Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 05:32 PM EDT

PDB ID	:	2QJG
Title	:	M. jannaschii ADH synthase complexed with F1,6P
Authors	:	Ealick, S.E.; Morar, M.
Deposited on	:	2007-07-07
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

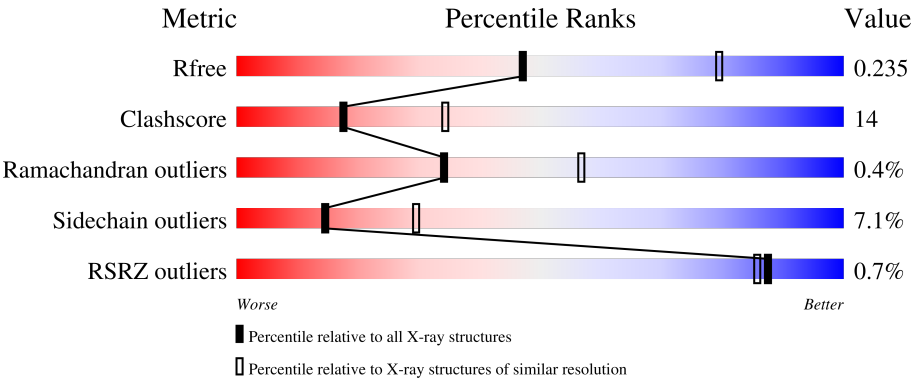
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	273	74% 22%
1	B	273	74% 19% 5%
1	C	273	73% 20%
1	D	273	76% 19%
1	E	273	75% 19%

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Mol	Chain	Length	Quality of chain
1	F	273	71% 21%
1	G	273	75% 19%
1	H	273	76% 18%
1	I	273	77% 17%
1	J	273	73% 23%
1	K	273	70% 24%
1	L	273	71% 24%
1	M	273	3% 74% 21%
1	N	273	73% 21%
1	O	273	75% 19%
1	P	273	68% 26%
1	Q	273	75% 21%
1	R	273	75% 20%
1	S	273	71% 22%
1	T	273	69% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F2P	A	501	X	-	-	-
2	F2P	B	501	X	-	-	-
2	F2P	C	501	X	-	-	-
2	F2P	D	501	X	-	-	-
2	F2P	E	501	X	-	-	-
2	F2P	F	501	X	-	-	-
2	F2P	G	501	X	-	-	-
2	F2P	H	501	X	-	-	-
2	F2P	I	501	X	-	-	-
2	F2P	J	501	X	-	-	-
2	F2P	K	501	X	-	-	-
2	F2P	L	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F2P	M	501	X	-	-	-
2	F2P	N	501	X	-	-	-
2	F2P	O	501	X	-	X	-
2	F2P	P	501	X	-	X	-
2	F2P	Q	501	X	-	-	-
2	F2P	R	501	X	-	-	-
2	F2P	S	501	X	-	-	-
2	F2P	T	501	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41023 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative aldolase MJ0400.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2014	1263	354	385	12			
1	B	268	Total	C	N	O	S	0	0	0
			1998	1253	352	381	12			
1	C	262	Total	C	N	O	S	0	0	0
			1968	1237	347	373	11			
1	D	267	Total	C	N	O	S	0	0	0
			2002	1256	352	382	12			
1	E	268	Total	C	N	O	S	0	0	0
			2004	1258	353	381	12			
1	K	266	Total	C	N	O	S	0	0	0
			1997	1253	354	379	11			
1	L	269	Total	C	N	O	S	0	0	0
			2008	1260	354	382	12			
1	M	265	Total	C	N	O	S	0	0	0
			1985	1247	350	376	12			
1	N	265	Total	C	N	O	S	0	0	0
			1985	1247	348	378	12			
1	O	266	Total	C	N	O	S	0	0	0
			2000	1255	354	379	12			
1	F	263	Total	C	N	O	S	0	0	0
			1983	1245	351	376	11			
1	G	268	Total	C	N	O	S	0	0	0
			2016	1264	357	383	12			
1	H	267	Total	C	N	O	S	0	0	0
			1998	1254	352	380	12			
1	I	265	Total	C	N	O	S	0	0	0
			1996	1252	353	380	11			
1	J	269	Total	C	N	O	S	0	0	0
			2021	1267	358	384	12			
1	P	268	Total	C	N	O	S	0	0	0
			2003	1256	353	383	11			

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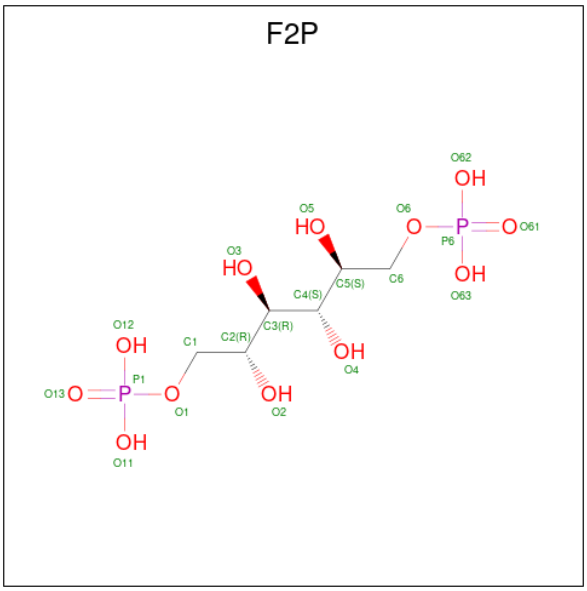
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	272	Total	C	N	O	S	0	0	0
			2035	1275	361	387	12			
1	R	269	Total	C	N	O	S	0	0	0
			2021	1267	360	382	12			
1	S	264	Total	C	N	O	S	0	0	0
			1988	1249	353	375	11			
1	T	267	Total	C	N	O	S	0	0	0
			2003	1257	353	382	11			

- Molecule 2 is 1,6-DI-O-PHOSPHONO-D-ALLITOL (three-letter code: F2P) (formula: $C_6H_{16}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			19	6	11	2		
2	B	1	Total	C	O	P	0	0
			19	6	11	2		
2	C	1	Total	C	O	P	0	0
			19	6	11	2		
2	D	1	Total	C	O	P	0	0
			19	6	11	2		
2	E	1	Total	C	O	P	0	0
			19	6	11	2		
2	K	1	Total	C	O	P	0	0
			19	6	11	2		
2	L	1	Total	C	O	P	0	0
			19	6	11	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	O	P	0	0
			19	6	11	2		
2	N	1	Total	C	O	P	0	0
			19	6	11	2		
2	O	1	Total	C	O	P	0	0
			19	6	11	2		
2	F	1	Total	C	O	P	0	0
			19	6	11	2		
2	G	1	Total	C	O	P	0	0
			19	6	11	2		
2	H	1	Total	C	O	P	0	0
			19	6	11	2		
2	I	1	Total	C	O	P	0	0
			19	6	11	2		
2	J	1	Total	C	O	P	0	0
			19	6	11	2		
2	P	1	Total	C	O	P	0	0
			19	6	11	2		
2	Q	1	Total	C	O	P	0	0
			19	6	11	2		
2	R	1	Total	C	O	P	0	0
			19	6	11	2		
2	S	1	Total	C	O	P	0	0
			19	6	11	2		
2	T	1	Total	C	O	P	0	0
			19	6	11	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	34	Total	O	0	0
			34	34		
3	C	35	Total	O	0	0
			35	35		
3	D	27	Total	O	0	0
			27	27		
3	E	31	Total	O	0	0
			31	31		
3	K	19	Total	O	0	0
			19	19		

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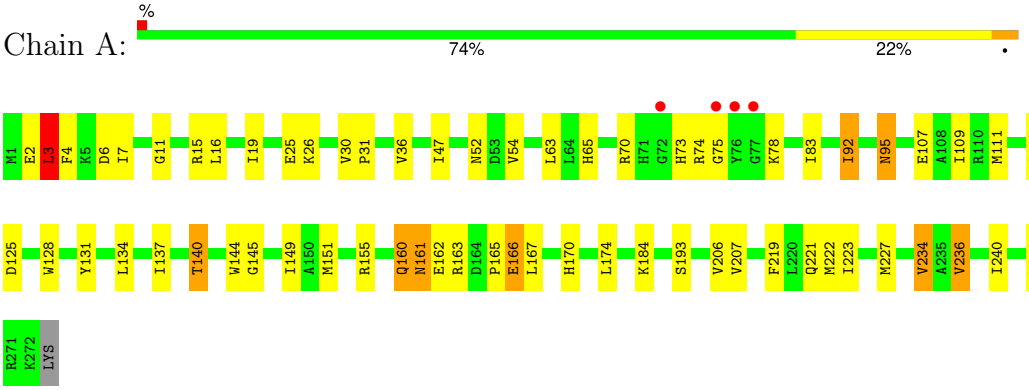
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	25	Total O 25 25	0	0
3	M	22	Total O 22 22	0	0
3	N	23	Total O 23 23	0	0
3	O	36	Total O 36 36	0	0
3	F	33	Total O 33 33	0	0
3	G	47	Total O 47 47	0	0
3	H	38	Total O 38 38	0	0
3	I	30	Total O 30 30	0	0
3	J	28	Total O 28 28	0	0
3	P	35	Total O 35 35	0	0
3	Q	29	Total O 29 29	0	0
3	R	39	Total O 39 39	0	0
3	S	18	Total O 18 18	0	0
3	T	36	Total O 36 36	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

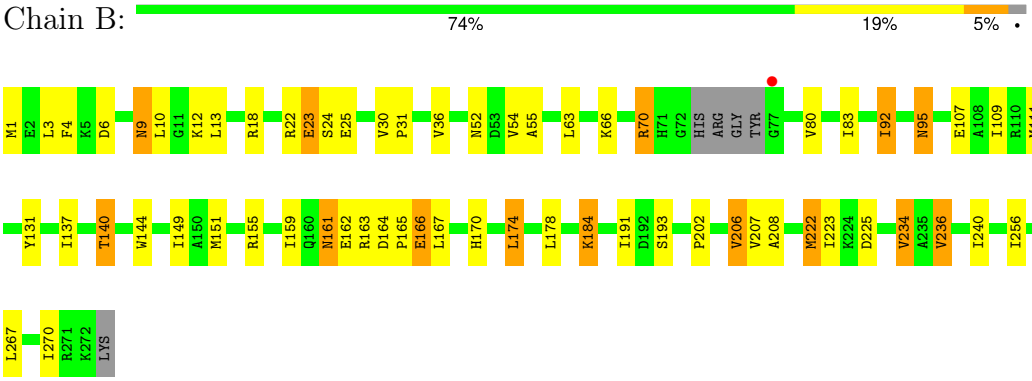
• Molecule 1: Putative aldolase MJ0400

Chain A:



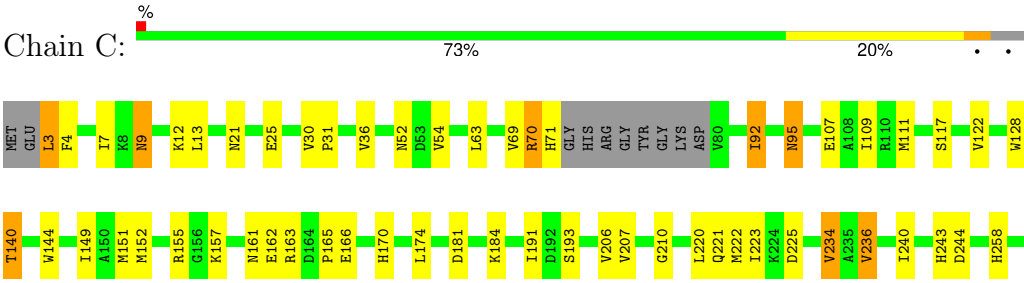
• Molecule 1: Putative aldolase MJ0400

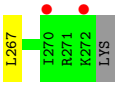
Chain B:



• Molecule 1: Putative aldolase MJ0400

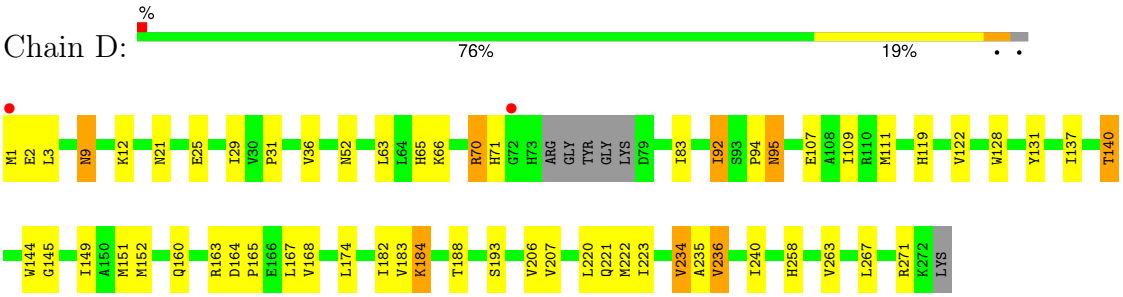
Chain C:





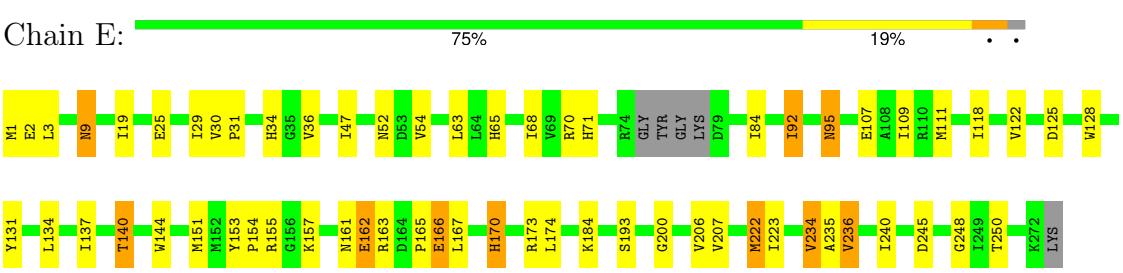
• Molecule 1: Putative aldolase MJ0400

Chain D:



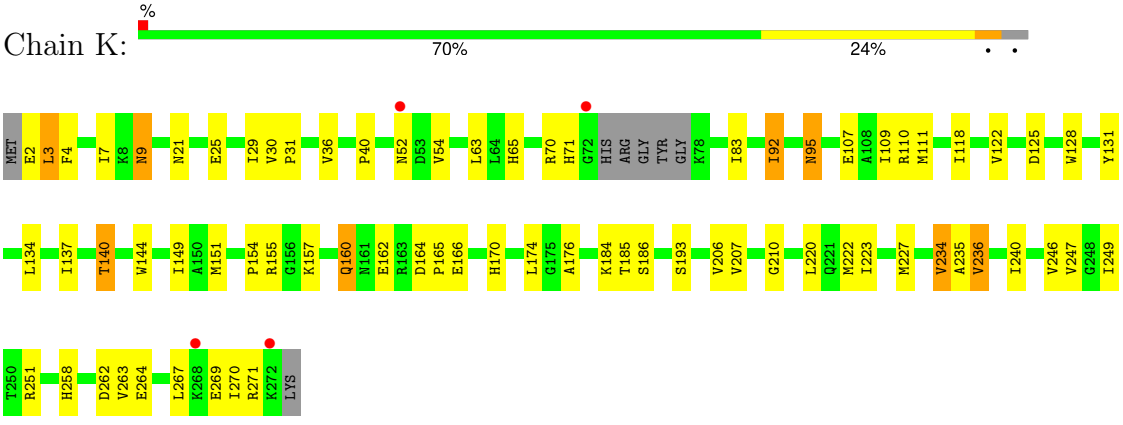
• Molecule 1: Putative aldolase MJ0400

Chain E:



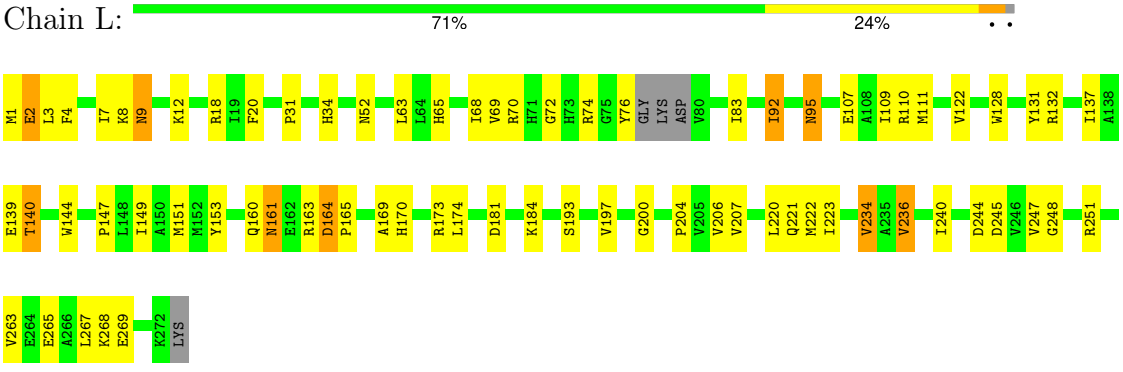
• Molecule 1: Putative aldolase MJ0400

Chain K:



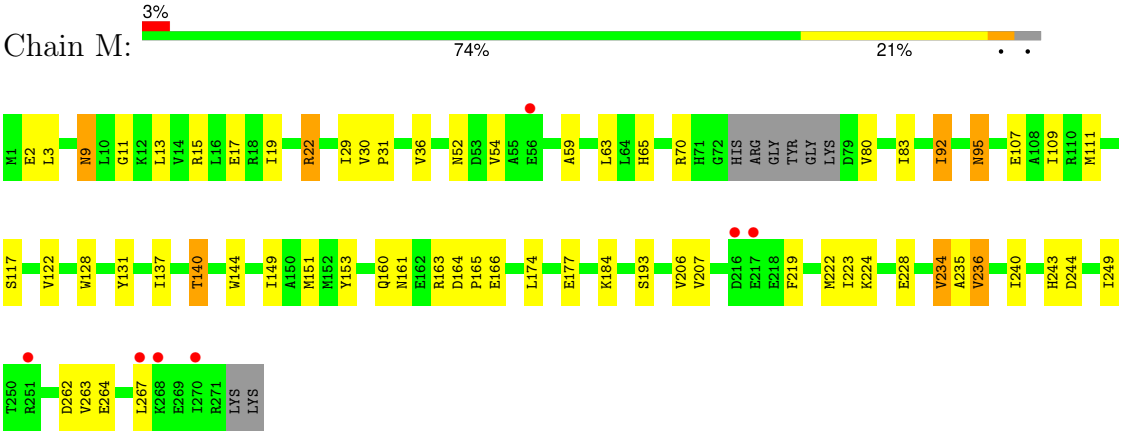
• Molecule 1: Putative aldolase MJ0400

Chain L:



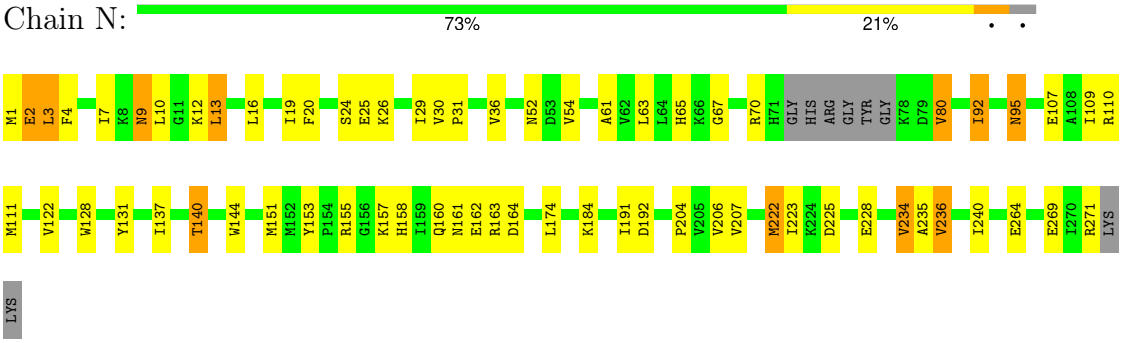
• Molecule 1: Putative aldolase MJ0400

Chain M:



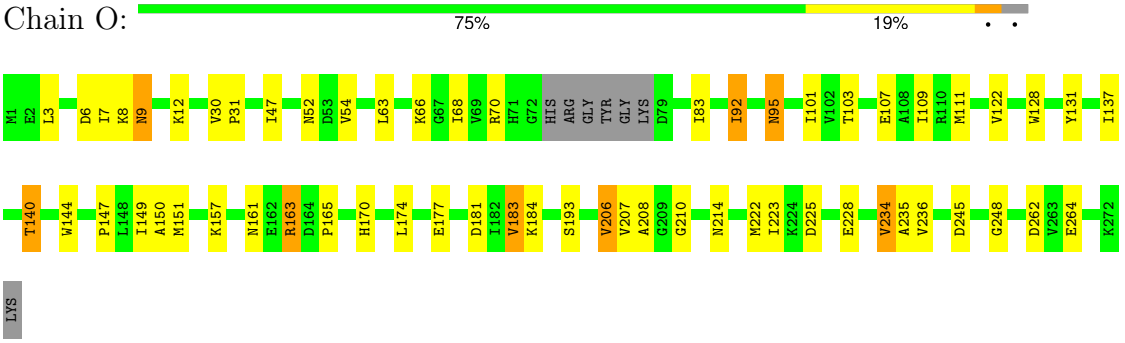
• Molecule 1: Putative aldolase MJ0400

Chain N:



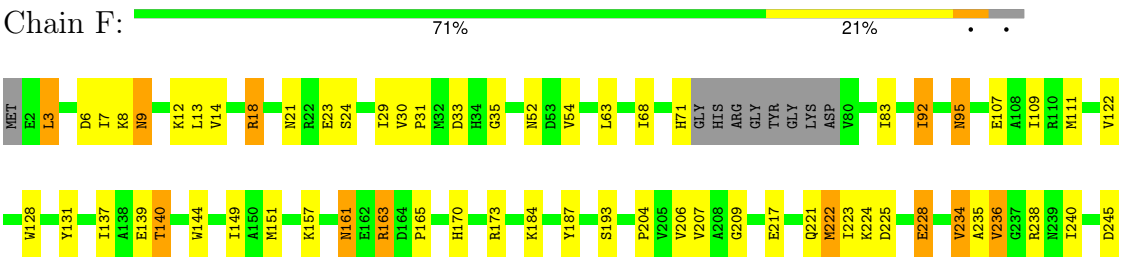
• Molecule 1: Putative aldolase MJ0400

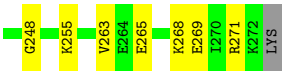
Chain O:



• Molecule 1: Putative aldolase MJ0400

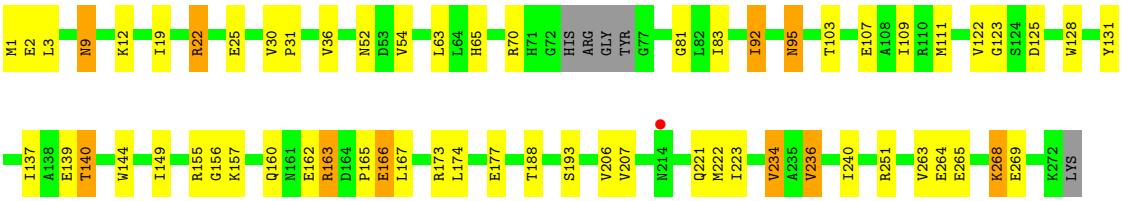
Chain F:





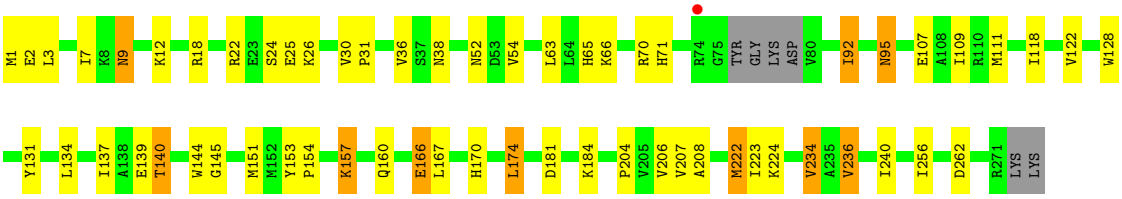
• Molecule 1: Putative aldolase MJ0400

Chain G:



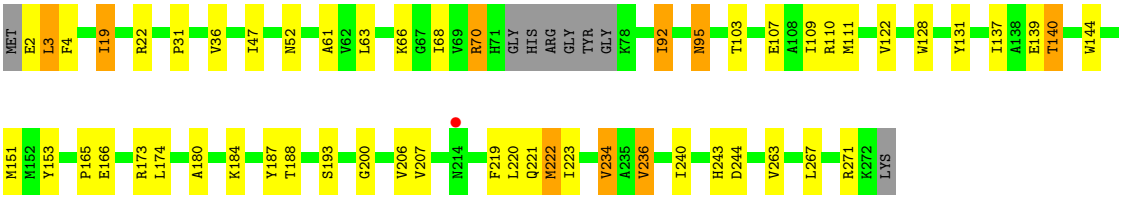
• Molecule 1: Putative aldolase MJ0400

Chain H:



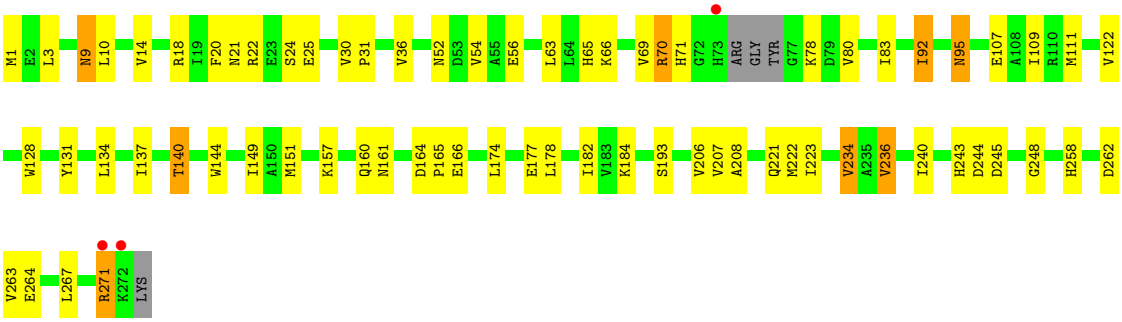
• Molecule 1: Putative aldolase MJ0400

Chain I:



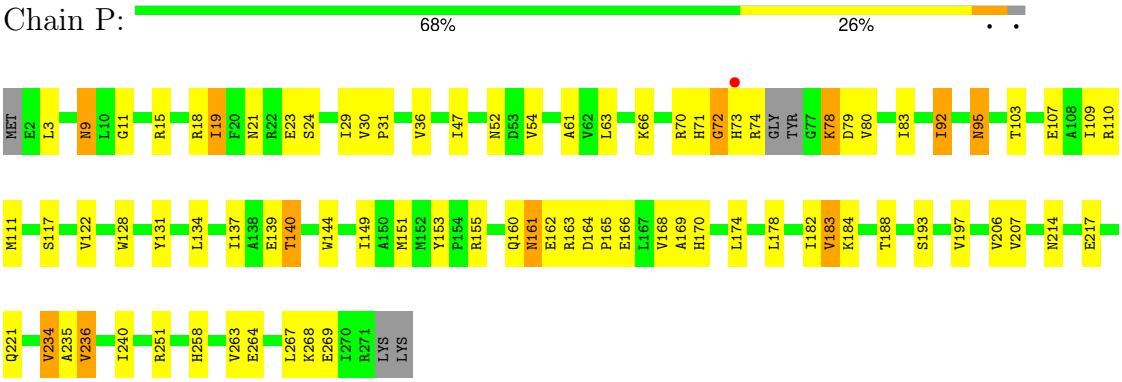
• Molecule 1: Putative aldolase MJ0400

Chain J:



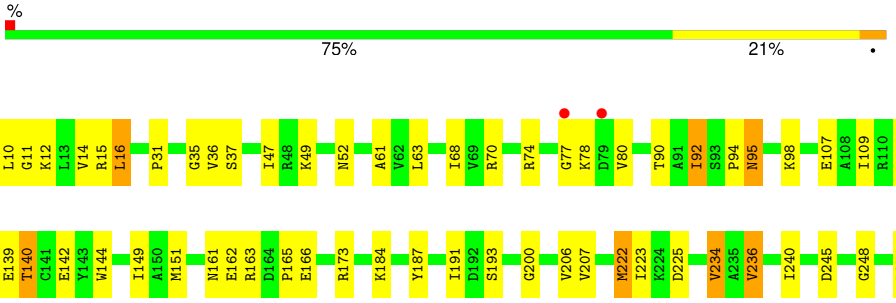
• Molecule 1: Putative aldolase MJ0400

Chain P:



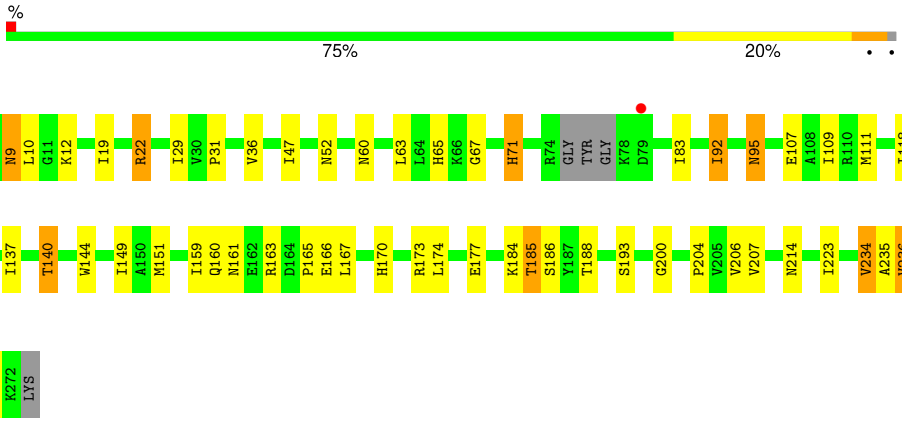
• Molecule 1: Putative aldolase MJ0400

Chain Q:



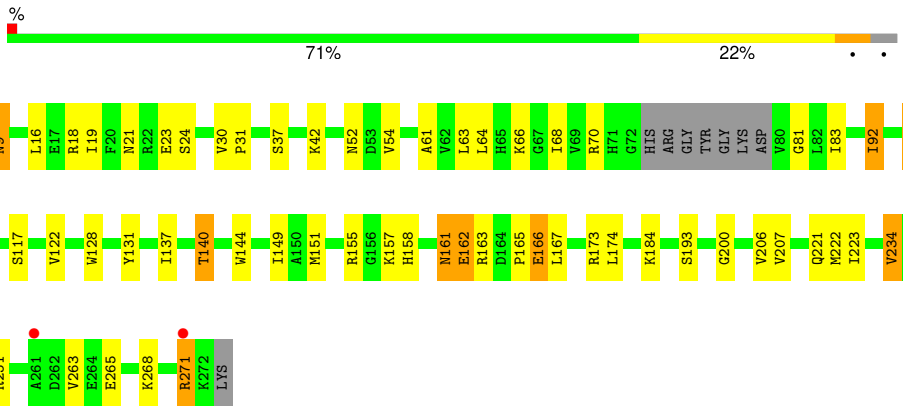
• Molecule 1: Putative aldolase MJ0400

Chain R:



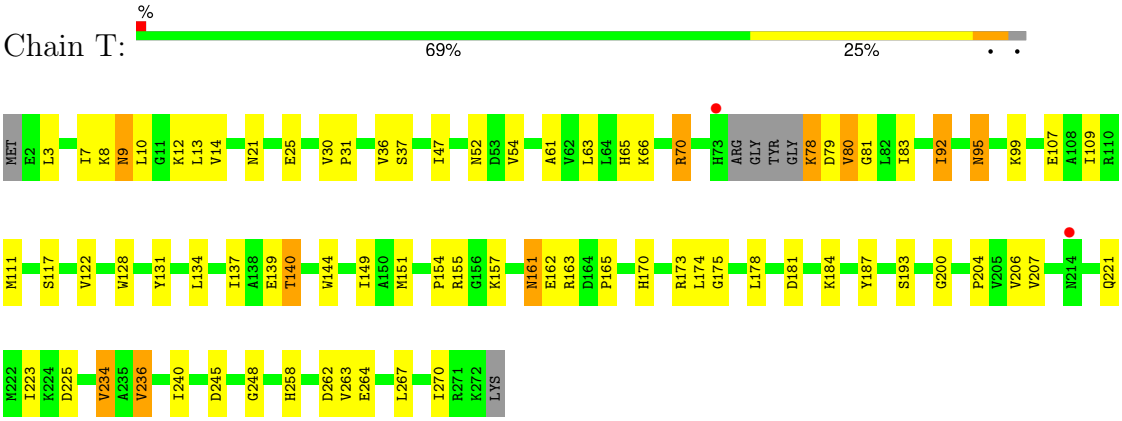
• Molecule 1: Putative aldolase MJ0400

Chain S:



• Molecule 1: Putative aldolase MJ0400

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	94.45Å 102.77Å 156.41Å 89.40° 85.83° 82.05°	Depositor
Resolution (Å)	46.31 – 2.60 48.54 – 2.36	Depositor EDS
% Data completeness (in resolution range)	89.8 (46.31-2.60) 89.8 (48.54-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.204 , 0.244 0.196 , 0.235	Depositor DCC
R_{free} test set	8749 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41023	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F2P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/2045	0.65	1/2770 (0.0%)
1	B	0.40	0/2028	0.63	0/2747
1	C	0.40	0/1998	0.63	0/2706
1	D	0.40	0/2032	0.63	0/2751
1	E	0.39	0/2034	0.64	0/2754
1	F	0.42	1/2013 (0.0%)	0.63	0/2725
1	G	0.42	0/2046	1.07	4/2767 (0.1%)
1	H	0.39	0/2028	0.63	0/2745
1	I	0.39	0/2026	0.62	0/2743
1	J	0.38	0/2051	0.64	0/2774
1	K	0.37	0/2027	0.62	0/2744
1	L	0.38	0/2038	0.63	0/2759
1	M	0.38	0/2015	0.62	0/2728
1	N	0.38	0/2014	0.62	0/2727
1	O	0.39	0/2030	0.65	1/2747 (0.0%)
1	P	0.40	1/2033 (0.0%)	0.66	2/2753 (0.1%)
1	Q	0.38	0/2066	0.63	0/2796
1	R	0.38	0/2051	0.62	0/2775
1	S	0.37	0/2018	0.62	0/2730
1	T	0.38	0/2033	0.64	0/2752
All	All	0.39	2/40626 (0.0%)	0.66	8/54993 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	183	VAL	C-N	5.92	1.47	1.34
1	F	228	GLU	CB-CG	-5.33	1.42	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	251	ARG	NE-CZ-NH1	-31.26	104.67	120.30
1	G	251	ARG	NE-CZ-NH2	28.28	134.44	120.30
1	G	251	ARG	CD-NE-CZ	14.89	144.44	123.60
1	G	251	ARG	CG-CD-NE	-10.04	90.70	111.80
1	P	183	VAL	C-N-CA	-9.70	97.45	121.70
1	A	3	LEU	CA-CB-CG	5.70	128.41	115.30
1	O	183	VAL	C-N-CA	-5.27	108.52	121.70
1	P	71	HIS	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2014	0	1996	50	0
1	B	1998	0	1987	61	0
1	C	1968	0	1971	59	0
1	D	2002	0	1999	52	0
1	E	2004	0	1998	51	0
1	F	1983	0	1989	58	0
1	G	2016	0	2023	53	0
1	H	1998	0	1998	58	0
1	I	1996	0	1994	51	0
1	J	2021	0	2026	58	0
1	K	1997	0	1995	59	0
1	L	2008	0	2002	61	0
1	M	1985	0	1989	43	0
1	N	1985	0	1987	71	0
1	O	2000	0	2006	58	0
1	P	2003	0	1992	88	0
1	Q	2035	0	2033	54	0
1	R	2021	0	2023	56	0
1	S	1988	0	2000	76	0
1	T	2003	0	1999	71	0
2	A	19	0	10	0	0
2	B	19	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	19	0	10	2	0
2	D	19	0	10	5	0
2	E	19	0	10	1	0
2	F	19	0	10	4	0
2	G	19	0	10	2	0
2	H	19	0	10	5	0
2	I	19	0	10	0	0
2	J	19	0	10	5	0
2	K	19	0	10	4	0
2	L	19	0	10	1	0
2	M	19	0	10	2	0
2	N	19	0	10	2	0
2	O	19	0	10	13	0
2	P	19	0	10	8	0
2	Q	19	0	10	3	0
2	R	19	0	10	0	0
2	S	19	0	10	3	0
2	T	19	0	10	3	0
3	A	33	0	0	6	0
3	B	34	0	0	1	0
3	C	35	0	0	4	0
3	D	27	0	0	3	0
3	E	31	0	0	3	0
3	F	33	0	0	5	0
3	G	47	0	0	4	0
3	H	38	0	0	2	0
3	I	30	0	0	0	0
3	J	28	0	0	3	0
3	K	19	0	0	0	0
3	L	25	0	0	1	0
3	M	22	0	0	1	0
3	N	23	0	0	1	0
3	O	36	0	0	6	0
3	P	35	0	0	3	0
3	Q	29	0	0	4	0
3	R	39	0	0	2	0
3	S	18	0	0	2	0
3	T	36	0	0	2	0
All	All	41023	0	40207	1108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:164:ASP:HB2	1:P:214:ASN:HD21	1.02	1.14
1:D:184:LYS:HE3	2:D:501:F2P:O4	1.40	1.11
2:D:501:F2P:O13	2:D:501:F2P:H2	1.45	1.11
1:S:21:ASN:ND2	1:S:24:SER:H	1.55	1.05
1:D:140:THR:HG21	3:D:522:HOH:O	1.56	1.04
1:H:208:ALA:HB1	2:H:501:F2P:H6C2	1.44	0.99
1:N:164:ASP:HB2	1:P:214:ASN:ND2	1.76	0.99
1:I:22:ARG:HH22	1:T:78:LYS:HZ3	1.09	0.97
1:E:250:THR:HA	3:E:522:HOH:O	1.66	0.95
1:D:151:MET:HG2	1:D:184:LYS:HG2	1.48	0.95
1:H:1:MET:HG3	1:H:25:GLU:HG2	1.49	0.95
1:T:140:THR:HG21	3:T:537:HOH:O	1.68	0.94
1:N:223:ILE:HD12	1:N:234:VAL:HG21	1.51	0.92
1:O:184:LYS:HE2	2:O:501:F2P:O4	1.68	0.92
1:H:208:ALA:CB	2:H:501:F2P:H6C2	2.03	0.89
1:D:184:LYS:CE	2:D:501:F2P:O4	2.22	0.88
1:I:22:ARG:HH22	1:T:78:LYS:NZ	1.71	0.88
1:J:140:THR:HB	3:J:522:HOH:O	1.71	0.88
2:H:501:F2P:O63	2:H:501:F2P:H4	1.73	0.88
1:E:222:MET:HE2	1:E:223:ILE:HD13	1.56	0.87
1:R:207:VAL:HG23	1:R:234:VAL:HG23	1.58	0.86
1:A:207:VAL:HG23	1:A:234:VAL:HG23	1.58	0.86
1:I:2:GLU:HG3	1:I:4:PHE:H	1.41	0.86
1:S:21:ASN:HD22	1:S:24:SER:H	1.20	0.86
1:T:207:VAL:HG23	1:T:234:VAL:HG23	1.57	0.85
1:I:207:VAL:HG23	1:I:234:VAL:HG23	1.58	0.85
1:K:207:VAL:HG23	1:K:234:VAL:HG23	1.56	0.85
1:P:207:VAL:HG23	1:P:234:VAL:HG23	1.59	0.85
1:C:207:VAL:HG23	1:C:234:VAL:HG23	1.59	0.85
1:M:207:VAL:HG23	1:M:234:VAL:HG23	1.59	0.85
1:S:207:VAL:HG23	1:S:234:VAL:HG23	1.57	0.84
1:B:207:VAL:HG23	1:B:234:VAL:HG23	1.56	0.84
1:Q:207:VAL:HG23	1:Q:234:VAL:HG23	1.57	0.84
1:N:207:VAL:HG23	1:N:234:VAL:HG23	1.59	0.84
1:L:207:VAL:HG23	1:L:234:VAL:HG23	1.58	0.83
1:D:207:VAL:HG23	1:D:234:VAL:HG23	1.59	0.83
1:J:223:ILE:HD12	1:J:234:VAL:HG21	1.60	0.83
1:E:207:VAL:HG23	1:E:234:VAL:HG23	1.60	0.83
1:J:1:MET:HG2	1:J:25:GLU:HG2	1.60	0.83
1:A:140:THR:HG21	3:A:527:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:VAL:HG23	1:H:234:VAL:HG23	1.58	0.82
1:H:224:LYS:NZ	1:H:262:ASP:HA	1.94	0.82
1:F:207:VAL:HG23	1:F:234:VAL:HG23	1.59	0.82
1:F:21:ASN:OD1	1:F:23:GLU:HG2	1.79	0.82
1:G:207:VAL:HG23	1:G:234:VAL:HG23	1.61	0.81
1:J:56:GLU:HA	1:J:78:LYS:HD3	1.62	0.81
1:L:223:ILE:HD12	1:L:234:VAL:HG21	1.63	0.81
1:H:222:MET:HE2	1:H:223:ILE:HD13	1.63	0.81
1:J:207:VAL:HG23	1:J:234:VAL:HG23	1.61	0.81
1:P:168:VAL:HG21	1:P:188:THR:CG2	2.11	0.81
2:O:501:F2P:O2	2:O:501:F2P:H6C2	1.81	0.80
1:S:21:ASN:HD21	1:S:23:GLU:HB2	1.47	0.80
1:E:223:ILE:HD12	1:E:234:VAL:HG21	1.64	0.80
1:M:17:GLU:HG2	1:M:22:ARG:NH2	1.98	0.78
1:N:164:ASP:CB	1:P:214:ASN:ND2	2.46	0.78
1:T:223:ILE:HD12	1:T:234:VAL:HG21	1.63	0.78
1:O:207:VAL:HG23	1:O:234:VAL:HG23	1.63	0.78
1:B:184:LYS:HE2	1:B:208:ALA:HB2	1.66	0.78
1:O:223:ILE:HD12	1:O:234:VAL:HG21	1.66	0.77
1:S:223:ILE:HD12	1:S:234:VAL:HG21	1.66	0.77
1:S:245:ASP:CB	1:S:271:ARG:HH22	1.96	0.77
1:L:220:LEU:HD12	1:L:267:LEU:HD23	1.66	0.77
1:B:184:LYS:C	1:B:184:LYS:HD3	2.03	0.77
1:K:223:ILE:HD12	1:K:234:VAL:HG21	1.66	0.77
1:N:164:ASP:CB	1:P:214:ASN:HD21	1.90	0.77
1:N:157:LYS:HG3	1:N:158:HIS:ND1	2.00	0.76
1:O:208:ALA:HB1	2:O:501:F2P:H6C1	1.68	0.76
1:C:223:ILE:HD12	1:C:234:VAL:HG21	1.69	0.75
2:F:501:F2P:H2	2:F:501:F2P:O12	1.86	0.75
1:C:220:LEU:HD12	1:C:267:LEU:HD23	1.67	0.75
1:S:21:ASN:HB2	3:S:510:HOH:O	1.85	0.75
1:D:223:ILE:HD12	1:D:234:VAL:HG21	1.69	0.75
1:P:19:ILE:O	1:P:19:ILE:HG13	1.87	0.75
1:R:9:ASN:HD22	1:R:12:LYS:H	1.36	0.74
1:K:154:PRO:O	1:K:162:GLU:HG2	1.88	0.74
1:S:271:ARG:H	1:S:271:ARG:HH21	1.35	0.74
1:S:161:ASN:ND2	1:S:163:ARG:H	1.85	0.74
1:N:153:TYR:OH	1:N:184:LYS:HE2	1.88	0.74
1:N:192:ASP:OD2	1:P:161:ASN:ND2	2.21	0.73
1:J:9:ASN:HD22	1:J:9:ASN:C	1.92	0.73
1:P:151:MET:CE	2:P:501:F2P:O4	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:37:SER:HB2	2:Q:501:F2P:O12	1.88	0.72
2:N:501:F2P:H6C2	2:N:501:F2P:O2	1.89	0.72
1:E:125:ASP:OD1	1:E:157:LYS:HE2	1.89	0.72
1:R:214:ASN:ND2	3:R:540:HOH:O	2.21	0.72
1:T:7:ILE:HG13	1:T:7:ILE:O	1.88	0.72
1:O:163:ARG:HG2	1:O:163:ARG:HH11	1.55	0.72
1:K:125:ASP:OD2	1:K:157:LYS:HE2	1.90	0.71
1:N:161:ASN:HB3	1:P:214:ASN:OD1	1.89	0.71
1:I:107:GLU:HG3	1:I:111:MET:HE2	1.73	0.71
1:T:7:ILE:HD11	1:T:13:LEU:HG	1.73	0.71
1:P:153:TYR:OH	1:P:184:LYS:HE3	1.90	0.71
1:F:221:GLN:OE1	1:F:263:VAL:HG21	1.91	0.71
1:I:22:ARG:NH2	1:T:78:LYS:HZ3	1.87	0.70
1:P:122:VAL:HG12	1:S:92:ILE:HG12	1.74	0.70
1:C:3:LEU:HD13	1:C:4:PHE:CE1	2.26	0.69
1:Q:223:ILE:HD12	1:Q:234:VAL:HG21	1.74	0.69
1:D:221:GLN:OE1	1:D:263:VAL:HG21	1.91	0.69
1:M:2:GLU:HG3	3:M:519:HOH:O	1.91	0.69
1:N:4:PHE:HB3	1:N:7:ILE:HG21	1.74	0.69
1:N:61:ALA:HA	1:N:80:VAL:HG23	1.74	0.69
1:O:228:GLU:HG3	3:O:529:HOH:O	1.93	0.69
1:H:224:LYS:HZ2	1:H:262:ASP:HA	1.57	0.69
1:G:223:ILE:HD12	1:G:234:VAL:HG21	1.75	0.69
1:N:192:ASP:OD2	1:P:161:ASN:HA	1.93	0.69
1:O:107:GLU:HG3	1:O:111:MET:HE2	1.74	0.69
1:P:184:LYS:HE2	2:P:501:F2P:O4	1.93	0.69
1:J:109:ILE:HD11	1:J:144:TRP:HB3	1.75	0.68
1:T:109:ILE:HD11	1:T:144:TRP:HB3	1.75	0.68
1:E:109:ILE:HD11	1:E:144:TRP:HB3	1.75	0.68
1:S:2:GLU:N	1:S:5:LYS:HZ2	1.90	0.68
1:C:122:VAL:HG21	3:C:535:HOH:O	1.92	0.68
1:D:109:ILE:HD11	1:D:144:TRP:HB3	1.76	0.68
1:B:1:MET:CG	1:B:25:GLU:HG2	2.24	0.68
1:M:153:TYR:OH	1:M:184:LYS:HE2	1.94	0.68
1:C:109:ILE:HD11	1:C:144:TRP:HB3	1.75	0.68
1:I:2:GLU:HG3	1:I:3:LEU:H	1.58	0.67
1:P:161:ASN:ND2	1:P:163:ARG:H	1.92	0.67
1:P:9:ASN:C	1:P:9:ASN:HD22	1.96	0.67
1:Q:109:ILE:HD11	1:Q:144:TRP:HB3	1.76	0.67
1:N:4:PHE:O	1:N:7:ILE:HG22	1.95	0.67
1:J:107:GLU:HG3	1:J:111:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:122:VAL:HG12	1:T:92:ILE:HG12	1.77	0.67
1:I:19:ILE:HG22	1:I:61:ALA:HB2	1.75	0.67
1:K:109:ILE:HD11	1:K:144:TRP:HB3	1.77	0.67
1:G:265:GLU:HA	1:G:268:LYS:HE3	1.75	0.67
1:P:109:ILE:HD11	1:P:144:TRP:HB3	1.76	0.67
1:B:222:MET:HE2	1:B:223:ILE:HD12	1.77	0.67
1:M:151:MET:HG2	1:M:184:LYS:HD3	1.75	0.67
1:N:151:MET:HG2	1:N:184:LYS:HD3	1.76	0.67
1:N:161:ASN:HD21	1:N:163:ARG:HB2	1.59	0.67
1:H:208:ALA:HB1	2:H:501:F2P:C6	2.21	0.67
1:H:222:MET:CE	1:H:223:ILE:HD13	2.24	0.67
1:C:7:ILE:CG2	1:C:13:LEU:HD21	2.25	0.67
1:H:223:ILE:HD12	1:H:234:VAL:HG21	1.77	0.67
2:M:501:F2P:H6C2	2:M:501:F2P:O2	1.95	0.66
1:A:151:MET:HG2	1:A:184:LYS:HD3	1.77	0.66
1:M:109:ILE:HD11	1:M:144:TRP:HB3	1.77	0.66
1:N:109:ILE:HD11	1:N:144:TRP:HB3	1.76	0.66
1:T:165:PRO:HB3	1:T:193:SER:HB2	1.78	0.66
1:C:4:PHE:O	1:C:7:ILE:HG22	1.95	0.66
1:D:107:GLU:HG3	1:D:111:MET:HE2	1.78	0.66
1:H:109:ILE:HD11	1:H:144:TRP:HB3	1.77	0.66
1:R:9:ASN:ND2	1:R:12:LYS:H	1.93	0.66
1:S:109:ILE:HD11	1:S:144:TRP:HB3	1.78	0.66
1:C:161:ASN:ND2	1:C:163:ARG:H	1.93	0.66
1:G:92:ILE:HG12	1:H:122:VAL:HG12	1.78	0.66
1:H:107:GLU:HG3	1:H:111:MET:HE2	1.77	0.66
1:T:161:ASN:ND2	1:T:163:ARG:H	1.93	0.66
1:I:271:ARG:HD3	1:I:271:ARG:N	2.11	0.66
1:L:122:VAL:HG12	1:O:92:ILE:HG12	1.78	0.65
1:N:7:ILE:HG23	1:N:7:ILE:O	1.95	0.65
1:B:262:ASP:OD2	1:B:264:GLU:HB2	1.96	0.65
1:O:163:ARG:HG2	1:O:163:ARG:NH1	2.12	0.65
1:H:92:ILE:HG12	1:I:122:VAL:HG12	1.78	0.65
1:A:73:HIS:O	1:A:75:GLY:N	2.29	0.65
1:G:125:ASP:OD1	1:G:157:LYS:HE2	1.96	0.65
1:S:2:GLU:HB3	1:S:5:LYS:HG3	1.79	0.65
1:T:107:GLU:HG3	1:T:111:MET:HE2	1.77	0.65
1:I:2:GLU:HG3	1:I:3:LEU:N	2.12	0.65
1:N:9:ASN:C	1:N:9:ASN:HD22	2.01	0.65
1:H:9:ASN:HD22	1:H:12:LYS:H	1.42	0.65
1:I:22:ARG:NH2	1:T:78:LYS:NZ	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:109:ILE:HD11	1:I:144:TRP:HB3	1.78	0.65
1:G:109:ILE:HD11	1:G:144:TRP:HB3	1.78	0.64
1:J:263:VAL:O	1:J:267:LEU:HG	1.96	0.64
1:S:19:ILE:HG22	1:S:61:ALA:HB2	1.79	0.64
1:Q:107:GLU:HG3	1:Q:111:MET:HE2	1.79	0.64
1:F:109:ILE:HD11	1:F:144:TRP:HB3	1.80	0.64
1:H:18:ARG:HH21	1:H:18:ARG:HG3	1.61	0.64
1:J:157:LYS:HD3	1:J:157:LYS:N	2.13	0.64
1:O:109:ILE:HD11	1:O:144:TRP:HB3	1.78	0.64
1:L:251:ARG:HB3	1:L:269:GLU:HG2	1.79	0.64
1:A:109:ILE:HD11	1:A:144:TRP:HB3	1.79	0.64
1:K:2:GLU:HA	1:K:25:GLU:OE1	1.98	0.64
1:B:107:GLU:HG3	1:B:111:MET:HE2	1.80	0.64
1:H:1:MET:HG3	1:H:25:GLU:CG	2.27	0.64
1:N:24:SER:O	1:N:26:LYS:HG2	1.98	0.63
1:B:109:ILE:HD11	1:B:144:TRP:HB3	1.80	0.63
1:E:151:MET:HG2	1:E:184:LYS:HD3	1.80	0.63
1:G:2:GLU:HB2	1:G:25:GLU:OE2	1.97	0.63
1:A:219:PHE:CZ	1:A:223:ILE:HD11	2.33	0.63
1:R:107:GLU:HG3	1:R:111:MET:HE2	1.80	0.63
1:L:220:LEU:HD12	1:L:267:LEU:CD2	2.29	0.63
1:P:264:GLU:O	1:P:268:LYS:HG3	1.98	0.63
1:T:173:ARG:HD3	1:T:200:GLY:O	1.98	0.63
1:N:107:GLU:HG3	1:N:111:MET:HE2	1.80	0.63
1:H:9:ASN:ND2	1:H:12:LYS:H	1.96	0.63
1:P:74:ARG:HA	3:P:524:HOH:O	1.97	0.63
1:M:165:PRO:HB3	1:M:193:SER:HB2	1.81	0.62
1:P:169:ALA:HB2	1:P:197:VAL:HG22	1.80	0.62
1:T:37:SER:HB2	2:T:501:F2P:O13	1.99	0.62
1:J:221:GLN:OE1	1:J:263:VAL:HG21	1.99	0.62
1:M:107:GLU:HG3	1:M:111:MET:HE2	1.80	0.62
1:P:107:GLU:HG3	1:P:111:MET:HE2	1.81	0.62
1:M:243:HIS:ND1	1:M:249:ILE:HB	2.14	0.62
1:G:107:GLU:HG3	1:G:111:MET:HE2	1.81	0.62
1:G:122:VAL:HG12	1:J:92:ILE:HG12	1.81	0.62
1:J:21:ASN:HD22	1:J:24:SER:H	1.45	0.62
1:F:223:ILE:HD12	1:F:234:VAL:HG21	1.81	0.62
1:Q:77:GLY:O	1:Q:78:LYS:HD2	2.00	0.62
1:R:151:MET:HG2	1:R:184:LYS:HD3	1.81	0.62
1:D:165:PRO:HB3	1:D:193:SER:HB2	1.82	0.62
1:T:7:ILE:HD11	1:T:13:LEU:CD2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:GLU:HG3	3:F:531:HOH:O	1.99	0.62
2:D:501:F2P:O13	2:D:501:F2P:C2	2.35	0.61
1:F:9:ASN:HD22	1:F:12:LYS:H	1.48	0.61
1:P:221:GLN:OE1	1:P:263:VAL:HG21	2.01	0.61
3:A:523:HOH:O	1:D:71:HIS:HD2	1.82	0.61
1:E:173:ARG:HD3	1:E:200:GLY:O	2.01	0.61
1:Q:9:ASN:C	1:Q:9:ASN:HD22	2.03	0.61
1:A:122:VAL:HG12	1:D:92:ILE:HG12	1.83	0.61
1:C:152:MET:HB3	3:C:535:HOH:O	2.00	0.61
1:K:92:ILE:O	1:K:92:ILE:HG13	2.00	0.61
1:N:160:GLN:HG2	3:N:517:HOH:O	2.00	0.61
1:E:107:GLU:HG3	1:E:111:MET:HE2	1.83	0.61
1:R:109:ILE:HD11	1:R:144:TRP:HB3	1.80	0.61
1:L:109:ILE:HD11	1:L:144:TRP:HB3	1.82	0.61
1:F:92:ILE:HG12	1:J:122:VAL:HG12	1.83	0.61
1:C:92:ILE:HG12	1:D:122:VAL:HG12	1.82	0.60
1:C:107:GLU:HG3	1:C:111:MET:HE2	1.82	0.60
1:T:66:LYS:O	1:T:70:ARG:HG2	2.02	0.60
1:G:92:ILE:HG13	1:G:92:ILE:O	2.01	0.60
1:P:92:ILE:HG13	1:P:92:ILE:O	2.01	0.60
1:K:4:PHE:CD2	1:K:7:ILE:HD12	2.35	0.60
1:O:214:ASN:ND2	3:O:530:HOH:O	2.33	0.60
1:R:163:ARG:HD3	3:R:531:HOH:O	2.00	0.60
1:B:161:ASN:ND2	1:B:163:ARG:H	2.00	0.60
1:O:6:ASP:HB3	3:O:526:HOH:O	2.01	0.60
1:H:38:ASN:ND2	3:H:523:HOH:O	2.34	0.60
1:P:217:GLU:HB2	3:P:522:HOH:O	2.00	0.60
1:E:92:ILE:O	1:E:92:ILE:HG13	2.01	0.60
1:N:228:GLU:OE2	1:P:160:GLN:NE2	2.34	0.60
1:Q:92:ILE:HG12	1:R:122:VAL:HG12	1.82	0.60
1:S:155:ARG:HG2	1:S:162:GLU:HG2	1.83	0.60
1:L:92:ILE:O	1:L:92:ILE:HG13	2.00	0.60
1:O:161:ASN:ND2	1:O:163:ARG:H	2.00	0.60
1:S:151:MET:HG2	1:S:184:LYS:HD3	1.83	0.59
1:K:270:ILE:HG22	1:K:271:ARG:N	2.18	0.59
1:M:164:ASP:OD2	1:M:166:GLU:HB2	2.03	0.59
1:K:107:GLU:HG3	1:K:111:MET:HE2	1.84	0.59
2:O:501:F2P:O2	2:O:501:F2P:C6	2.49	0.59
1:R:92:ILE:HG13	1:R:92:ILE:O	2.01	0.59
1:S:92:ILE:HG13	1:S:92:ILE:O	2.02	0.59
1:A:92:ILE:HD12	1:E:167:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:ARG:H	1:F:271:ARG:HD3	1.67	0.59
1:G:269:GLU:OE1	1:G:269:GLU:HA	2.02	0.59
1:O:184:LYS:HB2	1:O:206:VAL:HG12	1.85	0.59
1:F:107:GLU:HG3	1:F:111:MET:HE2	1.83	0.59
1:S:37:SER:CB	2:S:501:F2P:O12	2.50	0.59
1:D:92:ILE:O	1:D:92:ILE:HG13	2.03	0.59
1:E:153:TYR:OH	1:E:184:LYS:HE2	2.03	0.59
1:E:222:MET:CE	1:E:223:ILE:HD13	2.31	0.59
1:G:165:PRO:HB3	1:G:193:SER:HB2	1.85	0.59
1:H:1:MET:HA	1:H:25:GLU:OE2	2.02	0.59
1:Q:161:ASN:ND2	1:Q:163:ARG:H	2.00	0.59
1:N:222:MET:HE1	1:N:223:ILE:HA	1.85	0.59
1:H:166:GLU:HG3	1:H:167:LEU:N	2.17	0.58
1:S:9:ASN:C	1:S:9:ASN:HD22	2.07	0.58
1:A:92:ILE:HG13	1:A:92:ILE:O	2.03	0.58
1:Q:92:ILE:HG13	1:Q:92:ILE:O	2.03	0.58
1:A:65:HIS:HE1	3:A:528:HOH:O	1.86	0.58
1:K:128:TRP:HA	1:K:131:TYR:CD1	2.39	0.58
1:G:128:TRP:HA	1:G:131:TYR:CD1	2.38	0.58
1:S:137:ILE:HA	1:S:140:THR:HG23	1.85	0.58
1:O:151:MET:SD	2:O:501:F2P:H3	2.43	0.58
1:T:128:TRP:HA	1:T:131:TYR:CD1	2.38	0.58
1:A:128:TRP:HA	1:A:131:TYR:CD1	2.39	0.58
1:L:68:ILE:CD1	1:M:177:GLU:HA	2.33	0.58
2:O:501:F2P:O2	2:O:501:F2P:C5	2.51	0.58
1:F:224:LYS:HE3	3:F:521:HOH:O	2.03	0.58
1:H:92:ILE:HG13	1:H:92:ILE:O	2.04	0.58
2:N:501:F2P:O2	2:N:501:F2P:C6	2.50	0.58
1:P:92:ILE:HG12	1:T:122:VAL:HG12	1.84	0.58
1:A:107:GLU:HG3	1:A:111:MET:HE2	1.85	0.58
1:D:9:ASN:ND2	1:D:12:LYS:H	2.02	0.58
1:I:19:ILE:HG22	1:I:61:ALA:CB	2.32	0.58
1:C:92:ILE:O	1:C:92:ILE:HG13	2.04	0.58
1:N:92:ILE:O	1:N:92:ILE:HG13	2.03	0.58
1:N:157:LYS:HG3	1:N:158:HIS:CE1	2.38	0.58
1:P:78:LYS:HD2	1:P:79:ASP:H	1.68	0.58
1:S:37:SER:HB2	2:S:501:F2P:O12	2.04	0.58
1:O:66:LYS:O	1:O:70:ARG:HG3	2.04	0.57
1:B:223:ILE:HG13	1:B:234:VAL:HG21	1.86	0.57
1:G:160:GLN:HA	1:G:160:GLN:NE2	2.19	0.57
1:S:161:ASN:HD21	1:S:163:ARG:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:NH1	1:A:145:GLY:O	2.37	0.57
1:L:74:ARG:C	1:L:76:TYR:H	2.05	0.57
1:R:223:ILE:HD12	1:R:234:VAL:HG21	1.85	0.57
1:T:7:ILE:HD11	1:T:13:LEU:CG	2.33	0.57
1:D:151:MET:CG	1:D:184:LYS:HG2	2.29	0.57
1:F:9:ASN:ND2	1:F:12:LYS:H	2.02	0.57
1:I:92:ILE:HG13	1:I:92:ILE:O	2.03	0.57
1:M:137:ILE:HA	1:M:140:THR:HG23	1.85	0.57
1:N:4:PHE:HB3	1:N:7:ILE:CG2	2.35	0.57
1:F:92:ILE:O	1:F:92:ILE:HG13	2.03	0.57
1:A:26:LYS:HD2	1:A:227:MET:HE1	1.85	0.57
1:B:92:ILE:HG12	1:C:122:VAL:HG12	1.85	0.57
1:K:207:VAL:CG2	1:K:234:VAL:HG23	2.34	0.57
1:L:151:MET:HG2	1:L:184:LYS:HD3	1.86	0.57
1:S:42:LYS:HE2	3:S:509:HOH:O	2.04	0.57
1:B:122:VAL:HG12	1:E:92:ILE:HG12	1.86	0.57
1:K:236:VAL:HA	2:K:501:F2P:O61	2.05	0.57
1:M:59:ALA:O	1:M:80:VAL:HG12	2.04	0.57
1:J:137:ILE:HA	1:J:140:THR:HG23	1.87	0.57
1:S:221:GLN:OE1	1:S:263:VAL:HG21	2.05	0.57
1:T:134:LEU:HD23	1:T:178:LEU:HD12	1.85	0.57
1:D:137:ILE:HA	1:D:140:THR:HG23	1.87	0.57
1:K:247:VAL:O	1:K:251:ARG:HG3	2.05	0.57
1:O:137:ILE:HA	1:O:140:THR:HG23	1.87	0.57
1:Q:137:ILE:HA	1:Q:140:THR:HG23	1.87	0.57
1:B:92:ILE:HG13	1:B:92:ILE:O	2.03	0.56
1:L:128:TRP:HA	1:L:131:TYR:CD1	2.40	0.56
1:F:68:ILE:HD11	1:J:177:GLU:HG2	1.86	0.56
1:H:9:ASN:HB3	1:H:12:LYS:HB2	1.86	0.56
1:B:151:MET:SD	2:B:501:F2P:O4	2.64	0.56
1:E:128:TRP:HA	1:E:131:TYR:CD1	2.39	0.56
1:E:165:PRO:HB3	1:E:193:SER:HB2	1.87	0.56
1:M:92:ILE:HG13	1:M:92:ILE:O	2.03	0.56
1:M:219:PHE:CZ	1:M:223:ILE:HD11	2.40	0.56
1:N:128:TRP:HA	1:N:131:TYR:CD1	2.41	0.56
1:P:128:TRP:HA	1:P:131:TYR:CD1	2.40	0.56
1:S:107:GLU:HG3	1:S:111:MET:HE2	1.87	0.56
1:A:16:LEU:HD23	1:A:19:ILE:HD11	1.85	0.56
1:B:164:ASP:OD2	1:B:167:LEU:HG	2.06	0.56
1:L:221:GLN:OE1	1:L:263:VAL:HG21	2.05	0.56
1:F:271:ARG:HD3	1:F:271:ARG:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:VAL:CG2	1:H:234:VAL:HG23	2.35	0.56
1:Q:151:MET:HG2	1:Q:184:LYS:HD3	1.87	0.56
1:S:245:ASP:CB	1:S:271:ARG:NH2	2.65	0.56
1:B:151:MET:HG2	1:B:184:LYS:CG	2.35	0.56
1:C:221:GLN:OE1	1:C:263:VAL:HG21	2.05	0.56
1:E:2:GLU:N	1:E:2:GLU:OE2	2.39	0.56
1:E:137:ILE:HA	1:E:140:THR:HG23	1.87	0.56
1:H:137:ILE:HA	1:H:140:THR:HG23	1.88	0.56
1:I:128:TRP:HA	1:I:131:TYR:CD1	2.41	0.56
1:E:161:ASN:ND2	1:E:163:ARG:H	2.02	0.56
1:K:223:ILE:O	1:K:227:MET:HG2	2.06	0.56
1:L:92:ILE:HG12	1:M:122:VAL:HG12	1.88	0.56
1:J:92:ILE:HG13	1:J:92:ILE:O	2.04	0.56
1:T:12:LYS:HE2	1:T:181:ASP:OD2	2.06	0.56
1:C:7:ILE:O	1:C:7:ILE:HG23	2.05	0.56
2:M:501:F2P:O2	2:M:501:F2P:C6	2.53	0.56
1:R:128:TRP:HA	1:R:131:TYR:CD1	2.40	0.56
1:C:137:ILE:HA	1:C:140:THR:HG23	1.88	0.56
1:G:65:HIS:HE1	3:G:523:HOH:O	1.89	0.56
1:P:134:LEU:HD23	1:P:178:LEU:HD12	1.87	0.56
1:F:137:ILE:HA	1:F:140:THR:HG23	1.88	0.56
1:R:165:PRO:HB3	1:R:193:SER:HB2	1.87	0.56
1:D:65:HIS:HE1	3:D:516:HOH:O	1.87	0.56
1:O:184:LYS:CE	2:O:501:F2P:O4	2.50	0.56
1:F:170:HIS:HE1	1:I:36:VAL:O	1.89	0.56
1:S:128:TRP:HA	1:S:131:TYR:CD1	2.40	0.56
1:L:220:LEU:CD1	1:L:267:LEU:HD23	2.35	0.55
1:F:122:VAL:HG12	1:I:92:ILE:HG12	1.87	0.55
1:Q:37:SER:CB	2:Q:501:F2P:O12	2.53	0.55
1:Q:128:TRP:HA	1:Q:131:TYR:CD1	2.42	0.55
1:M:9:ASN:C	1:M:9:ASN:HD22	2.10	0.55
1:H:224:LYS:HZ1	1:H:262:ASP:HA	1.71	0.55
1:P:207:VAL:CG2	1:P:234:VAL:HG23	2.35	0.55
1:K:137:ILE:HA	1:K:140:THR:HG23	1.89	0.55
1:G:166:GLU:HG3	1:G:167:LEU:N	2.21	0.55
1:S:2:GLU:N	1:S:5:LYS:NZ	2.55	0.55
1:B:159:ILE:HD13	1:B:167:LEU:HD13	1.88	0.55
1:L:107:GLU:HG3	1:L:111:MET:HE2	1.87	0.55
1:M:128:TRP:HA	1:M:131:TYR:CD1	2.41	0.55
1:N:164:ASP:CG	1:P:214:ASN:ND2	2.60	0.55
1:F:165:PRO:HB3	1:F:193:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:LYS:HG2	3:G:504:HOH:O	2.07	0.55
1:D:128:TRP:HA	1:D:131:TYR:CD1	2.42	0.55
1:M:151:MET:CG	1:M:184:LYS:HD3	2.37	0.55
1:O:161:ASN:HD21	1:O:163:ARG:HB2	1.72	0.55
1:C:69:VAL:O	1:C:71:HIS:N	2.40	0.55
1:Q:142:GLU:HG2	1:T:70:ARG:HH12	1.71	0.55
1:Q:245:ASP:OD2	1:Q:248:GLY:HA3	2.05	0.55
1:R:137:ILE:HA	1:R:140:THR:HG23	1.88	0.55
1:B:128:TRP:HA	1:B:131:TYR:CD1	2.41	0.55
1:L:165:PRO:HB3	1:L:193:SER:HB2	1.89	0.55
1:L:207:VAL:CG2	1:L:234:VAL:HG23	2.33	0.55
1:O:128:TRP:HA	1:O:131:TYR:CD1	2.42	0.55
1:F:128:TRP:HA	1:F:131:TYR:CD1	2.42	0.55
1:H:1:MET:CE	1:H:22:ARG:HA	2.37	0.55
1:I:66:LYS:O	1:I:70:ARG:HG2	2.06	0.55
1:E:1:MET:HG3	1:E:25:GLU:HG2	1.89	0.55
1:S:21:ASN:HD22	1:S:24:SER:N	1.99	0.55
1:I:2:GLU:HG3	1:I:4:PHE:N	2.15	0.55
1:I:2:GLU:CG	1:I:3:LEU:H	2.20	0.55
1:I:207:VAL:CG2	1:I:234:VAL:HG23	2.34	0.55
1:A:270:ILE:HB	3:A:517:HOH:O	2.05	0.54
1:B:10:LEU:HD21	1:L:69:VAL:HG12	1.89	0.54
1:B:151:MET:HG2	1:B:184:LYS:HG2	1.89	0.54
1:K:92:ILE:HG12	1:O:122:VAL:HG12	1.88	0.54
1:A:207:VAL:CG2	1:A:234:VAL:HG23	2.34	0.54
1:B:137:ILE:HA	1:B:140:THR:HG23	1.88	0.54
1:L:251:ARG:CB	1:L:269:GLU:HG2	2.38	0.54
1:M:92:ILE:HG12	1:N:122:VAL:HG12	1.89	0.54
1:N:192:ASP:OD2	1:P:161:ASN:CG	2.46	0.54
1:O:31:PRO:CB	2:O:501:F2P:O4	2.55	0.54
1:J:21:ASN:HB2	1:J:258:HIS:CE1	2.42	0.54
1:R:36:VAL:HG13	1:S:174:LEU:CD1	2.36	0.54
1:S:271:ARG:HH21	1:S:271:ARG:N	2.06	0.54
1:H:157:LYS:HB3	1:H:157:LYS:NZ	2.23	0.54
1:I:110:ARG:HD3	3:T:514:HOH:O	2.08	0.54
1:J:245:ASP:OD2	1:J:248:GLY:HA3	2.08	0.54
1:D:9:ASN:HD22	1:D:12:LYS:H	1.56	0.54
1:F:187:TYR:HB2	1:F:222:MET:HE3	1.90	0.54
1:F:207:VAL:CG2	1:F:234:VAL:HG23	2.34	0.54
1:C:7:ILE:HD11	1:C:12:LYS:CB	2.38	0.54
1:L:137:ILE:HA	1:L:140:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:262:ASP:OD2	1:M:264:GLU:HB3	2.08	0.54
1:N:9:ASN:ND2	1:N:12:LYS:H	2.06	0.54
1:N:137:ILE:HA	1:N:140:THR:HG23	1.89	0.54
1:T:37:SER:CB	2:T:501:F2P:O13	2.55	0.54
1:T:92:ILE:O	1:T:92:ILE:HG13	2.06	0.54
1:T:137:ILE:HA	1:T:140:THR:HG23	1.90	0.54
1:A:137:ILE:HA	1:A:140:THR:HG23	1.90	0.54
1:N:223:ILE:CD1	1:N:234:VAL:HG21	2.33	0.54
1:I:151:MET:HG2	1:I:184:LYS:HD3	1.88	0.54
1:D:182:ILE:HG22	1:D:183:VAL:N	2.22	0.54
1:D:263:VAL:O	1:D:267:LEU:HG	2.08	0.54
1:K:240:ILE:O	1:K:246:VAL:HG22	2.08	0.54
1:I:137:ILE:HA	1:I:140:THR:HG23	1.89	0.54
1:Q:162:GLU:HG3	3:Q:510:HOH:O	2.08	0.54
1:T:207:VAL:CG2	1:T:234:VAL:HG23	2.36	0.54
1:T:221:GLN:OE1	1:T:263:VAL:HG21	2.07	0.54
1:E:161:ASN:C	1:E:163:ARG:H	2.11	0.53
1:N:207:VAL:CG2	1:N:234:VAL:HG23	2.35	0.53
1:F:35:GLY:HA3	1:J:177:GLU:OE2	2.07	0.53
1:G:22:ARG:HG2	1:G:22:ARG:HH11	1.73	0.53
1:P:161:ASN:HD22	1:P:163:ARG:H	1.55	0.53
1:S:157:LYS:HB2	1:S:157:LYS:NZ	2.23	0.53
1:C:30:VAL:HG21	1:C:54:VAL:CG1	2.39	0.53
1:L:245:ASP:OD2	1:L:248:GLY:HA3	2.08	0.53
1:G:137:ILE:HA	1:G:140:THR:HG23	1.89	0.53
1:P:151:MET:SD	2:P:501:F2P:O3	2.60	0.53
1:Q:36:VAL:HG13	1:R:174:LEU:CD1	2.38	0.53
1:R:207:VAL:CG2	1:R:234:VAL:HG23	2.35	0.53
1:B:23:GLU:HG2	1:B:24:SER:N	2.23	0.53
1:O:92:ILE:O	1:O:92:ILE:HG13	2.08	0.53
1:F:18:ARG:HE	1:P:18:ARG:CZ	2.22	0.53
1:B:222:MET:CE	1:B:223:ILE:HD12	2.38	0.53
1:C:128:TRP:HA	1:C:131:TYR:CD1	2.44	0.53
1:C:207:VAL:CG2	1:C:234:VAL:HG23	2.35	0.53
1:A:151:MET:CG	1:A:184:LYS:HD3	2.38	0.53
1:B:184:LYS:HA	1:B:206:VAL:O	2.09	0.53
1:O:31:PRO:HB3	2:O:501:F2P:O4	2.07	0.53
1:C:92:ILE:HD12	1:D:167:LEU:HD22	1.89	0.53
1:Q:2:GLU:HA	3:Q:522:HOH:O	2.09	0.53
1:A:31:PRO:HA	1:A:63:LEU:HB3	1.91	0.53
1:B:1:MET:HG2	1:B:25:GLU:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:PRO:HB3	1:I:193:SER:HB2	1.91	0.53
1:R:4:PHE:CD2	1:R:7:ILE:HD12	2.44	0.53
1:R:161:ASN:HD21	1:R:163:ARG:HB2	1.74	0.53
1:C:69:VAL:C	1:C:71:HIS:H	2.11	0.53
1:K:151:MET:HG2	1:K:184:LYS:HD3	1.90	0.53
1:N:164:ASP:OD2	1:P:214:ASN:ND2	2.42	0.53
1:H:128:TRP:HA	1:H:131:TYR:CD1	2.44	0.53
1:T:99:LYS:NZ	2:T:501:F2P:O11	2.33	0.53
1:N:31:PRO:HA	1:N:63:LEU:HB3	1.91	0.52
1:T:267:LEU:HD23	1:T:270:ILE:HD12	1.90	0.52
1:K:71:HIS:HE1	3:O:528:HOH:O	1.92	0.52
1:S:236:VAL:HA	2:S:501:F2P:O61	2.08	0.52
1:B:223:ILE:CG1	1:B:234:VAL:HG21	2.39	0.52
1:L:153:TYR:OH	1:L:184:LYS:HE2	2.10	0.52
1:R:3:LEU:HD22	1:R:204:PRO:HG3	1.92	0.52
1:C:31:PRO:HA	1:C:63:LEU:HB3	1.92	0.52
1:N:151:MET:CG	1:N:184:LYS:HD3	2.39	0.52
1:D:31:PRO:HA	1:D:63:LEU:HB3	1.91	0.52
1:L:1:MET:HE3	1:L:20:PHE:HB3	1.92	0.52
1:L:3:LEU:HD22	1:L:204:PRO:HG3	1.92	0.52
1:L:34:HIS:CE1	2:L:501:F2P:O2	2.62	0.52
1:N:164:ASP:CG	1:P:214:ASN:HD22	2.13	0.52
1:J:207:VAL:CG2	1:J:234:VAL:HG23	2.35	0.52
1:T:245:ASP:OD2	1:T:248:GLY:HA3	2.10	0.52
1:D:165:PRO:HA	1:D:188:THR:HG21	1.92	0.52
1:N:191:ILE:CD1	1:P:160:GLN:HG2	2.39	0.52
1:F:161:ASN:ND2	1:F:163:ARG:H	2.07	0.52
1:P:137:ILE:HA	1:P:140:THR:HG23	1.90	0.52
1:D:31:PRO:HB2	2:D:501:F2P:H6C2	1.92	0.52
1:O:262:ASP:OD2	1:O:264:GLU:HB3	2.09	0.52
1:P:164:ASP:OD1	1:P:166:GLU:HB3	2.10	0.52
1:O:6:ASP:O	1:O:8:LYS:HG3	2.09	0.52
1:H:224:LYS:HD3	1:H:256:ILE:HG23	1.91	0.52
1:I:165:PRO:HG3	1:I:188:THR:HB	1.91	0.52
1:K:164:ASP:OD1	1:K:166:GLU:HB3	2.10	0.52
1:L:265:GLU:HA	1:L:268:LYS:CE	2.40	0.52
1:G:207:VAL:CG2	1:G:234:VAL:HG23	2.38	0.52
1:P:161:ASN:HD22	1:P:161:ASN:C	2.12	0.52
1:O:245:ASP:OD2	1:O:248:GLY:HA3	2.09	0.51
1:J:70:ARG:HH11	1:J:70:ARG:HG3	1.75	0.51
1:C:9:ASN:C	1:C:9:ASN:HD22	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:ILE:HD12	1:L:68:ILE:N	2.24	0.51
1:J:262:ASP:OD2	1:J:264:GLU:HB2	2.11	0.51
1:K:122:VAL:HG12	1:N:92:ILE:HG12	1.91	0.51
1:P:184:LYS:CE	2:P:501:F2P:H3	2.41	0.51
1:S:207:VAL:CG2	1:S:234:VAL:HG23	2.34	0.51
1:B:107:GLU:HG3	1:B:111:MET:CE	2.41	0.51
1:D:160:GLN:HA	1:D:160:GLN:NE2	2.26	0.51
1:K:31:PRO:HA	1:K:63:LEU:HB3	1.93	0.51
1:F:31:PRO:HA	1:F:63:LEU:HB3	1.93	0.51
1:J:128:TRP:HA	1:J:131:TYR:CD1	2.45	0.51
1:Q:61:ALA:HA	1:Q:80:VAL:HG22	1.91	0.51
1:T:262:ASP:OD2	1:T:264:GLU:HB3	2.10	0.51
1:E:207:VAL:CG2	1:E:234:VAL:HG23	2.34	0.51
1:O:31:PRO:HA	1:O:63:LEU:HB3	1.92	0.51
1:P:168:VAL:HG21	1:P:188:THR:HG23	1.90	0.51
1:D:109:ILE:CD1	1:D:144:TRP:HB3	2.41	0.51
1:P:251:ARG:CB	1:P:269:GLU:HG2	2.40	0.51
1:Q:139:GLU:HG3	1:T:66:LYS:HE3	1.92	0.51
1:R:3:LEU:HD22	1:R:204:PRO:CG	2.41	0.51
1:R:165:PRO:HA	1:R:188:THR:HG21	1.93	0.51
1:B:207:VAL:CG2	1:B:234:VAL:HG23	2.33	0.51
1:O:47:ILE:CD1	1:O:68:ILE:HD12	2.40	0.51
1:T:151:MET:HG2	1:T:184:LYS:HD3	1.93	0.51
1:F:14:VAL:HG12	1:F:18:ARG:NH2	2.26	0.51
1:S:21:ASN:ND2	1:S:24:SER:N	2.41	0.51
3:F:515:HOH:O	1:P:110:ARG:HD3	2.10	0.51
1:P:21:ASN:HB2	1:P:258:HIS:CE1	2.46	0.51
1:P:31:PRO:HA	1:P:63:LEU:HB3	1.92	0.51
1:T:10:LEU:O	1:T:14:VAL:HG23	2.10	0.51
1:C:157:LYS:HE2	1:C:157:LYS:H	1.76	0.51
1:C:262:ASP:OD1	1:C:265:GLU:HB2	2.10	0.51
1:G:163:ARG:HD3	1:G:163:ARG:N	2.26	0.51
1:Q:151:MET:HA	1:Q:184:LYS:HB3	1.91	0.51
1:T:9:ASN:C	1:T:9:ASN:HD22	2.15	0.51
1:M:207:VAL:CG2	1:M:234:VAL:HG23	2.37	0.50
1:N:19:ILE:HG13	1:N:20:PHE:HD1	1.75	0.50
1:O:151:MET:SD	1:O:184:LYS:HE3	2.50	0.50
1:G:221:GLN:OE1	1:G:263:VAL:HG21	2.11	0.50
1:B:4:PHE:C	1:B:6:ASP:H	2.14	0.50
1:K:160:GLN:OE1	1:K:160:GLN:N	2.43	0.50
1:L:31:PRO:HA	1:L:63:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ILE:CD1	1:O:144:TRP:HB3	2.42	0.50
1:F:209:GLY:N	2:F:501:F2P:O61	2.41	0.50
1:I:187:TYR:HB2	1:I:222:MET:HE3	1.93	0.50
1:Q:92:ILE:HD11	1:R:122:VAL:O	2.12	0.50
1:N:160:GLN:NE2	1:N:160:GLN:HA	2.26	0.50
1:O:184:LYS:HD2	1:O:235:ALA:HB3	1.93	0.50
1:F:151:MET:HA	1:F:184:LYS:HB3	1.92	0.50
1:I:31:PRO:HA	1:I:63:LEU:HB3	1.91	0.50
1:I:187:TYR:HB2	1:I:222:MET:CE	2.42	0.50
1:J:109:ILE:CD1	1:J:144:TRP:HB3	2.41	0.50
1:E:245:ASP:OD2	1:E:248:GLY:HA3	2.11	0.50
1:M:17:GLU:HG2	1:M:22:ARG:HH22	1.74	0.50
1:M:31:PRO:HA	1:M:63:LEU:HB3	1.94	0.50
1:H:107:GLU:HG3	1:H:111:MET:CE	2.42	0.50
1:A:221:GLN:OE1	1:A:263:VAL:HG21	2.11	0.50
2:K:501:F2P:H2	2:K:501:F2P:O13	2.11	0.50
1:L:139:GLU:HG3	1:O:66:LYS:HE3	1.92	0.50
1:R:92:ILE:HD12	1:S:167:LEU:HD22	1.92	0.50
1:K:36:VAL:HG23	1:O:177:GLU:OE1	2.11	0.50
1:M:109:ILE:CD1	1:M:144:TRP:HB3	2.42	0.50
2:H:501:F2P:H4	2:H:501:F2P:P6	2.51	0.50
1:J:31:PRO:HA	1:J:63:LEU:HB3	1.93	0.50
1:R:7:ILE:O	1:R:7:ILE:HG22	2.11	0.50
1:C:157:LYS:H	1:C:157:LYS:CE	2.23	0.50
1:N:2:GLU:HB2	1:N:25:GLU:OE2	2.11	0.50
1:J:236:VAL:HA	2:J:501:F2P:O61	2.11	0.50
1:Q:10:LEU:O	1:Q:14:VAL:HG23	2.12	0.50
1:C:165:PRO:HB3	1:C:193:SER:HB2	1.93	0.50
1:K:263:VAL:O	1:K:267:LEU:HG	2.11	0.50
1:P:23:GLU:HG3	1:P:24:SER:N	2.27	0.50
1:Q:31:PRO:HA	1:Q:63:LEU:HB3	1.94	0.50
1:T:161:ASN:ND2	1:T:161:ASN:C	2.65	0.50
1:B:31:PRO:HA	1:B:63:LEU:HB3	1.93	0.50
1:B:66:LYS:O	1:B:70:ARG:HG2	2.12	0.50
1:C:155:ARG:HG2	1:C:162:GLU:CD	2.32	0.50
1:E:109:ILE:CD1	1:E:144:TRP:HB3	2.41	0.50
1:G:31:PRO:HA	1:G:63:LEU:HB3	1.93	0.50
1:G:264:GLU:HG3	3:G:521:HOH:O	2.12	0.50
2:G:501:F2P:H2	2:G:501:F2P:O13	2.12	0.50
1:K:220:LEU:HD12	1:K:267:LEU:CD2	2.41	0.49
1:N:160:GLN:HA	1:N:160:GLN:HE21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:ASN:HD22	1:O:9:ASN:C	2.15	0.49
1:G:163:ARG:NH2	3:G:514:HOH:O	2.45	0.49
1:C:151:MET:HA	1:C:184:LYS:HB3	1.93	0.49
1:P:151:MET:HE1	2:P:501:F2P:O4	2.12	0.49
1:D:207:VAL:CG2	1:D:234:VAL:HG23	2.37	0.49
1:F:6:ASP:O	1:F:8:LYS:N	2.45	0.49
1:F:109:ILE:CD1	1:F:144:TRP:HB3	2.41	0.49
1:A:92:ILE:HG12	1:E:122:VAL:HG12	1.94	0.49
1:F:245:ASP:OD2	1:F:248:GLY:HA3	2.13	0.49
1:H:109:ILE:CD1	1:H:144:TRP:HB3	2.42	0.49
1:T:31:PRO:HA	1:T:63:LEU:HB3	1.94	0.49
1:C:109:ILE:CD1	1:C:144:TRP:HB3	2.42	0.49
1:C:161:ASN:HD21	1:C:163:ARG:HB2	1.77	0.49
1:F:14:VAL:CG1	1:F:18:ARG:NH2	2.76	0.49
1:J:65:HIS:HE1	3:J:513:HOH:O	1.94	0.49
1:P:78:LYS:HD2	1:P:79:ASP:N	2.27	0.49
1:S:31:PRO:HA	1:S:63:LEU:HB3	1.94	0.49
1:K:151:MET:SD	2:K:501:F2P:O3	2.70	0.49
1:L:107:GLU:HG3	1:L:111:MET:CE	2.42	0.49
1:P:109:ILE:CD1	1:P:144:TRP:HB3	2.42	0.49
1:D:107:GLU:HG3	1:D:111:MET:CE	2.42	0.49
1:K:9:ASN:C	1:K:9:ASN:HD22	2.16	0.49
1:K:160:GLN:N	1:K:160:GLN:CD	2.66	0.49
1:R:31:PRO:HA	1:R:63:LEU:HB3	1.93	0.49
1:C:4:PHE:HB3	1:C:7:ILE:CG2	2.43	0.49
1:G:173:ARG:HD2	1:G:173:ARG:O	2.13	0.49
1:T:107:GLU:HG3	1:T:111:MET:CE	2.41	0.49
1:K:210:GLY:N	2:K:501:F2P:O63	2.44	0.49
1:H:160:GLN:HA	1:H:160:GLN:HE21	1.77	0.49
1:T:3:LEU:HD22	1:T:204:PRO:HG3	1.95	0.49
1:K:40:PRO:HG3	3:O:527:HOH:O	2.13	0.48
1:K:262:ASP:OD2	1:K:264:GLU:HB3	2.12	0.48
1:L:161:ASN:ND2	1:L:163:ARG:H	2.10	0.48
1:J:9:ASN:C	1:J:9:ASN:ND2	2.65	0.48
1:B:22:ARG:HH21	1:L:76:TYR:C	2.17	0.48
1:N:109:ILE:CD1	1:N:144:TRP:HB3	2.42	0.48
1:O:207:VAL:CG2	1:O:234:VAL:HG23	2.38	0.48
1:C:7:ILE:HD11	1:C:12:LYS:HB3	1.95	0.48
1:K:246:VAL:HA	1:K:249:ILE:HG22	1.95	0.48
1:H:151:MET:HA	1:H:184:LYS:HB3	1.94	0.48
1:T:95:ASN:HD22	1:T:95:ASN:C	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:GLU:HG2	1:M:22:ARG:CZ	2.43	0.48
1:O:9:ASN:ND2	1:O:12:LYS:H	2.11	0.48
1:F:238:ARG:NH2	2:F:501:F2P:O62	2.39	0.48
1:S:107:GLU:HG3	1:S:111:MET:CE	2.44	0.48
1:S:161:ASN:ND2	1:S:161:ASN:C	2.66	0.48
1:K:165:PRO:HB3	1:K:193:SER:HB2	1.94	0.48
1:I:109:ILE:CD1	1:I:144:TRP:HB3	2.44	0.48
1:T:21:ASN:O	1:T:25:GLU:N	2.41	0.48
1:A:170:HIS:HE1	1:D:36:VAL:O	1.97	0.48
1:O:225:ASP:HA	3:O:529:HOH:O	2.14	0.48
1:H:1:MET:HE2	1:H:22:ARG:HA	1.96	0.48
1:P:47:ILE:HD11	1:T:173:ARG:NH2	2.28	0.48
1:Q:107:GLU:HG3	1:Q:111:MET:CE	2.43	0.48
1:Q:207:VAL:CG2	1:Q:234:VAL:HG23	2.37	0.48
1:R:109:ILE:CD1	1:R:144:TRP:HB3	2.43	0.48
1:Q:94:PRO:HG2	1:R:125:ASP:HA	1.95	0.48
1:I:221:GLN:OE1	1:I:263:VAL:HG21	2.14	0.48
1:T:61:ALA:HA	1:T:80:VAL:HG23	1.95	0.48
1:A:161:ASN:ND2	1:A:163:ARG:H	2.12	0.48
1:L:139:GLU:OE2	1:O:103:THR:HA	2.14	0.48
1:S:157:LYS:HD2	1:S:158:HIS:NE2	2.29	0.48
1:C:243:HIS:ND1	1:C:244:ASP:N	2.62	0.48
1:E:151:MET:HA	1:E:184:LYS:HB3	1.96	0.48
1:L:151:MET:HA	1:L:184:LYS:HB3	1.96	0.48
1:H:160:GLN:HA	1:H:160:GLN:NE2	2.28	0.48
1:Q:47:ILE:CD1	1:Q:68:ILE:HD12	2.43	0.48
1:M:224:LYS:O	1:M:228:GLU:HG3	2.14	0.47
1:J:1:MET:HG2	1:J:25:GLU:CG	2.38	0.47
1:T:109:ILE:CD1	1:T:144:TRP:HB3	2.43	0.47
1:B:184:LYS:HE2	1:B:208:ALA:CB	2.42	0.47
1:M:151:MET:HA	1:M:184:LYS:HB3	1.95	0.47
1:N:191:ILE:HD13	1:P:160:GLN:HG2	1.95	0.47
1:F:33:ASP:OD2	2:F:501:F2P:O2	2.32	0.47
1:F:151:MET:HG2	1:F:184:LYS:HD3	1.95	0.47
1:F:255:LYS:HE3	1:F:269:GLU:OE2	2.13	0.47
1:G:22:ARG:HG2	1:G:22:ARG:NH1	2.30	0.47
1:J:21:ASN:HB3	1:J:24:SER:OG	2.13	0.47
1:R:92:ILE:HG12	1:S:122:VAL:HG12	1.96	0.47
1:S:265:GLU:HA	1:S:268:LYS:NZ	2.30	0.47
1:B:184:LYS:C	1:B:184:LYS:CD	2.72	0.47
1:C:7:ILE:HG21	1:C:13:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:16:LEU:HD23	1:N:19:ILE:HD11	1.94	0.47
1:N:151:MET:HA	1:N:184:LYS:HB3	1.97	0.47
1:F:107:GLU:HG3	1:F:111:MET:CE	2.43	0.47
1:Q:187:TYR:HB2	1:Q:222:MET:HE3	1.96	0.47
1:P:107:GLU:HG3	1:P:111:MET:CE	2.44	0.47
1:S:30:VAL:HG21	1:S:54:VAL:CG1	2.44	0.47
1:R:22:ARG:HD3	1:R:22:ARG:C	2.35	0.47
1:R:151:MET:HA	1:R:184:LYS:HB3	1.95	0.47
1:C:95:ASN:HD22	1:C:95:ASN:C	2.18	0.47
1:P:267:LEU:C	1:P:269:GLU:H	2.18	0.47
1:B:70:ARG:HG2	1:B:70:ARG:H	1.54	0.47
1:B:166:GLU:HG3	1:B:167:LEU:N	2.29	0.47
1:E:31:PRO:HA	1:E:63:LEU:HB3	1.96	0.47
1:E:151:MET:CG	1:E:184:LYS:HD3	2.44	0.47
1:E:157:LYS:HG3	3:E:529:HOH:O	2.14	0.47
1:L:4:PHE:HB3	1:L:7:ILE:HD13	1.96	0.47
1:N:7:ILE:CG2	1:N:13:LEU:HD13	2.45	0.47
1:O:107:GLU:HG3	1:O:111:MET:CE	2.43	0.47
1:G:155:ARG:HG2	1:G:162:GLU:CD	2.35	0.47
1:I:243:HIS:ND1	1:I:244:ASP:N	2.63	0.47
1:J:151:MET:SD	2:J:501:F2P:O3	2.69	0.47
1:R:4:PHE:HD2	1:R:7:ILE:HD12	1.79	0.47
1:S:21:ASN:ND2	1:S:23:GLU:HB2	2.24	0.47
1:T:161:ASN:C	1:T:161:ASN:HD22	2.17	0.47
1:C:107:GLU:HG3	1:C:111:MET:CE	2.43	0.47
1:J:165:PRO:HB3	1:J:193:SER:HB2	1.97	0.47
1:T:21:ASN:HB2	1:T:258:HIS:CE1	2.50	0.47
3:A:515:HOH:O	1:N:110:ARG:HD3	2.13	0.47
1:N:191:ILE:HG12	1:N:225:ASP:HB3	1.97	0.47
1:A:166:GLU:HG3	1:A:167:LEU:N	2.30	0.47
1:B:95:ASN:C	1:B:95:ASN:HD22	2.19	0.47
1:C:30:VAL:HG21	1:C:54:VAL:HG13	1.97	0.47
1:G:103:THR:HA	1:H:139:GLU:OE2	2.14	0.47
1:G:109:ILE:CD1	1:G:144:TRP:HB3	2.43	0.47
1:Q:61:ALA:HA	1:Q:80:VAL:CG2	2.44	0.47
1:R:67:GLY:O	1:R:71:HIS:HB2	2.16	0.47
1:A:7:ILE:O	1:A:7:ILE:HG22	2.14	0.46
1:B:9:ASN:C	1:B:9:ASN:HD22	2.19	0.46
1:B:109:ILE:CD1	1:B:144:TRP:HB3	2.44	0.46
1:E:155:ARG:HG2	1:E:162:GLU:CD	2.35	0.46
1:K:107:GLU:HG3	1:K:111:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:GLU:HG3	1:I:111:MET:CE	2.44	0.46
1:J:95:ASN:C	1:J:95:ASN:HD22	2.18	0.46
1:S:173:ARG:HD3	1:S:200:GLY:O	2.16	0.46
1:K:30:VAL:HG21	1:K:54:VAL:CG1	2.46	0.46
1:L:207:VAL:HG23	1:L:234:VAL:CG2	2.39	0.46
1:P:155:ARG:HG2	1:P:162:GLU:CD	2.35	0.46
1:S:95:ASN:C	1:S:95:ASN:HD22	2.17	0.46
1:M:107:GLU:HG3	1:M:111:MET:CE	2.43	0.46
1:N:1:MET:HG3	1:N:25:GLU:HG2	1.96	0.46
1:G:70:ARG:HG3	3:H:528:HOH:O	2.16	0.46
1:I:153:TYR:OH	1:I:184:LYS:HE2	2.16	0.46
1:T:78:LYS:HD3	1:T:78:LYS:N	2.30	0.46
1:A:107:GLU:HG3	1:A:111:MET:CE	2.45	0.46
1:L:122:VAL:HG12	1:O:92:ILE:CD1	2.46	0.46
1:H:9:ASN:HD21	1:H:145:GLY:HA2	1.79	0.46
1:E:107:GLU:HG3	1:E:111:MET:CE	2.45	0.46
1:F:165:PRO:HG2	3:F:512:HOH:O	2.14	0.46
1:L:109:ILE:CD1	1:L:144:TRP:HB3	2.45	0.46
1:R:159:ILE:HD13	1:R:167:LEU:HD13	1.98	0.46
1:R:173:ARG:HD3	1:R:200:GLY:O	2.15	0.46
1:A:151:MET:HA	1:A:184:LYS:HB3	1.98	0.46
1:K:262:ASP:OD2	1:K:264:GLU:CB	2.63	0.46
1:H:31:PRO:HA	1:H:63:LEU:HB3	1.97	0.46
1:J:22:ARG:NH1	1:J:22:ARG:HG2	2.31	0.46
1:S:19:ILE:HG22	1:S:81:GLY:HA3	1.96	0.46
1:C:4:PHE:HB3	1:C:7:ILE:HG21	1.98	0.46
1:C:220:LEU:HD12	1:C:267:LEU:CD2	2.42	0.46
1:K:95:ASN:C	1:K:95:ASN:HD22	2.19	0.46
1:L:122:VAL:HG12	1:O:92:ILE:CG1	2.45	0.46
1:N:192:ASP:OD2	1:P:161:ASN:CA	2.64	0.46
1:F:207:VAL:HG23	1:F:234:VAL:CG2	2.40	0.46
1:G:92:ILE:CG1	1:H:122:VAL:HG12	2.45	0.46
1:J:18:ARG:NH2	1:S:18:ARG:NE	2.64	0.46
1:Q:98:LYS:NZ	3:Q:513:HOH:O	2.28	0.46
1:S:64:LEU:HD22	1:S:68:ILE:HG21	1.97	0.46
1:T:154:PRO:O	1:T:162:GLU:HG2	2.16	0.46
1:Q:90:THR:HG23	1:R:131:TYR:CE1	2.51	0.46
1:Q:142:GLU:HG2	1:T:70:ARG:NH1	2.30	0.46
1:C:152:MET:CE	3:C:535:HOH:O	2.64	0.45
1:K:36:VAL:HG21	1:K:65:HIS:CE1	2.51	0.45
1:K:109:ILE:CD1	1:K:144:TRP:HB3	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:LEU:HD12	1:K:267:LEU:HD23	1.98	0.45
1:N:207:VAL:HG23	1:N:234:VAL:CG2	2.40	0.45
1:O:165:PRO:HB3	1:O:193:SER:HB2	1.98	0.45
1:I:165:PRO:HA	1:I:188:THR:HG21	1.98	0.45
1:I:220:LEU:HD12	1:I:267:LEU:HD23	1.99	0.45
1:D:109:ILE:HD11	1:D:144:TRP:CB	2.46	0.45
1:D:164:ASP:O	1:D:168:VAL:HG23	2.16	0.45
1:L:95:ASN:C	1:L:95:ASN:HD22	2.18	0.45
1:O:95:ASN:C	1:O:95:ASN:HD22	2.18	0.45
1:F:21:ASN:HA	3:F:532:HOH:O	2.16	0.45
1:S:155:ARG:HG2	1:S:162:GLU:CD	2.36	0.45
1:O:184:LYS:HA	1:O:206:VAL:O	2.17	0.45
1:O:210:GLY:N	2:O:501:F2P:O62	2.41	0.45
1:G:92:ILE:CD1	1:H:122:VAL:HG12	2.46	0.45
1:H:207:VAL:HG23	1:H:234:VAL:CG2	2.40	0.45
1:R:236:VAL:CG2	1:R:240:ILE:HG13	2.47	0.45
1:S:109:ILE:CD1	1:S:144:TRP:HB3	2.44	0.45
1:S:155:ARG:HG2	1:S:162:GLU:CG	2.44	0.45
1:I:47:ILE:CD1	1:I:68:ILE:HD12	2.47	0.45
1:R:107:GLU:HG3	1:R:111:MET:CE	2.46	0.45
1:B:30:VAL:HG21	1:B:54:VAL:CG1	2.47	0.45
1:N:7:ILE:O	1:N:7:ILE:CG2	2.64	0.45
1:Q:11:GLY:O	1:Q:15:ARG:HG3	2.17	0.45
1:Q:173:ARG:HD3	1:Q:200:GLY:O	2.16	0.45
1:I:207:VAL:HG23	1:I:234:VAL:CG2	2.40	0.45
1:P:36:VAL:O	1:T:170:HIS:HE1	1.98	0.45
1:T:83:ILE:HD13	1:T:149:ILE:HD12	1.99	0.45
1:T:187:TYR:OH	1:T:225:ASP:HB3	2.17	0.45
3:A:513:HOH:O	1:D:71:HIS:CE1	2.69	0.45
1:B:151:MET:HA	1:B:184:LYS:HG3	1.97	0.45
1:N:30:VAL:HG21	1:N:54:VAL:CG1	2.47	0.45
1:O:31:PRO:CG	2:O:501:F2P:O4	2.64	0.45
2:O:501:F2P:H6C2	2:O:501:F2P:HA	1.77	0.45
1:F:95:ASN:C	1:F:95:ASN:HD22	2.20	0.45
1:J:22:ARG:HG2	1:J:22:ARG:HH11	1.81	0.45
1:T:134:LEU:HD21	1:T:175:GLY:HA2	1.99	0.45
1:K:270:ILE:CG2	1:K:271:ARG:N	2.80	0.45
1:L:74:ARG:C	1:L:76:TYR:N	2.69	0.45
1:L:132:ARG:NH1	1:O:101:ILE:O	2.48	0.45
1:M:244:ASP:OD2	1:M:244:ASP:N	2.38	0.45
1:N:107:GLU:HG3	1:N:111:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:ILE:O	1:F:235:ALA:HA	2.17	0.45
1:P:251:ARG:HB3	1:P:269:GLU:HG2	1.99	0.45
1:R:185:THR:HG23	1:R:186:SER:N	2.32	0.45
1:E:9:ASN:HD22	1:E:9:ASN:C	2.20	0.45
1:G:107:GLU:HG3	1:G:111:MET:CE	2.44	0.45
1:Q:90:THR:HG23	1:R:131:TYR:CZ	2.52	0.45
1:T:7:ILE:CD1	1:T:13:LEU:HG	2.43	0.45
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.81	0.44
3:D:511:HOH:O	1:K:110:ARG:HD3	2.16	0.44
1:K:267:LEU:C	1:K:269:GLU:H	2.20	0.44
1:M:95:ASN:HD22	1:M:95:ASN:C	2.20	0.44
1:J:10:LEU:O	1:J:14:VAL:HG23	2.16	0.44
1:A:122:VAL:O	1:D:92:ILE:HD11	2.17	0.44
1:D:164:ASP:OD1	1:D:167:LEU:HG	2.18	0.44
1:F:3:LEU:HD22	1:F:204:PRO:HG3	1.99	0.44
1:Q:35:GLY:HA3	1:R:177:GLU:OE2	2.17	0.44
1:T:13:LEU:HD23	1:T:13:LEU:HA	1.84	0.44
1:M:11:GLY:O	1:M:15:ARG:HG3	2.17	0.44
1:T:236:VAL:CG2	1:T:240:ILE:HG13	2.47	0.44
1:D:152:MET:CE	1:D:174:LEU:HD12	2.47	0.44
1:D:163:ARG:HG2	1:D:163:ARG:HH11	1.83	0.44
1:L:65:HIS:HE1	3:L:503:HOH:O	1.98	0.44
1:L:160:GLN:HA	1:L:160:GLN:NE2	2.33	0.44
1:F:265:GLU:O	1:F:268:LYS:HB2	2.18	0.44
1:G:139:GLU:HG3	1:J:66:LYS:HE3	1.99	0.44
1:J:30:VAL:HG21	1:J:54:VAL:CG1	2.47	0.44
1:J:109:ILE:HD11	1:J:144:TRP:CB	2.46	0.44
1:P:9:ASN:C	1:P:9:ASN:ND2	2.67	0.44
1:A:30:VAL:HG21	1:A:54:VAL:CG1	2.48	0.44
1:O:109:ILE:HD11	1:O:144:TRP:CB	2.47	0.44
1:J:107:GLU:HG3	1:J:111:MET:CE	2.43	0.44
1:A:11:GLY:O	1:A:15:ARG:HG3	2.18	0.44
1:M:161:ASN:ND2	1:M:163:ARG:H	2.16	0.44
1:O:30:VAL:HG21	1:O:54:VAL:CG1	2.47	0.44
1:O:147:PRO:HA	1:O:181:ASP:OD2	2.17	0.44
1:J:134:LEU:HD23	1:J:178:LEU:HD12	1.98	0.44
1:P:83:ILE:HD13	1:P:149:ILE:HD12	1.99	0.44
1:M:263:VAL:O	1:M:267:LEU:HG	2.18	0.44
1:G:36:VAL:HG13	1:H:174:LEU:HD21	2.00	0.44
1:G:236:VAL:CG2	1:G:240:ILE:HG13	2.47	0.44
1:R:271:ARG:HD2	1:R:271:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:161:ASN:C	1:S:161:ASN:HD22	2.19	0.44
1:A:3:LEU:HD13	1:A:4:PHE:CD1	2.53	0.44
1:C:210:GLY:N	2:C:501:F2P:O63	2.50	0.44
1:D:1:MET:CB	1:D:25:GLU:HG2	2.47	0.44
1:K:21:ASN:HB2	1:K:258:HIS:CE1	2.53	0.44
1:K:185:THR:OG1	1:K:186:SER:N	2.51	0.44
1:I:95:ASN:C	1:I:95:ASN:HD22	2.20	0.44
1:A:125:ASP:HA	1:D:94:PRO:HG2	1.99	0.44
1:K:170:HIS:HE1	1:N:36:VAL:O	1.99	0.44
1:M:19:ILE:O	1:M:19:ILE:HG22	2.18	0.44
1:F:71:HIS:HE1	3:J:523:HOH:O	2.00	0.44
1:F:109:ILE:HD11	1:F:144:TRP:CB	2.47	0.44
1:F:225:ASP:O	1:F:228:GLU:HB2	2.18	0.44
1:G:177:GLU:OE1	1:J:36:VAL:HG23	2.17	0.44
1:G:265:GLU:O	1:G:268:LYS:HB2	2.18	0.44
1:A:36:VAL:O	1:E:170:HIS:HE1	2.01	0.43
1:C:3:LEU:HB2	1:C:25:GLU:OE1	2.18	0.43
1:K:223:ILE:HD12	1:K:234:VAL:CG2	2.43	0.43
1:M:109:ILE:HD11	1:M:144:TRP:CB	2.47	0.43
1:J:18:ARG:NH2	1:S:18:ARG:CZ	2.81	0.43
1:P:103:THR:HA	1:T:139:GLU:OE2	2.17	0.43
1:S:271:ARG:NH2	1:S:271:ARG:HB2	2.33	0.43
1:N:9:ASN:C	1:N:9:ASN:ND2	2.70	0.43
1:N:236:VAL:CG2	1:N:240:ILE:HG13	2.48	0.43
2:J:501:F2P:HA	2:J:501:F2P:P1	2.41	0.43
1:P:117:SER:HA	1:P:149:ILE:O	2.18	0.43
1:Q:10:LEU:HD23	1:Q:10:LEU:HA	1.78	0.43
1:Q:236:VAL:CG2	1:Q:240:ILE:HG13	2.48	0.43
1:R:151:MET:CG	1:R:184:LYS:HD3	2.48	0.43
1:S:30:VAL:HG21	1:S:54:VAL:HG13	2.00	0.43
1:E:30:VAL:HG21	1:E:54:VAL:CG1	2.48	0.43
1:H:95:ASN:C	1:H:95:ASN:HD22	2.21	0.43
1:J:151:MET:HG2	1:J:184:LYS:HD3	2.01	0.43
1:P:151:MET:SD	2:P:501:F2P:O4	2.76	0.43
1:Q:9:ASN:C	1:Q:9:ASN:ND2	2.71	0.43
1:A:117:SER:HA	1:A:149:ILE:O	2.19	0.43
1:B:223:ILE:HG22	1:B:256:ILE:HG21	2.00	0.43
1:C:236:VAL:CG2	1:C:240:ILE:HG13	2.49	0.43
1:E:47:ILE:CD1	1:E:68:ILE:HD12	2.49	0.43
1:N:109:ILE:HD11	1:N:144:TRP:CB	2.46	0.43
1:O:184:LYS:HD2	1:O:235:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:HIS:HE1	1:I:180:ALA:O	2.00	0.43
1:P:95:ASN:C	1:P:95:ASN:HD22	2.20	0.43
1:R:95:ASN:C	1:R:95:ASN:HD22	2.21	0.43
1:B:208:ALA:HB1	2:B:501:F2P:H6C2	2.00	0.43
1:B:236:VAL:CG2	1:B:240:ILE:HG13	2.48	0.43
1:B:267:LEU:HD23	1:B:270:ILE:HD12	1.99	0.43
1:J:20:PHE:HE1	1:J:182:ILE:HD11	1.83	0.43
1:Q:95:ASN:C	1:Q:95:ASN:HD22	2.21	0.43
1:B:18:ARG:NH1	1:L:18:ARG:HD2	2.34	0.43
1:C:236:VAL:HA	2:C:501:F2P:O61	2.18	0.43
1:E:166:GLU:HG3	1:E:167:LEU:N	2.33	0.43
1:N:7:ILE:HG23	1:N:13:LEU:HD13	2.01	0.43
1:J:207:VAL:HG23	1:J:234:VAL:CG2	2.41	0.43
1:P:236:VAL:CG2	1:P:240:ILE:HG13	2.49	0.43
1:S:21:ASN:HD22	1:S:24:SER:CB	2.31	0.43
1:S:161:ASN:C	1:S:163:ARG:H	2.21	0.43
1:A:165:PRO:HB3	1:A:193:SER:HB2	1.99	0.43
1:D:29:ILE:O	1:D:235:ALA:HA	2.19	0.43
1:H:181:ASP:O	1:H:204:PRO:HD2	2.19	0.43
1:Q:9:ASN:ND2	1:Q:12:LYS:H	2.16	0.43
1:C:36:VAL:HG13	1:D:174:LEU:CD2	2.48	0.43
1:L:169:ALA:HB2	1:L:197:VAL:HG22	2.01	0.43
1:J:83:ILE:HD13	1:J:149:ILE:HD12	2.00	0.43
1:J:236:VAL:CG2	1:J:240:ILE:HG13	2.49	0.43
1:Q:49:LYS:HE3	3:Q:520:HOH:O	2.17	0.43
1:T:109:ILE:HD11	1:T:144:TRP:CB	2.46	0.43
1:B:155:ARG:HG2	1:B:162:GLU:CD	2.38	0.43
1:H:236:VAL:CG2	1:H:240:ILE:HG13	2.48	0.43
1:Q:207:VAL:HG23	1:Q:234:VAL:CG2	2.40	0.43
1:S:207:VAL:HG23	1:S:234:VAL:CG2	2.39	0.43
1:S:236:VAL:CG2	1:S:240:ILE:HG13	2.48	0.43
1:K:176:ALA:O	1:N:67:GLY:HA3	2.18	0.43
1:B:36:VAL:O	1:C:170:HIS:HE1	2.02	0.42
3:B:525:HOH:O	1:L:110:ARG:HD3	2.19	0.42
1:E:84:ILE:HD13	1:E:111:MET:HE1	2.01	0.42
1:E:95:ASN:C	1:E:95:ASN:HD22	2.21	0.42
1:N:3:LEU:CD2	1:N:204:PRO:HG3	2.49	0.42
1:H:18:ARG:HG3	1:H:18:ARG:NH2	2.28	0.42
1:H:30:VAL:HG21	1:H:54:VAL:CG1	2.48	0.42
1:R:3:LEU:CD2	1:R:204:PRO:HG3	2.49	0.42
1:B:165:PRO:HB3	1:B:193:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ILE:HG12	1:C:225:ASP:HB3	2.01	0.42
1:E:161:ASN:ND2	1:E:161:ASN:C	2.73	0.42
1:E:236:VAL:CG2	1:E:240:ILE:HG13	2.48	0.42
1:E:240:ILE:CD1	3:E:522:HOH:O	2.67	0.42
1:K:83:ILE:HD13	1:K:149:ILE:HD12	2.02	0.42
1:L:147:PRO:HA	1:L:181:ASP:OD2	2.19	0.42
1:N:155:ARG:HG2	1:N:162:GLU:CD	2.39	0.42
1:F:83:ILE:HD13	1:F:149:ILE:HD12	2.00	0.42
1:H:2:GLU:O	1:H:2:GLU:CG	2.66	0.42
1:J:157:LYS:N	1:J:157:LYS:CD	2.78	0.42
1:P:122:VAL:HG12	1:S:92:ILE:CG1	2.46	0.42
1:C:122:VAL:CG2	3:C:535:HOH:O	2.61	0.42
1:N:30:VAL:HG21	1:N:54:VAL:HG13	2.01	0.42
1:G:19:ILE:HG22	1:G:81:GLY:HA3	2.01	0.42
1:O:83:ILE:HD13	1:O:149:ILE:HD12	2.01	0.42
1:G:1:MET:O	1:G:2:GLU:HG2	2.19	0.42
1:H:109:ILE:HD11	1:H:144:TRP:CB	2.48	0.42
1:H:223:ILE:HD12	1:H:234:VAL:CG2	2.48	0.42
1:J:69:VAL:C	1:J:71:HIS:H	2.23	0.42
1:R:118:ILE:HG21	1:R:134:LEU:HD13	2.00	0.42
1:S:83:ILE:HD13	1:S:149:ILE:CD1	2.49	0.42
1:M:30:VAL:HG21	1:M:54:VAL:CG1	2.49	0.42
1:N:95:ASN:C	1:N:95:ASN:HD22	2.22	0.42
1:F:139:GLU:OE2	1:I:103:THR:HA	2.18	0.42
1:G:9:ASN:ND2	1:G:12:LYS:H	2.17	0.42
1:P:151:MET:HE2	2:P:501:F2P:O4	2.17	0.42
1:T:95:ASN:C	1:T:95:ASN:ND2	2.72	0.42
1:A:236:VAL:CG2	1:A:240:ILE:HG13	2.50	0.42
1:B:222:MET:HE2	1:B:223:ILE:HA	2.02	0.42
1:E:36:VAL:HG21	1:E:65:HIS:CE1	2.53	0.42
1:L:2:GLU:OE2	1:L:2:GLU:N	2.45	0.42
1:L:236:VAL:CG2	1:L:240:ILE:HG13	2.49	0.42
1:G:236:VAL:HA	2:G:501:F2P:O61	2.19	0.42
1:H:66:LYS:HE3	1:I:139:GLU:HG3	2.01	0.42
1:P:11:GLY:O	1:P:15:ARG:HG3	2.19	0.42
1:Q:109:ILE:CD1	1:Q:144:TRP:HB3	2.44	0.42
1:T:8:LYS:HD2	1:T:8:LYS:N	2.35	0.42
1:T:30:VAL:HG21	1:T:54:VAL:CG1	2.49	0.42
1:A:95:ASN:C	1:A:95:ASN:HD22	2.21	0.42
1:A:109:ILE:CD1	1:A:144:TRP:HB3	2.46	0.42
1:C:157:LYS:H	1:C:157:LYS:NZ	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:7:ILE:O	1:K:7:ILE:HG22	2.18	0.42
1:M:83:ILE:HD13	1:M:149:ILE:CD1	2.50	0.42
1:M:236:VAL:CG2	1:M:240:ILE:HG13	2.50	0.42
1:O:208:ALA:CB	2:O:501:F2P:H6C1	2.46	0.42
1:G:95:ASN:C	1:G:95:ASN:HD22	2.22	0.42
1:I:173:ARG:HD3	1:I:200:GLY:O	2.19	0.42
1:P:30:VAL:HG21	1:P:54:VAL:CG1	2.49	0.42
1:P:161:ASN:ND2	1:P:161:ASN:C	2.72	0.42
1:E:29:ILE:O	1:E:235:ALA:HA	2.20	0.42
1:E:207:VAL:HG23	1:E:234:VAL:CG2	2.39	0.42
1:P:72:GLY:O	1:P:74:ARG:N	2.53	0.42
1:S:95:ASN:C	1:S:95:ASN:ND2	2.73	0.42
1:T:83:ILE:HD13	1:T:149:ILE:CD1	2.50	0.42
1:A:118:ILE:HG21	1:A:134:LEU:HD13	2.02	0.42
1:D:21:ASN:HB2	1:D:258:HIS:CE1	2.54	0.42
1:E:161:ASN:O	1:E:163:ARG:N	2.53	0.42
1:O:95:ASN:C	1:O:95:ASN:ND2	2.74	0.42
1:J:69:VAL:O	1:J:71:HIS:N	2.53	0.42
1:A:2:GLU:H	1:A:25:GLU:CD	2.23	0.42
1:B:174:LEU:HD22	1:B:178:LEU:CD1	2.50	0.42
1:F:236:VAL:CG2	1:F:240:ILE:HG13	2.49	0.42
1:P:165:PRO:HB3	1:P:193:SER:HB2	2.02	0.42
1:Q:151:MET:CG	1:Q:184:LYS:HD3	2.49	0.42
1:S:16:LEU:HD23	1:S:16:LEU:HA	1.92	0.42
1:S:18:ARG:HD2	1:S:114:ASP:OD1	2.20	0.42
1:B:151:MET:HG2	1:B:184:LYS:HG3	2.02	0.41
1:B:191:ILE:HG12	1:B:225:ASP:HB3	2.01	0.41
1:K:3:LEU:HD13	1:K:4:PHE:CD1	2.55	0.41
1:L:247:VAL:O	1:L:251:ARG:HG3	2.20	0.41
1:M:117:SER:HA	1:M:149:ILE:O	2.19	0.41
1:P:18:ARG:HD2	3:P:532:HOH:O	2.20	0.41
1:A:4:PHE:CD2	1:A:7:ILE:HD12	2.55	0.41
1:A:109:ILE:HD11	1:A:144:TRP:CB	2.50	0.41
1:L:3:LEU:HD23	1:L:3:LEU:HA	1.90	0.41
1:L:9:ASN:ND2	1:L:12:LYS:H	2.17	0.41
1:G:30:VAL:HG21	1:G:54:VAL:CG1	2.49	0.41
1:G:83:ILE:HD13	1:G:149:ILE:CD1	2.50	0.41
1:I:219:PHE:CZ	1:I:223:ILE:HD11	2.55	0.41
1:J:271:ARG:HD3	1:J:271:ARG:H	1.85	0.41
1:P:184:LYS:HE3	2:P:501:F2P:H3	2.02	0.41
1:S:166:GLU:HG3	1:S:167:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:HG2	1:A:265:GLU:N	2.34	0.41
1:K:30:VAL:HG21	1:K:54:VAL:HG13	2.02	0.41
1:O:30:VAL:HG21	1:O:54:VAL:HG13	2.01	0.41
1:O:184:LYS:CB	1:O:206:VAL:HG12	2.49	0.41
1:G:92:ILE:O	1:G:92:ILE:CG1	2.68	0.41
1:G:165:PRO:HA	1:G:188:THR:HG21	2.02	0.41
1:H:118:ILE:HG21	1:H:134:LEU:HD13	2.02	0.41
1:P:83:ILE:HD13	1:P:149:ILE:CD1	2.50	0.41
1:P:161:ASN:HB3	1:P:164:ASP:HB2	2.01	0.41
1:S:83:ILE:HD13	1:S:149:ILE:HD12	2.01	0.41
1:S:247:VAL:O	1:S:251:ARG:HG3	2.21	0.41
1:T:36:VAL:HG21	1:T:65:HIS:CE1	2.54	0.41
1:T:80:VAL:HG23	1:T:81:GLY:O	2.20	0.41
1:A:151:MET:HG2	1:A:184:LYS:CD	2.48	0.41
1:A:155:ARG:HG2	1:A:162:GLU:CD	2.40	0.41
1:K:118:ILE:HG21	1:K:134:LEU:HD13	2.03	0.41
1:Q:117:SER:HA	1:Q:149:ILE:O	2.20	0.41
1:Q:165:PRO:HB3	1:Q:193:SER:HB2	2.03	0.41
1:S:243:HIS:ND1	1:S:244:ASP:N	2.68	0.41
1:T:155:ARG:HG2	1:T:162:GLU:CD	2.40	0.41
1:A:30:VAL:HG21	1:A:54:VAL:HG13	2.03	0.41
1:A:47:ILE:H	1:A:47:ILE:HG13	1.61	0.41
1:E:118:ILE:HG21	1:E:134:LEU:HD13	2.02	0.41
1:K:109:ILE:HD11	1:K:144:TRP:CB	2.49	0.41
1:K:155:ARG:HG2	1:K:162:GLU:CD	2.40	0.41
1:J:83:ILE:HD13	1:J:149:ILE:CD1	2.51	0.41
1:P:149:ILE:HG12	1:P:182:ILE:HB	2.02	0.41
1:P:251:ARG:HB2	1:P:269:GLU:HG2	2.02	0.41
1:R:109:ILE:HD11	1:R:144:TRP:CB	2.49	0.41
1:S:109:ILE:HD11	1:S:144:TRP:CB	2.48	0.41
1:B:30:VAL:HG21	1:B:54:VAL:HG13	2.01	0.41
1:B:55:ALA:CB	1:B:80:VAL:HG11	2.50	0.41
1:B:202:PRO:O	1:E:71:HIS:HD2	2.03	0.41
1:B:207:VAL:HG23	1:B:234:VAL:CG2	2.38	0.41
1:D:220:LEU:HD12	1:D:267:LEU:HD23	2.03	0.41
1:G:30:VAL:HG21	1:G:54:VAL:HG13	2.03	0.41
1:G:123:GLY:O	1:G:156:GLY:HA3	2.20	0.41
1:P:207:VAL:HG23	1:P:234:VAL:CG2	2.41	0.41
1:C:95:ASN:C	1:C:95:ASN:ND2	2.74	0.41
1:D:66:LYS:O	1:D:70:ARG:HG3	2.20	0.41
1:E:109:ILE:HD11	1:E:144:TRP:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ASN:C	1:E:163:ARG:N	2.73	0.41
1:L:92:ILE:O	1:L:92:ILE:CG1	2.68	0.41
1:I:92:ILE:O	1:I:92:ILE:CG1	2.68	0.41
1:P:139:GLU:HG3	1:S:66:LYS:HE3	2.02	0.41
1:B:83:ILE:HD13	1:B:149:ILE:HD12	2.03	0.41
1:C:117:SER:HA	1:C:149:ILE:O	2.21	0.41
1:N:36:VAL:HG21	1:N:65:HIS:CE1	2.55	0.41
1:N:161:ASN:ND2	1:N:163:ARG:H	2.19	0.41
1:F:14:VAL:CG1	1:F:18:ARG:HH22	2.33	0.41
1:R:19:ILE:O	1:R:60:ASN:HB3	2.21	0.41
1:S:117:SER:HA	1:S:149:ILE:O	2.20	0.41
1:D:207:VAL:HG23	1:D:234:VAL:CG2	2.41	0.41
1:E:34:HIS:CE1	2:E:501:F2P:O2	2.74	0.41
1:K:236:VAL:CG2	1:K:240:ILE:HG13	2.49	0.41
1:L:151:MET:CG	1:L:184:LYS:HD3	2.48	0.41
1:L:164:ASP:HA	1:L:165:PRO:HD2	1.88	0.41
1:L:173:ARG:HD3	1:L:200:GLY:O	2.21	0.41
1:M:29:ILE:O	1:M:235:ALA:HA	2.20	0.41
1:F:18:ARG:HG2	1:P:18:ARG:NH1	2.36	0.41
1:I:2:GLU:CG	1:I:3:LEU:N	2.76	0.41
1:I:236:VAL:CG2	1:I:240:ILE:HG13	2.51	0.41
1:P:182:ILE:HG22	1:P:183:VAL:N	2.36	0.41
1:Q:12:LYS:O	1:Q:16:LEU:HB2	2.21	0.41
1:R:29:ILE:O	1:R:235:ALA:HA	2.21	0.41
1:R:47:ILE:H	1:R:47:ILE:HG13	1.59	0.41
1:R:83:ILE:HD13	1:R:149:ILE:HD12	2.02	0.41
1:S:165:PRO:HB3	1:S:193:SER:HB2	2.02	0.41
1:T:117:SER:HA	1:T:149:ILE:O	2.20	0.41
1:B:109:ILE:HD11	1:B:144:TRP:CB	2.49	0.41
1:C:21:ASN:HB2	1:C:258:HIS:CE1	2.55	0.41
1:D:236:VAL:CG2	1:D:240:ILE:HG13	2.51	0.41
1:L:83:ILE:HD13	1:L:149:ILE:HD12	2.03	0.41
1:F:30:VAL:HG21	1:F:54:VAL:CG1	2.50	0.41
1:J:208:ALA:HB1	2:J:501:F2P:H6C2	2.03	0.41
1:J:243:HIS:ND1	1:J:244:ASP:N	2.69	0.41
1:P:139:GLU:OE2	1:S:103:THR:HA	2.21	0.41
1:R:83:ILE:HD13	1:R:149:ILE:CD1	2.51	0.41
1:F:151:MET:CG	1:F:184:LYS:HD3	2.51	0.40
1:F:173:ARG:NH2	1:I:47:ILE:HD11	2.37	0.40
1:G:2:GLU:HB2	1:G:25:GLU:CD	2.41	0.40
1:G:36:VAL:HG21	1:G:65:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:SER:O	1:H:26:LYS:HG2	2.21	0.40
1:I:109:ILE:HD11	1:I:144:TRP:CB	2.49	0.40
1:J:164:ASP:HA	1:J:165:PRO:HD3	1.94	0.40
2:J:501:F2P:P1	2:J:501:F2P:O2	2.79	0.40
1:P:21:ASN:HB3	1:P:24:SER:OG	2.21	0.40
1:Q:236:VAL:HA	2:Q:501:F2P:O63	2.21	0.40
1:B:83:ILE:HD13	1:B:149:ILE:CD1	2.51	0.40
1:C:7:ILE:HG23	1:C:13:LEU:HD21	2.00	0.40
1:D:95:ASN:C	1:D:95:ASN:HD22	2.23	0.40
1:L:4:PHE:HD2	1:L:7:ILE:HD13	1.86	0.40
1:L:95:ASN:C	1:L:95:ASN:ND2	2.74	0.40
1:N:29:ILE:O	1:N:235:ALA:HA	2.21	0.40
1:P:61:ALA:HA	1:P:80:VAL:HG22	2.02	0.40
1:S:151:MET:CG	1:S:184:LYS:HD3	2.50	0.40
1:S:157:LYS:HB2	1:S:157:LYS:HZ3	1.84	0.40
1:E:153:TYR:HA	1:E:154:PRO:HD3	1.87	0.40
1:F:23:GLU:HG3	1:F:24:SER:N	2.37	0.40
1:F:83:ILE:HD13	1:F:149:ILE:CD1	2.51	0.40
1:R:36:VAL:HG21	1:R:65:HIS:CE1	2.56	0.40
1:B:9:ASN:ND2	1:B:12:LYS:H	2.19	0.40
1:C:12:LYS:HZ3	1:C:181:ASP:CG	2.24	0.40
1:D:9:ASN:HD21	1:D:145:GLY:HA2	1.86	0.40
1:D:83:ILE:HD13	1:D:149:ILE:CD1	2.52	0.40
1:D:83:ILE:HD13	1:D:149:ILE:HD12	2.03	0.40
1:D:119:HIS:CD2	1:D:119:HIS:C	2.94	0.40
1:K:29:ILE:O	1:K:235:ALA:HA	2.21	0.40
1:G:111:MET:HG2	1:R:10:LEU:HD23	2.04	0.40
1:H:36:VAL:HG21	1:H:65:HIS:CE1	2.56	0.40
1:H:153:TYR:HA	1:H:154:PRO:HD3	1.92	0.40
1:T:163:ARG:HD2	1:T:187:TYR:O	2.22	0.40
1:A:83:ILE:HD13	1:A:149:ILE:HD12	2.02	0.40
1:C:207:VAL:HG23	1:C:234:VAL:CG2	2.41	0.40
1:M:30:VAL:HG21	1:M:54:VAL:HG13	2.03	0.40
1:M:36:VAL:HG21	1:M:65:HIS:CE1	2.57	0.40
1:O:150:ALA:O	1:O:183:VAL:HA	2.22	0.40
1:H:92:ILE:O	1:H:92:ILE:CG1	2.70	0.40
1:I:19:ILE:CG2	1:I:61:ALA:HB2	2.46	0.40
1:P:29:ILE:O	1:P:235:ALA:HA	2.21	0.40
1:P:66:LYS:HE3	1:T:139:GLU:HG3	2.04	0.40
1:Q:36:VAL:O	1:R:170:HIS:HE1	2.04	0.40
1:Q:191:ILE:HG12	1:Q:225:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:243:HIS:ND1	1:R:244:ASP:N	2.70	0.40
1:T:47:ILE:H	1:T:47:ILE:HG13	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/273 (99%)	256 (95%)	12 (4%)	2 (1%)	22	43
1	B	264/273 (97%)	249 (94%)	15 (6%)	0	100	100
1	C	258/273 (94%)	246 (95%)	11 (4%)	1 (0%)	34	57
1	D	263/273 (96%)	250 (95%)	11 (4%)	2 (1%)	19	39
1	E	264/273 (97%)	249 (94%)	14 (5%)	1 (0%)	34	57
1	F	259/273 (95%)	247 (95%)	11 (4%)	1 (0%)	34	57
1	G	264/273 (97%)	253 (96%)	11 (4%)	0	100	100
1	H	263/273 (96%)	252 (96%)	11 (4%)	0	100	100
1	I	261/273 (96%)	250 (96%)	11 (4%)	0	100	100
1	J	265/273 (97%)	249 (94%)	15 (6%)	1 (0%)	34	57
1	K	262/273 (96%)	246 (94%)	16 (6%)	0	100	100
1	L	265/273 (97%)	249 (94%)	14 (5%)	2 (1%)	19	39
1	M	261/273 (96%)	247 (95%)	14 (5%)	0	100	100
1	N	261/273 (96%)	247 (95%)	11 (4%)	3 (1%)	14	30
1	O	262/273 (96%)	248 (95%)	13 (5%)	1 (0%)	34	57
1	P	264/273 (97%)	251 (95%)	11 (4%)	2 (1%)	19	39
1	Q	270/273 (99%)	256 (95%)	12 (4%)	2 (1%)	22	43
1	R	265/273 (97%)	256 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	S	260/273 (95%)	245 (94%)	14 (5%)	1 (0%)	34 57
1	T	263/273 (96%)	247 (94%)	16 (6%)	0	100 100
All	All	5264/5460 (96%)	4993 (95%)	252 (5%)	19 (0%)	34 57

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	78	LYS
1	C	70	ARG
1	Q	74	ARG
1	L	72	GLY
1	N	2	GLU
1	F	7	ILE
1	P	73	HIS
1	Q	7	ILE
1	D	70	ARG
1	E	162	GLU
1	N	269	GLU
1	D	2	GLU
1	N	70	ARG
1	O	7	ILE
1	J	70	ARG
1	S	162	GLU
1	L	2	GLU
1	P	72	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	208/220 (94%)	192 (92%)	16 (8%)	13 25
1	B	208/220 (94%)	190 (91%)	18 (9%)	10 20
1	C	207/220 (94%)	193 (93%)	14 (7%)	16 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	210/220 (96%)	198 (94%)	12 (6%)	20	41
1	E	209/220 (95%)	194 (93%)	15 (7%)	14	29
1	F	209/220 (95%)	194 (93%)	15 (7%)	14	29
1	G	212/220 (96%)	197 (93%)	15 (7%)	14	29
1	H	209/220 (95%)	193 (92%)	16 (8%)	13	25
1	I	210/220 (96%)	197 (94%)	13 (6%)	18	37
1	J	212/220 (96%)	196 (92%)	16 (8%)	13	27
1	K	209/220 (95%)	196 (94%)	13 (6%)	18	37
1	L	209/220 (95%)	193 (92%)	16 (8%)	13	25
1	M	208/220 (94%)	193 (93%)	15 (7%)	14	29
1	N	208/220 (94%)	192 (92%)	16 (8%)	13	25
1	O	210/220 (96%)	196 (93%)	14 (7%)	16	33
1	P	209/220 (95%)	194 (93%)	15 (7%)	14	29
1	Q	212/220 (96%)	198 (93%)	14 (7%)	16	33
1	R	211/220 (96%)	197 (93%)	14 (7%)	16	33
1	S	209/220 (95%)	195 (93%)	14 (7%)	16	33
1	T	210/220 (96%)	195 (93%)	15 (7%)	14	29
All	All	4189/4400 (95%)	3893 (93%)	296 (7%)	14	29

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	6	ASP
1	A	52	ASN
1	A	70	ARG
1	A	92	ILE
1	A	95	ASN
1	A	140	THR
1	A	160	GLN
1	A	161	ASN
1	A	166	GLU
1	A	174	LEU
1	A	206	VAL
1	A	222	MET
1	A	234	VAL

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Mol	Chain	Res	Type
1	A	236	VAL
1	A	264	GLU
1	B	3	LEU
1	B	9	ASN
1	B	13	LEU
1	B	23	GLU
1	B	52	ASN
1	B	70	ARG
1	B	92	ILE
1	B	95	ASN
1	B	140	THR
1	B	161	ASN
1	B	166	GLU
1	B	170	HIS
1	B	174	LEU
1	B	184	LYS
1	B	206	VAL
1	B	222	MET
1	B	234	VAL
1	B	236	VAL
1	C	3	LEU
1	C	9	ASN
1	C	52	ASN
1	C	70	ARG
1	C	92	ILE
1	C	95	ASN
1	C	140	THR
1	C	166	GLU
1	C	174	LEU
1	C	206	VAL
1	C	222	MET
1	C	234	VAL
1	C	236	VAL
1	C	265	GLU
1	D	3	LEU
1	D	9	ASN
1	D	52	ASN
1	D	92	ILE
1	D	95	ASN
1	D	140	THR
1	D	184	LYS
1	D	206	VAL

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Mol	Chain	Res	Type
1	D	222	MET
1	D	234	VAL
1	D	236	VAL
1	D	271	ARG
1	E	3	LEU
1	E	9	ASN
1	E	19	ILE
1	E	52	ASN
1	E	70	ARG
1	E	92	ILE
1	E	95	ASN
1	E	140	THR
1	E	166	GLU
1	E	170	HIS
1	E	174	LEU
1	E	206	VAL
1	E	222	MET
1	E	234	VAL
1	E	236	VAL
1	K	3	LEU
1	K	9	ASN
1	K	52	ASN
1	K	70	ARG
1	K	92	ILE
1	K	95	ASN
1	K	140	THR
1	K	160	GLN
1	K	174	LEU
1	K	206	VAL
1	K	222	MET
1	K	234	VAL
1	K	236	VAL
1	L	8	LYS
1	L	9	ASN
1	L	52	ASN
1	L	70	ARG
1	L	92	ILE
1	L	95	ASN
1	L	140	THR
1	L	161	ASN
1	L	164	ASP
1	L	170	HIS

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Mol	Chain	Res	Type
1	L	174	LEU
1	L	206	VAL
1	L	222	MET
1	L	234	VAL
1	L	236	VAL
1	L	244	ASP
1	M	3	LEU
1	M	9	ASN
1	M	13	LEU
1	M	22	ARG
1	M	52	ASN
1	M	70	ARG
1	M	92	ILE
1	M	95	ASN
1	M	140	THR
1	M	160	GLN
1	M	174	LEU
1	M	206	VAL
1	M	222	MET
1	M	234	VAL
1	M	236	VAL
1	N	3	LEU
1	N	9	ASN
1	N	10	LEU
1	N	13	LEU
1	N	52	ASN
1	N	80	VAL
1	N	92	ILE
1	N	95	ASN
1	N	140	THR
1	N	174	LEU
1	N	206	VAL
1	N	222	MET
1	N	234	VAL
1	N	236	VAL
1	N	264	GLU
1	N	271	ARG
1	O	3	LEU
1	O	9	ASN
1	O	52	ASN
1	O	92	ILE
1	O	95	ASN

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Mol	Chain	Res	Type
1	O	140	THR
1	O	157	LYS
1	O	163	ARG
1	O	170	HIS
1	O	174	LEU
1	O	206	VAL
1	O	222	MET
1	O	234	VAL
1	O	236	VAL
1	F	3	LEU
1	F	9	ASN
1	F	13	LEU
1	F	18	ARG
1	F	52	ASN
1	F	92	ILE
1	F	95	ASN
1	F	140	THR
1	F	157	LYS
1	F	161	ASN
1	F	163	ARG
1	F	206	VAL
1	F	222	MET
1	F	234	VAL
1	F	236	VAL
1	G	3	LEU
1	G	9	ASN
1	G	22	ARG
1	G	52	ASN
1	G	92	ILE
1	G	95	ASN
1	G	140	THR
1	G	163	ARG
1	G	166	GLU
1	G	174	LEU
1	G	206	VAL
1	G	222	MET
1	G	234	VAL
1	G	236	VAL
1	G	268	LYS
1	H	3	LEU
1	H	7	ILE
1	H	9	ASN

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Mol	Chain	Res	Type
1	H	52	ASN
1	H	70	ARG
1	H	92	ILE
1	H	95	ASN
1	H	140	THR
1	H	157	LYS
1	H	166	GLU
1	H	170	HIS
1	H	174	LEU
1	H	206	VAL
1	H	222	MET
1	H	234	VAL
1	H	236	VAL
1	I	3	LEU
1	I	19	ILE
1	I	52	ASN
1	I	70	ARG
1	I	92	ILE
1	I	95	ASN
1	I	140	THR
1	I	166	GLU
1	I	174	LEU
1	I	206	VAL
1	I	222	MET
1	I	234	VAL
1	I	236	VAL
1	J	3	LEU
1	J	9	ASN
1	J	52	ASN
1	J	80	VAL
1	J	92	ILE
1	J	95	ASN
1	J	140	THR
1	J	160	GLN
1	J	161	ASN
1	J	166	GLU
1	J	174	LEU
1	J	206	VAL
1	J	222	MET
1	J	234	VAL
1	J	236	VAL
1	J	271	ARG

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Mol	Chain	Res	Type
1	P	3	LEU
1	P	9	ASN
1	P	19	ILE
1	P	52	ASN
1	P	70	ARG
1	P	78	LYS
1	P	92	ILE
1	P	95	ASN
1	P	140	THR
1	P	161	ASN
1	P	170	HIS
1	P	174	LEU
1	P	206	VAL
1	P	234	VAL
1	P	236	VAL
1	Q	3	LEU
1	Q	9	ASN
1	Q	16	LEU
1	Q	52	ASN
1	Q	70	ARG
1	Q	92	ILE
1	Q	95	ASN
1	Q	140	THR
1	Q	166	GLU
1	Q	206	VAL
1	Q	222	MET
1	Q	234	VAL
1	Q	236	VAL
1	Q	271	ARG
1	R	3	LEU
1	R	9	ASN
1	R	22	ARG
1	R	52	ASN
1	R	71	HIS
1	R	92	ILE
1	R	95	ASN
1	R	140	THR
1	R	160	GLN
1	R	166	GLU
1	R	185	THR
1	R	206	VAL
1	R	234	VAL

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Mol	Chain	Res	Type
1	R	236	VAL
1	S	3	LEU
1	S	9	ASN
1	S	52	ASN
1	S	70	ARG
1	S	92	ILE
1	S	95	ASN
1	S	140	THR
1	S	161	ASN
1	S	166	GLU
1	S	206	VAL
1	S	222	MET
1	S	234	VAL
1	S	236	VAL
1	S	271	ARG
1	T	9	ASN
1	T	52	ASN
1	T	70	ARG
1	T	78	LYS
1	T	79	ASP
1	T	80	VAL
1	T	92	ILE
1	T	95	ASN
1	T	140	THR
1	T	157	LYS
1	T	161	ASN
1	T	174	LEU
1	T	206	VAL
1	T	234	VAL
1	T	236	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	95	ASN
1	A	160	GLN
1	A	161	ASN
1	B	9	ASN
1	B	95	ASN
1	B	161	ASN
1	C	9	ASN

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Mol	Chain	Res	Type
1	C	95	ASN
1	C	161	ASN
1	D	9	ASN
1	D	65	HIS
1	D	71	HIS
1	D	95	ASN
1	D	160	GLN
1	D	161	ASN
1	D	214	ASN
1	E	9	ASN
1	E	71	HIS
1	E	95	ASN
1	E	161	ASN
1	K	9	ASN
1	K	71	HIS
1	K	95	ASN
1	K	161	ASN
1	L	9	ASN
1	L	95	ASN
1	L	160	GLN
1	L	161	ASN
1	M	9	ASN
1	M	71	HIS
1	M	95	ASN
1	M	160	GLN
1	M	161	ASN
1	N	9	ASN
1	N	95	ASN
1	N	160	GLN
1	N	161	ASN
1	N	260	ASN
1	O	9	ASN
1	O	95	ASN
1	O	161	ASN
1	O	170	HIS
1	F	9	ASN
1	F	95	ASN
1	F	161	ASN
1	G	9	ASN
1	G	65	HIS
1	G	95	ASN
1	G	160	GLN

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Mol	Chain	Res	Type
1	G	161	ASN
1	H	9	ASN
1	H	38	ASN
1	H	95	ASN
1	H	160	GLN
1	I	95	ASN
1	I	158	HIS
1	J	9	ASN
1	J	21	ASN
1	J	65	HIS
1	J	95	ASN
1	J	160	GLN
1	J	161	ASN
1	P	9	ASN
1	P	95	ASN
1	P	160	GLN
1	P	161	ASN
1	P	170	HIS
1	Q	9	ASN
1	Q	95	ASN
1	Q	161	ASN
1	R	9	ASN
1	R	71	HIS
1	R	95	ASN
1	R	160	GLN
1	R	161	ASN
1	S	9	ASN
1	S	21	ASN
1	S	95	ASN
1	S	161	ASN
1	T	9	ASN
1	T	95	ASN
1	T	161	ASN
1	T	170	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	F2P	Q	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	O	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	C	501	1	18,18,19	1.22	1 (5%)	23,26,28	1.16	3 (13%)
2	F2P	F	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	L	501	1	18,18,19	1.26	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	J	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	R	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	D	501	1	18,18,19	1.07	2 (11%)	23,26,28	1.49	5 (21%)
2	F2P	A	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	K	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	M	501	1	18,18,19	1.26	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	H	501	1	18,18,19	1.26	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	P	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	N	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	T	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	E	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.09	3 (13%)
2	F2P	I	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	B	501	1	18,18,19	1.26	1 (5%)	23,26,28	1.10	3 (13%)
2	F2P	G	501	1	18,18,19	1.22	1 (5%)	23,26,28	1.16	3 (13%)
2	F2P	S	501	1	18,18,19	1.25	1 (5%)	23,26,28	1.10	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F2P	Q	501	1	2/2/5/6	1/21/21/24	-
2	F2P	O	501	1	2/2/5/6	5/21/21/24	-
2	F2P	C	501	1	2/2/5/6	2/21/21/24	-
2	F2P	F	501	1	2/2/5/6	5/21/21/24	-
2	F2P	L	501	1	2/2/5/6	5/21/21/24	-
2	F2P	J	501	1	2/2/5/6	9/21/21/24	-
2	F2P	R	501	1	2/2/5/6	6/21/21/24	-
2	F2P	D	501	1	2/2/5/6	10/21/21/24	-
2	F2P	A	501	1	2/2/5/6	4/21/21/24	-
2	F2P	K	501	1	2/2/5/6	5/21/21/24	-
2	F2P	M	501	1	2/2/5/6	3/21/21/24	-
2	F2P	H	501	1	2/2/5/6	2/21/21/24	-
2	F2P	P	501	1	2/2/5/6	7/21/21/24	-
2	F2P	N	501	1	2/2/5/6	2/21/21/24	-
2	F2P	T	501	1	2/2/5/6	5/21/21/24	-
2	F2P	E	501	1	2/2/5/6	6/21/21/24	-
2	F2P	I	501	1	2/2/5/6	4/21/21/24	-
2	F2P	B	501	1	2/2/5/6	3/21/21/24	-
2	F2P	G	501	1	2/2/5/6	5/21/21/24	-
2	F2P	S	501	1	2/2/5/6	4/21/21/24	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	F2P	P6-O61	3.54	1.61	1.50
2	B	501	F2P	P6-O61	3.54	1.61	1.50
2	L	501	F2P	P6-O61	3.54	1.61	1.50
2	P	501	F2P	P6-O61	3.54	1.61	1.50
2	H	501	F2P	P6-O61	3.53	1.61	1.50
2	T	501	F2P	P6-O61	3.53	1.61	1.50
2	E	501	F2P	P6-O61	3.53	1.61	1.50
2	O	501	F2P	P6-O61	3.53	1.61	1.50
2	R	501	F2P	P6-O61	3.53	1.61	1.50
2	F	501	F2P	P6-O61	3.53	1.61	1.50
2	I	501	F2P	P6-O61	3.52	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	501	F2P	P6-O61	3.52	1.61	1.50
2	A	501	F2P	P6-O61	3.52	1.61	1.50
2	S	501	F2P	P6-O61	3.52	1.61	1.50
2	K	501	F2P	P6-O61	3.52	1.61	1.50
2	M	501	F2P	P6-O61	3.51	1.61	1.50
2	Q	501	F2P	P6-O61	3.51	1.61	1.50
2	C	501	F2P	P6-O61	3.41	1.61	1.50
2	G	501	F2P	P6-O61	3.41	1.61	1.50
2	D	501	F2P	P6-O61	2.24	1.57	1.50
2	D	501	F2P	P6-O62	2.14	1.62	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	F2P	O6-P6-O61	4.08	117.46	106.44
2	C	501	F2P	C5-C4-C3	-3.59	108.28	113.97
2	G	501	F2P	C5-C4-C3	-3.54	108.36	113.97
2	D	501	F2P	C5-C4-C3	-2.99	109.22	113.97
2	O	501	F2P	C5-C4-C3	-2.84	109.47	113.97
2	S	501	F2P	C5-C4-C3	-2.84	109.47	113.97
2	J	501	F2P	C5-C4-C3	-2.84	109.47	113.97
2	R	501	F2P	C5-C4-C3	-2.83	109.48	113.97
2	L	501	F2P	C5-C4-C3	-2.83	109.48	113.97
2	B	501	F2P	C5-C4-C3	-2.82	109.49	113.97
2	P	501	F2P	C5-C4-C3	-2.82	109.49	113.97
2	I	501	F2P	C5-C4-C3	-2.82	109.50	113.97
2	H	501	F2P	C5-C4-C3	-2.82	109.50	113.97
2	M	501	F2P	C5-C4-C3	-2.81	109.51	113.97
2	E	501	F2P	C5-C4-C3	-2.81	109.52	113.97
2	F	501	F2P	C5-C4-C3	-2.81	109.52	113.97
2	T	501	F2P	C5-C4-C3	-2.80	109.53	113.97
2	A	501	F2P	C5-C4-C3	-2.80	109.53	113.97
2	N	501	F2P	C5-C4-C3	-2.80	109.54	113.97
2	K	501	F2P	C5-C4-C3	-2.79	109.55	113.97
2	Q	501	F2P	C5-C4-C3	-2.78	109.56	113.97
2	G	501	F2P	O1-P1-O13	2.62	113.52	106.44
2	C	501	F2P	O1-P1-O13	2.52	113.24	106.44
2	M	501	F2P	O63-P6-O6	2.38	112.87	106.67
2	J	501	F2P	O63-P6-O6	2.38	112.87	106.67
2	H	501	F2P	O1-P1-O13	2.38	112.87	106.44
2	L	501	F2P	O1-P1-O13	2.38	112.86	106.44
2	R	501	F2P	O1-P1-O13	2.37	112.85	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	501	F2P	O1-P1-O13	2.37	112.85	106.44
2	O	501	F2P	O1-P1-O13	2.37	112.85	106.44
2	S	501	F2P	O63-P6-O6	2.37	112.85	106.67
2	B	501	F2P	O1-P1-O13	2.37	112.84	106.44
2	F	501	F2P	O63-P6-O6	2.37	112.85	106.67
2	B	501	F2P	O63-P6-O6	2.37	112.84	106.67
2	E	501	F2P	O1-P1-O13	2.37	112.84	106.44
2	O	501	F2P	O63-P6-O6	2.37	112.84	106.67
2	S	501	F2P	O1-P1-O13	2.37	112.84	106.44
2	N	501	F2P	O1-P1-O13	2.37	112.84	106.44
2	Q	501	F2P	O1-P1-O13	2.37	112.84	106.44
2	R	501	F2P	O63-P6-O6	2.37	112.84	106.67
2	A	501	F2P	O1-P1-O13	2.37	112.83	106.44
2	M	501	F2P	O1-P1-O13	2.37	112.83	106.44
2	F	501	F2P	O1-P1-O13	2.37	112.83	106.44
2	P	501	F2P	O1-P1-O13	2.36	112.83	106.44
2	I	501	F2P	O1-P1-O13	2.36	112.83	106.44
2	P	501	F2P	O63-P6-O6	2.36	112.83	106.67
2	H	501	F2P	O63-P6-O6	2.36	112.83	106.67
2	N	501	F2P	O63-P6-O6	2.36	112.83	106.67
2	K	501	F2P	O1-P1-O13	2.36	112.82	106.44
2	J	501	F2P	O1-P1-O13	2.36	112.82	106.44
2	L	501	F2P	O63-P6-O6	2.36	112.82	106.67
2	Q	501	F2P	O63-P6-O6	2.36	112.82	106.67
2	A	501	F2P	O63-P6-O6	2.36	112.82	106.67
2	I	501	F2P	O63-P6-O6	2.36	112.82	106.67
2	T	501	F2P	O63-P6-O6	2.36	112.82	106.67
2	E	501	F2P	O63-P6-O6	2.35	112.80	106.67
2	K	501	F2P	O63-P6-O6	2.35	112.80	106.67
2	D	501	F2P	O1-P1-O13	2.21	112.41	106.44
2	D	501	F2P	O63-P6-O6	-2.17	101.02	106.67
2	G	501	F2P	O63-P6-O6	2.16	112.31	106.67
2	C	501	F2P	O63-P6-O6	2.13	112.22	106.67
2	D	501	F2P	O62-P6-O6	2.00	111.90	106.67

All (40) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	F2P	C5
2	A	501	F2P	C4
2	B	501	F2P	C5
2	B	501	F2P	C4

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Mol	Chain	Res	Type	Atom
2	C	501	F2P	C5
2	C	501	F2P	C4
2	D	501	F2P	C5
2	D	501	F2P	C4
2	E	501	F2P	C5
2	E	501	F2P	C4
2	K	501	F2P	C5
2	K	501	F2P	C4
2	L	501	F2P	C5
2	L	501	F2P	C4
2	M	501	F2P	C5
2	M	501	F2P	C4
2	N	501	F2P	C5
2	N	501	F2P	C4
2	O	501	F2P	C5
2	O	501	F2P	C4
2	F	501	F2P	C5
2	F	501	F2P	C4
2	G	501	F2P	C5
2	G	501	F2P	C4
2	H	501	F2P	C5
2	H	501	F2P	C4
2	I	501	F2P	C5
2	I	501	F2P	C4
2	J	501	F2P	C5
2	J	501	F2P	C4
2	P	501	F2P	C5
2	P	501	F2P	C4
2	Q	501	F2P	C5
2	Q	501	F2P	C4
2	R	501	F2P	C5
2	R	501	F2P	C4
2	S	501	F2P	C5
2	S	501	F2P	C4
2	T	501	F2P	C5
2	T	501	F2P	C4

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	F2P	C2-C1-O1-P1
2	C	501	F2P	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	501	F2P	C6-O6-P6-O62
2	D	501	F2P	C1-O1-P1-O11
2	D	501	F2P	C1-O1-P1-O12
2	D	501	F2P	C2-C1-O1-P1
2	D	501	F2P	C4-C5-C6-O6
2	D	501	F2P	C6-O6-P6-O61
2	D	501	F2P	C6-O6-P6-O62
2	D	501	F2P	C6-O6-P6-O63
2	E	501	F2P	C1-O1-P1-O11
2	E	501	F2P	C1-O1-P1-O12
2	E	501	F2P	C6-O6-P6-O61
2	E	501	F2P	C6-O6-P6-O62
2	E	501	F2P	C6-O6-P6-O63
2	K	501	F2P	C2-C1-O1-P1
2	K	501	F2P	C4-C5-C6-O6
2	K	501	F2P	C6-O6-P6-O62
2	L	501	F2P	C1-O1-P1-O12
2	L	501	F2P	C4-C5-C6-O6
2	L	501	F2P	C6-O6-P6-O62
2	O	501	F2P	C2-C1-O1-P1
2	F	501	F2P	C2-C1-O1-P1
2	F	501	F2P	C4-C5-C6-O6
2	F	501	F2P	C6-O6-P6-O62
2	G	501	F2P	C2-C1-O1-P1
2	G	501	F2P	C4-C5-C6-O6
2	G	501	F2P	C6-O6-P6-O62
2	I	501	F2P	C1-O1-P1-O11
2	I	501	F2P	C1-O1-P1-O12
2	J	501	F2P	C1-O1-P1-O11
2	J	501	F2P	C2-C1-O1-P1
2	J	501	F2P	C4-C5-C6-O6
2	J	501	F2P	C6-O6-P6-O62
2	P	501	F2P	C1-O1-P1-O11
2	P	501	F2P	C1-O1-P1-O12
2	P	501	F2P	C1-O1-P1-O13
2	P	501	F2P	C4-C5-C6-O6
2	Q	501	F2P	C4-C5-C6-O6
2	R	501	F2P	C1-O1-P1-O11
2	R	501	F2P	C1-O1-P1-O12
2	R	501	F2P	C4-C5-C6-O6
2	S	501	F2P	C1-O1-P1-O11
2	S	501	F2P	C1-O1-P1-O12

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Mol	Chain	Res	Type	Atoms
2	S	501	F2P	C4-C5-C6-O6
2	S	501	F2P	C6-O6-P6-O62
2	T	501	F2P	C1-O1-P1-O11
2	T	501	F2P	C1-O1-P1-O12
2	F	501	F2P	O4-C4-C5-C6
2	P	501	F2P	C2-C1-O1-P1
2	A	501	F2P	C4-C5-C6-O6
2	B	501	F2P	C4-C5-C6-O6
2	M	501	F2P	C4-C5-C6-O6
2	N	501	F2P	C4-C5-C6-O6
2	H	501	F2P	C4-C5-C6-O6
2	I	501	F2P	C4-C5-C6-O6
2	T	501	F2P	C4-C5-C6-O6
2	D	501	F2P	O3-C3-C4-O4
2	D	501	F2P	C2-C3-C4-O4
2	K	501	F2P	O4-C4-C5-C6
2	G	501	F2P	O4-C4-C5-C6
2	P	501	F2P	O4-C4-C5-C6
2	K	501	F2P	C3-C4-C5-C6
2	F	501	F2P	C3-C4-C5-C6
2	G	501	F2P	C3-C4-C5-C6
2	P	501	F2P	C3-C4-C5-C6
2	I	501	F2P	C1-O1-P1-O13
2	R	501	F2P	C1-O1-P1-O13
2	T	501	F2P	C1-O1-P1-O13
2	O	501	F2P	C3-C4-C5-C6
2	A	501	F2P	C1-O1-P1-O12
2	B	501	F2P	C1-O1-P1-O12
2	L	501	F2P	C1-O1-P1-O11
2	M	501	F2P	C1-O1-P1-O12
2	O	501	F2P	C6-O6-P6-O63
2	O	501	F2P	O4-C4-C5-C6
2	J	501	F2P	O4-C4-C5-C6
2	A	501	F2P	C1-O1-P1-O13
2	B	501	F2P	C1-O1-P1-O13
2	L	501	F2P	C1-O1-P1-O13
2	M	501	F2P	C1-O1-P1-O13
2	O	501	F2P	C6-O6-P6-O61
2	R	501	F2P	O4-C4-C5-C6
2	T	501	F2P	O4-C4-C5-C6
2	J	501	F2P	C3-C4-C5-C6
2	R	501	F2P	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	E	501	F2P	C1-O1-P1-O13
2	N	501	F2P	C1-O1-P1-O12
2	J	501	F2P	C1-O1-P1-O12
2	H	501	F2P	O4-C4-C5-C6
2	J	501	F2P	C2-C3-C4-O4
2	J	501	F2P	O3-C3-C4-O4
2	D	501	F2P	C3-C4-C5-C6

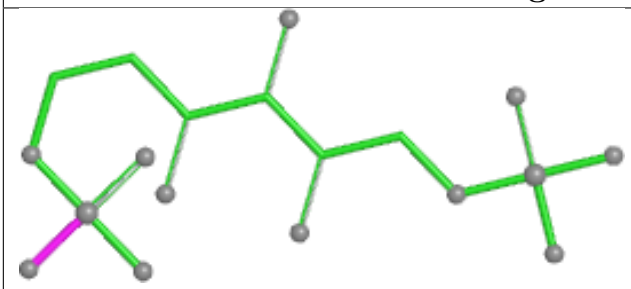
There are no ring outliers.

17 monomers are involved in 65 short contacts:

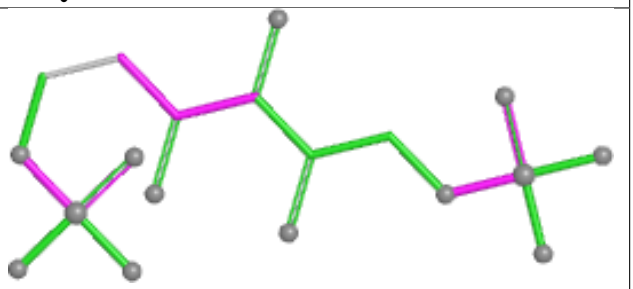
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	501	F2P	3	0
2	O	501	F2P	13	0
2	C	501	F2P	2	0
2	F	501	F2P	4	0
2	L	501	F2P	1	0
2	J	501	F2P	5	0
2	D	501	F2P	5	0
2	K	501	F2P	4	0
2	M	501	F2P	2	0
2	H	501	F2P	5	0
2	P	501	F2P	8	0
2	N	501	F2P	2	0
2	T	501	F2P	3	0
2	E	501	F2P	1	0
2	B	501	F2P	2	0
2	G	501	F2P	2	0
2	S	501	F2P	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

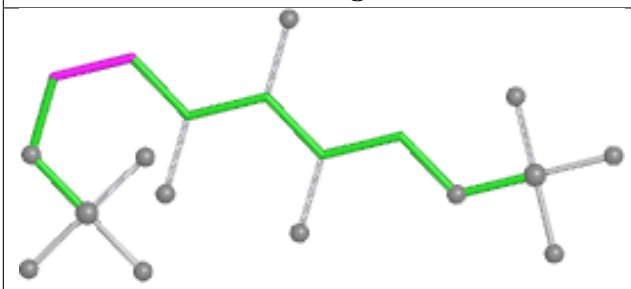
Ligand F2P Q 501



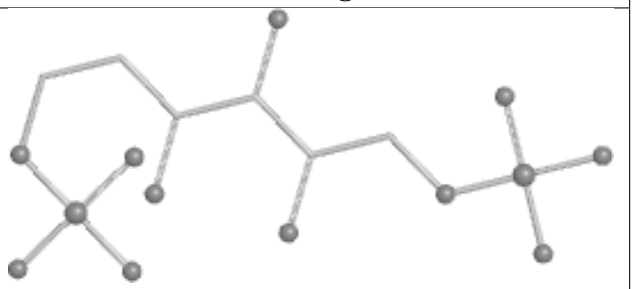
Bond lengths



Bond angles

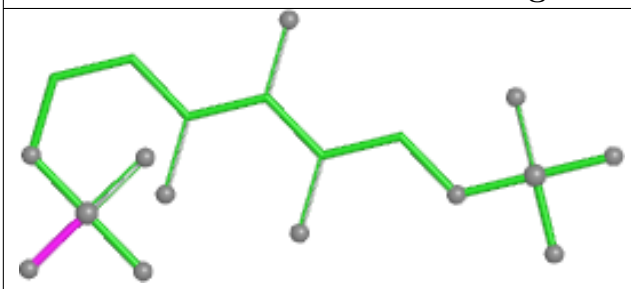


Torsions

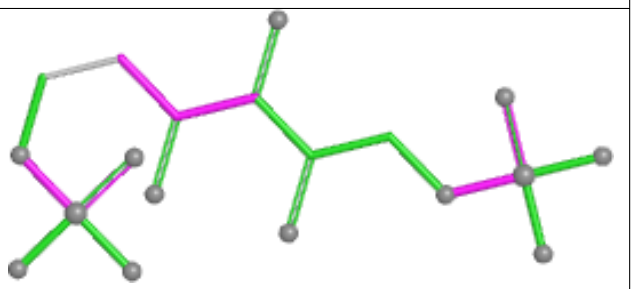


Rings

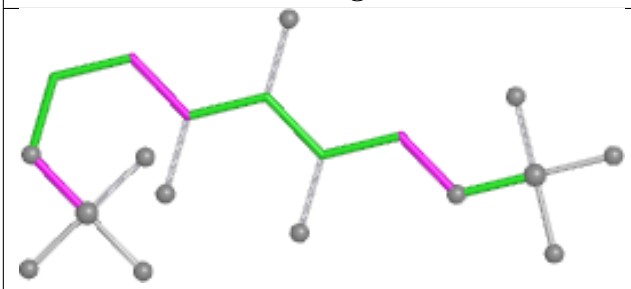
Ligand F2P O 501



Bond lengths



Bond angles



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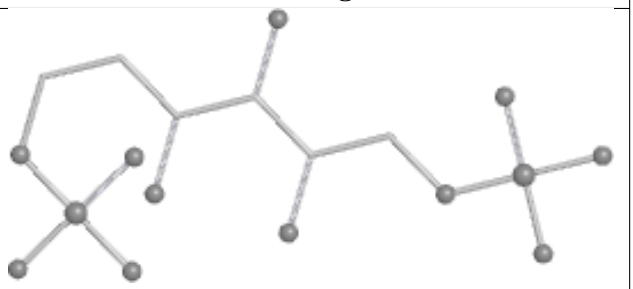
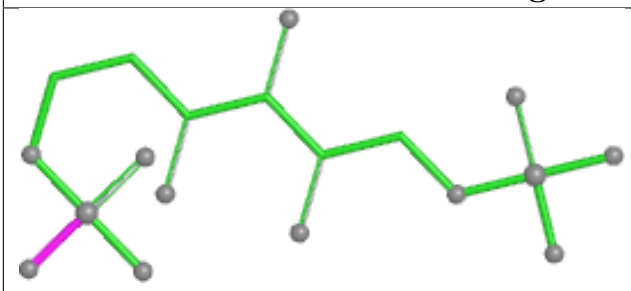
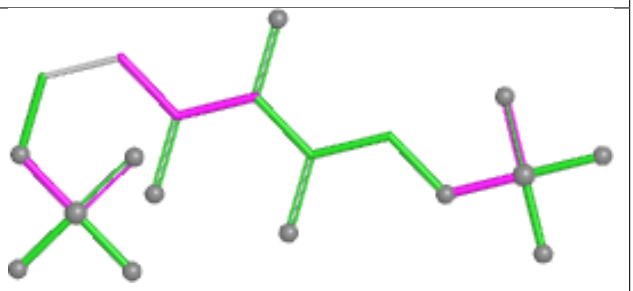


Rings

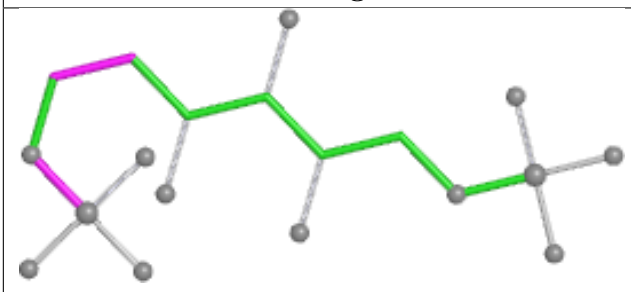
Ligand F2P C 501



Bond lengths



Bond angles



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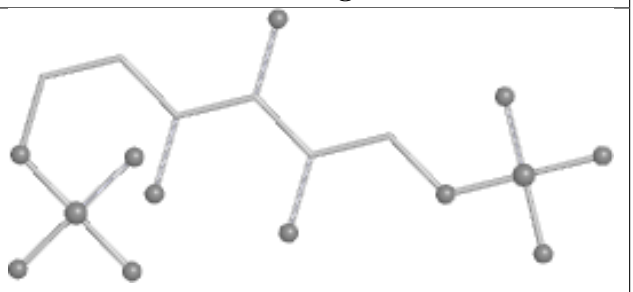
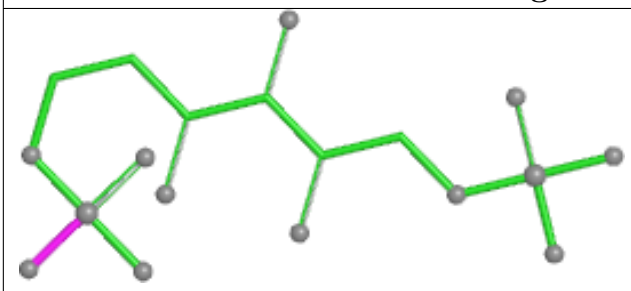
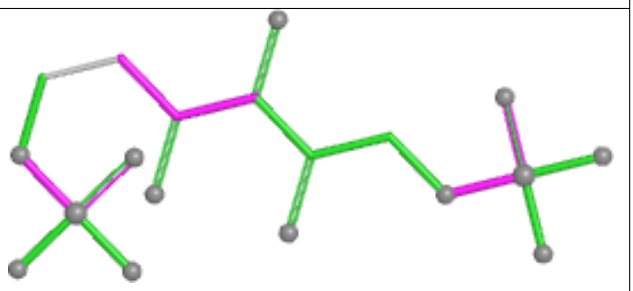


Rings

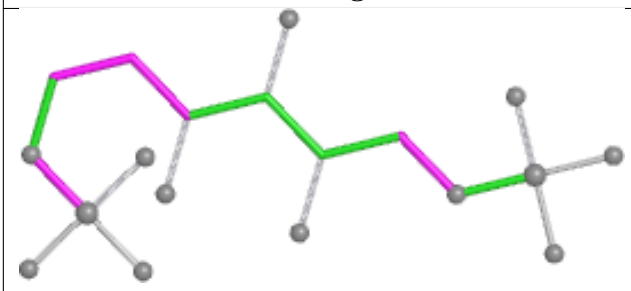
Ligand F2P F 501



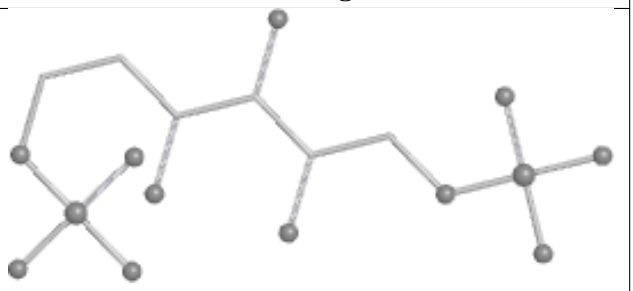
Bond lengths



Bond angles

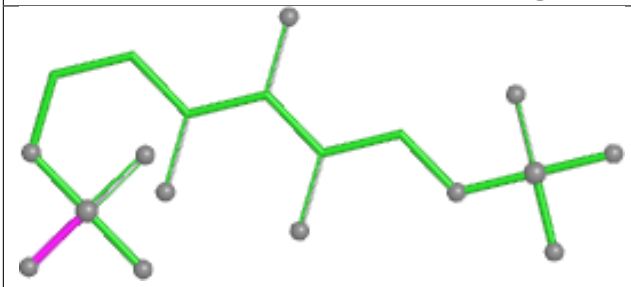


Torsions

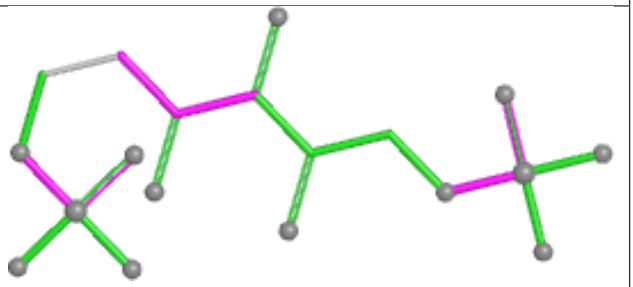


Rings

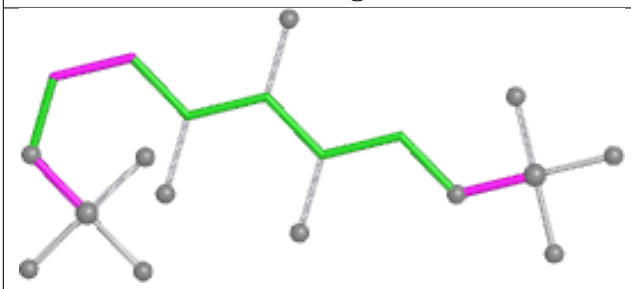
Ligand F2P L 501



Bond lengths



Bond angles



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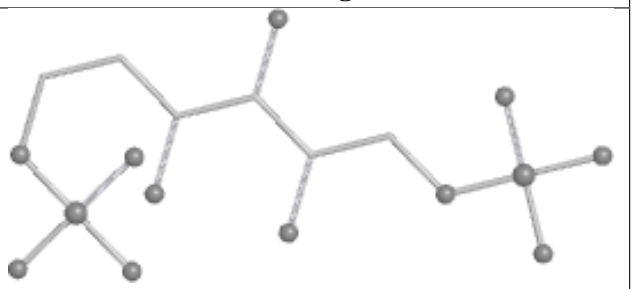
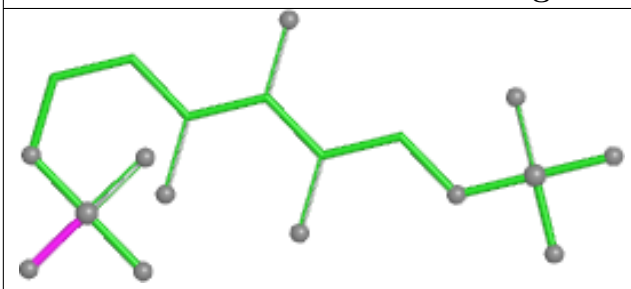


Rings

Ligand F2P J 501



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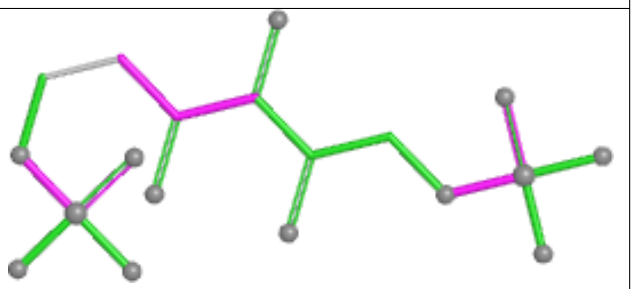
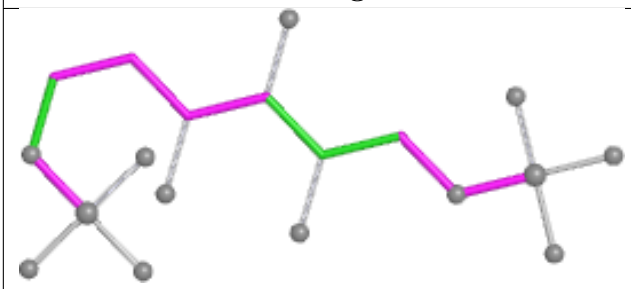


Bond angles



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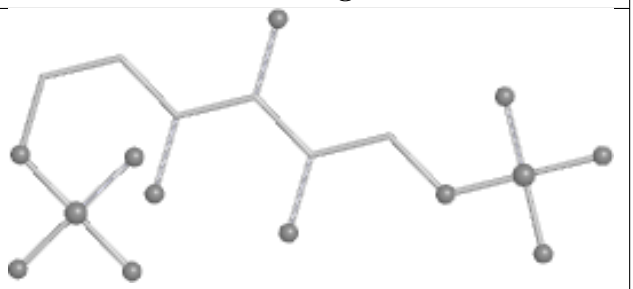
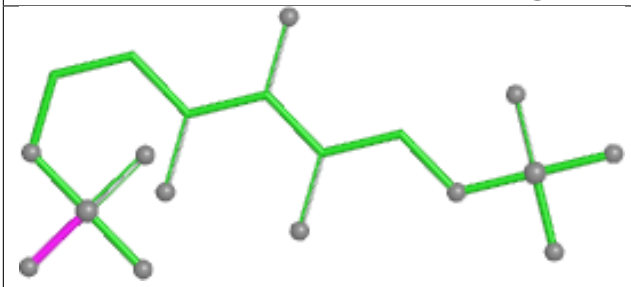
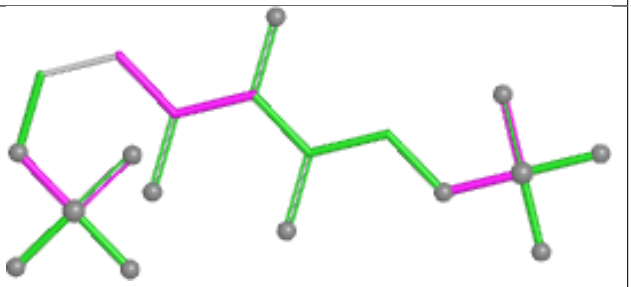


Rings

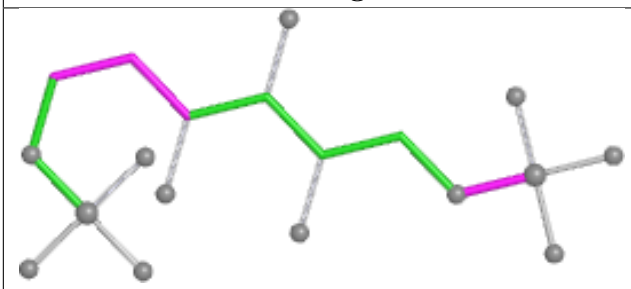
Ligand F2P R 501



Bond lengths



Bond angles



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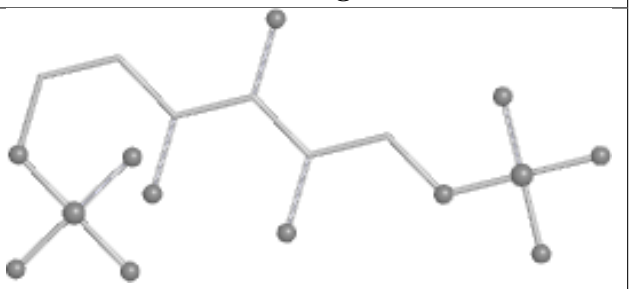
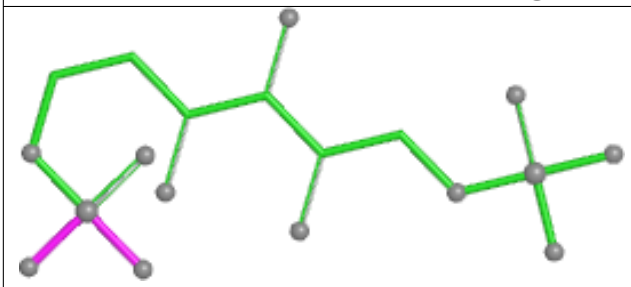
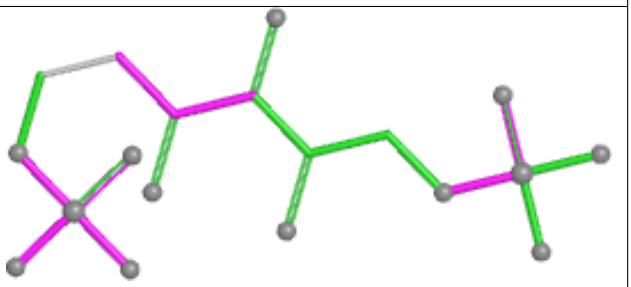


Rings

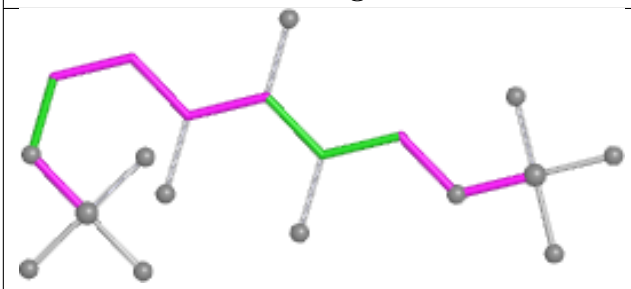
Ligand F2P D 501



Bond lengths



Bond angles



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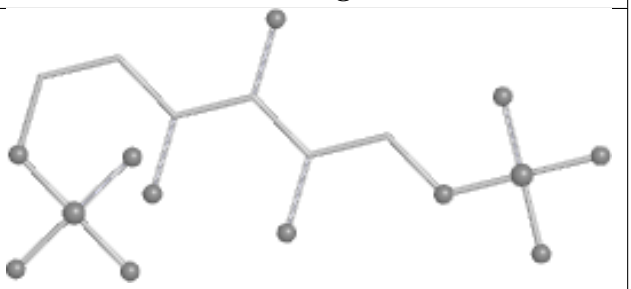
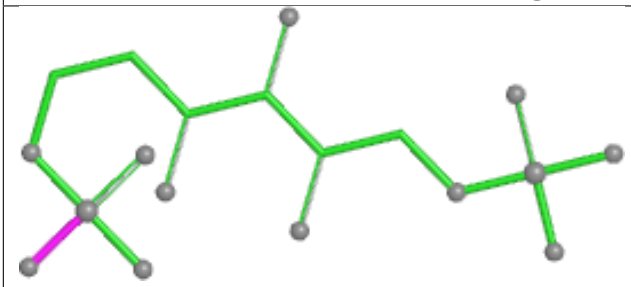
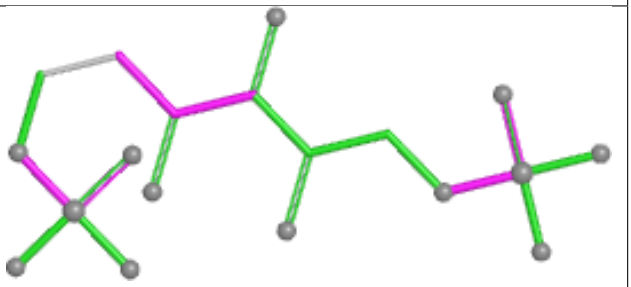


Rings

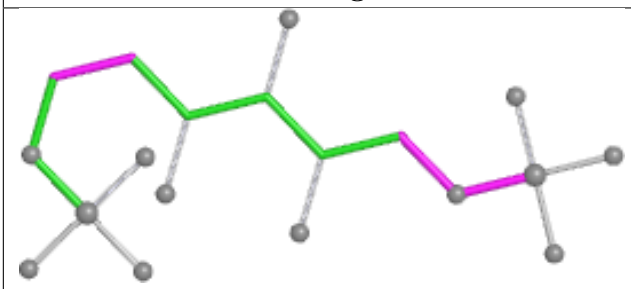
Ligand F2P A 501



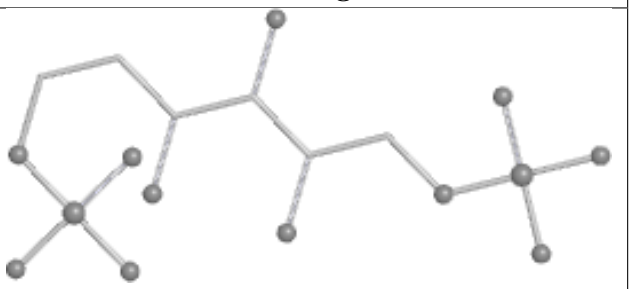
Bond lengths



Bond angles

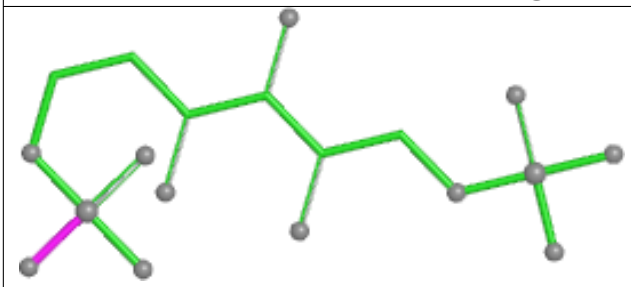


Torsions

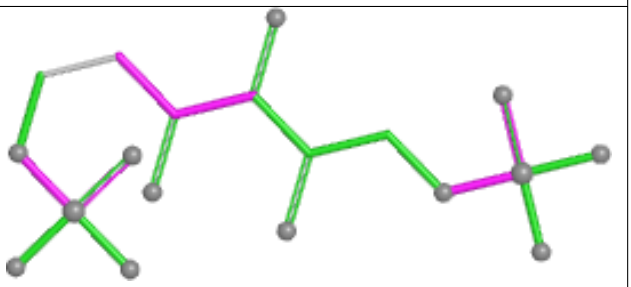


Rings

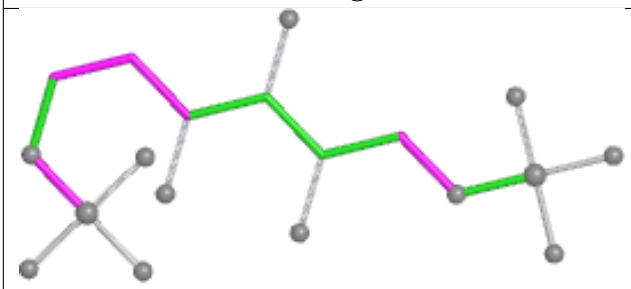
Ligand F2P K 501



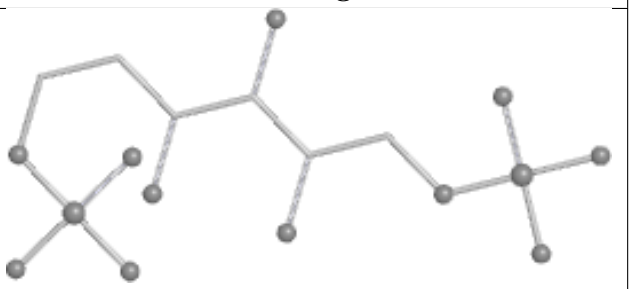
Bond lengths



Bond angles

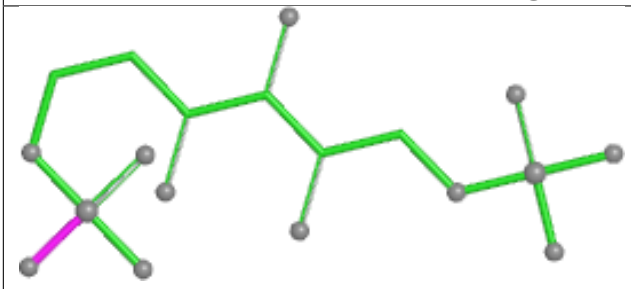


Torsions



Rings

Ligand F2P M 501



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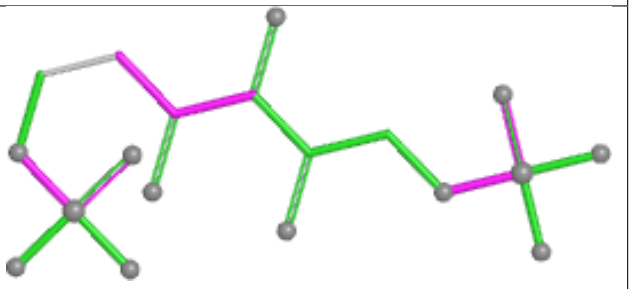
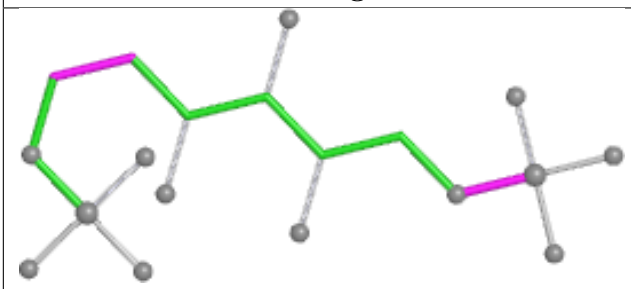
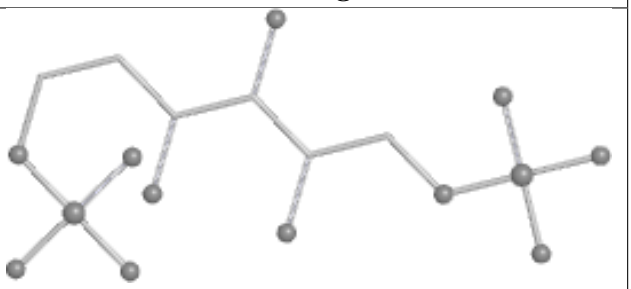


Bond angles

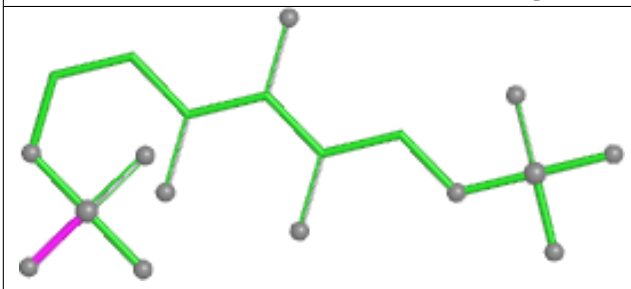


Torsions



Rings

Ligand F2P H 501



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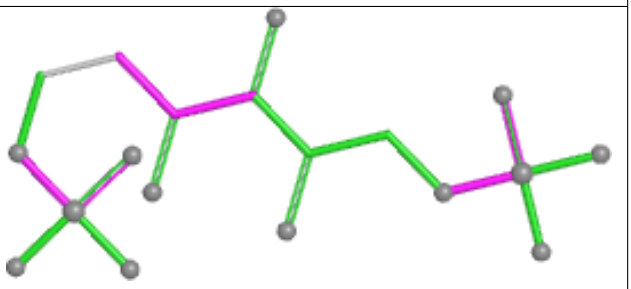
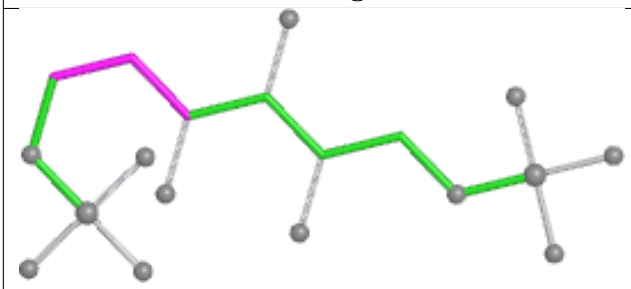
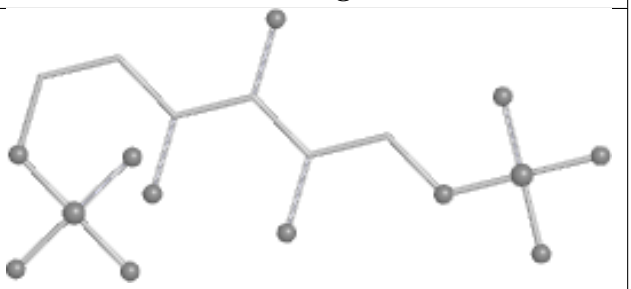


Bond angles

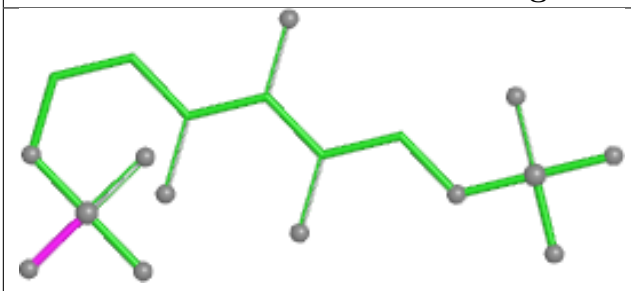


Torsions

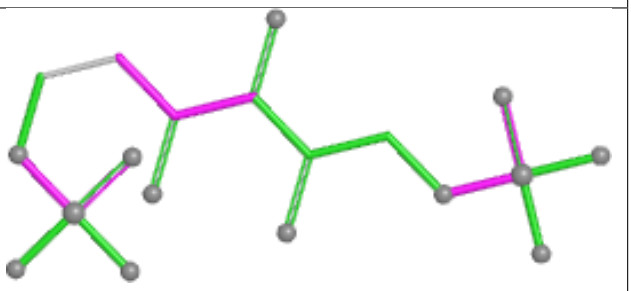


Rings

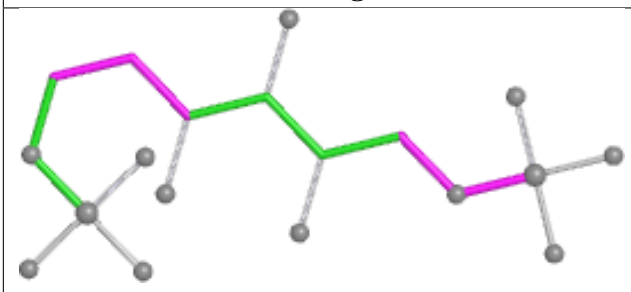
Ligand F2P P 501



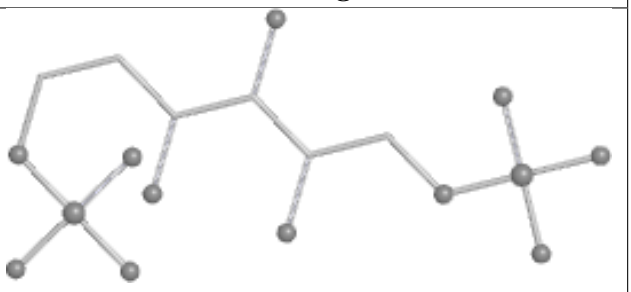
Bond lengths



Bond angles

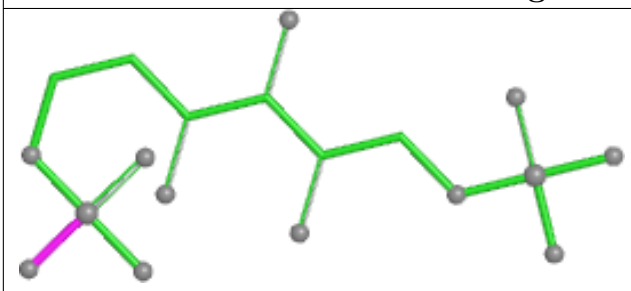


Torsions

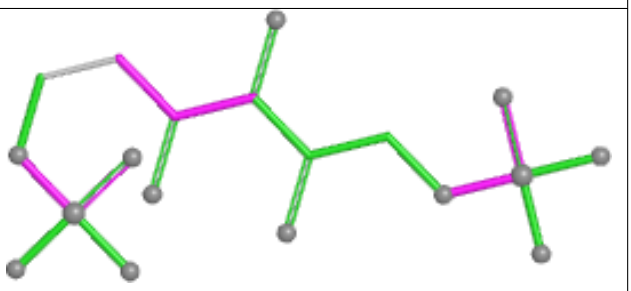


Rings

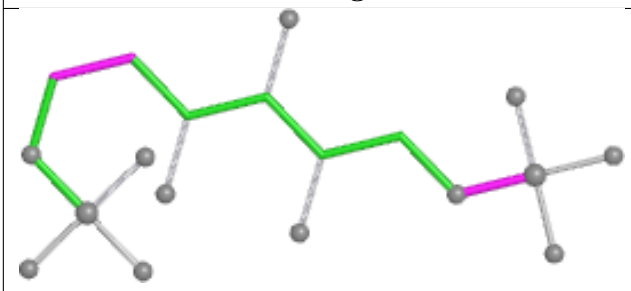
Ligand F2P N 501



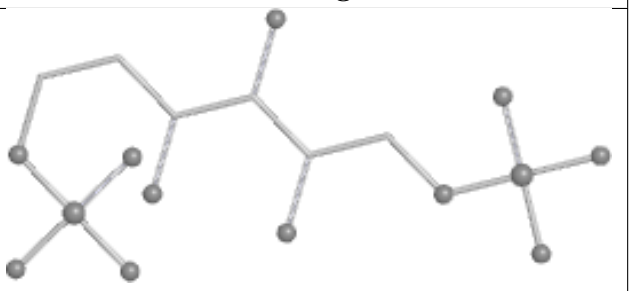
Bond lengths



Bond angles

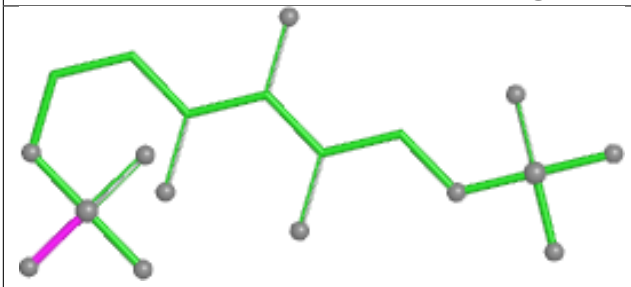


Torsions

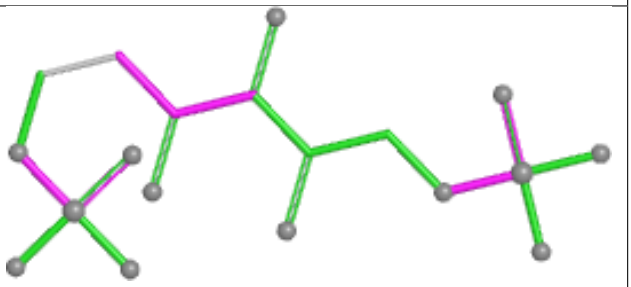


Rings

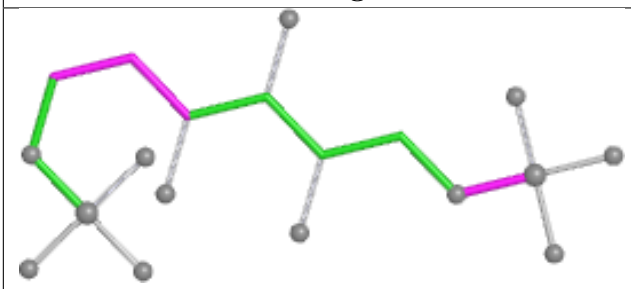
Ligand F2P T 501



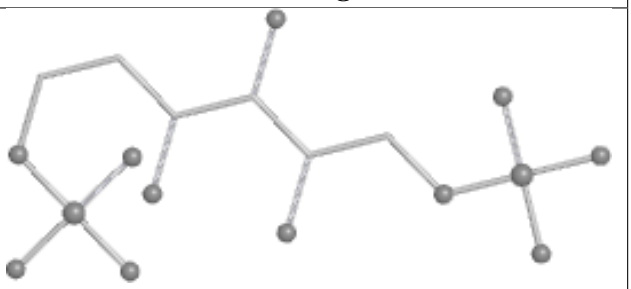
Bond lengths



Bond angles

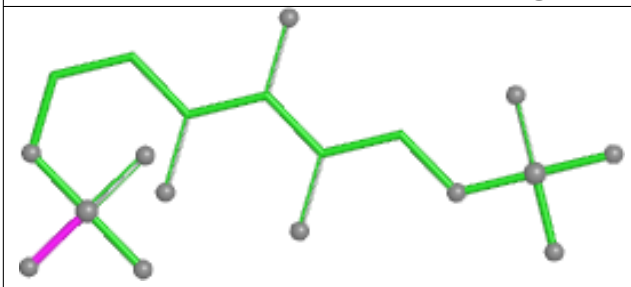


Torsions



Rings

Ligand F2P E 501



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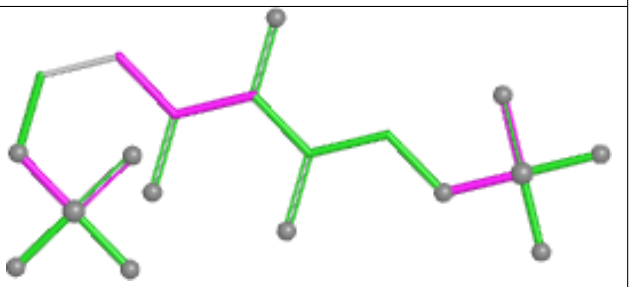
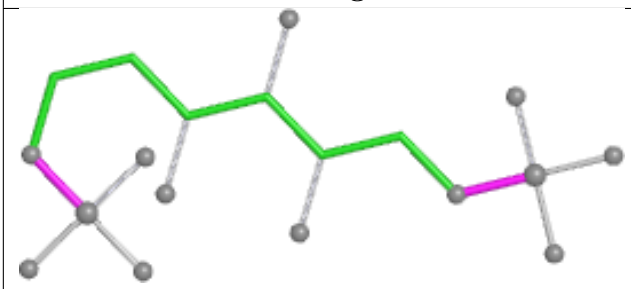
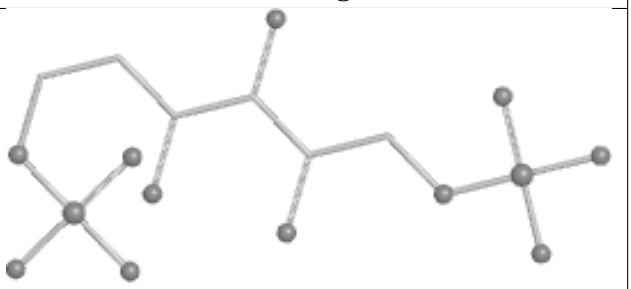


Bond angles

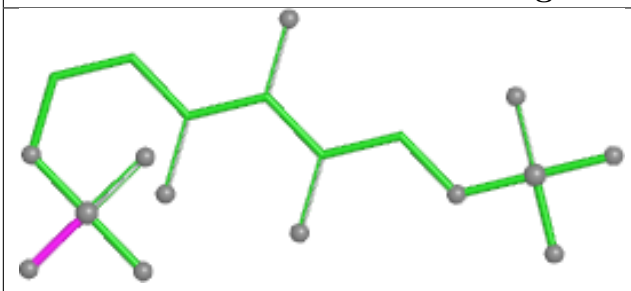


Torsions

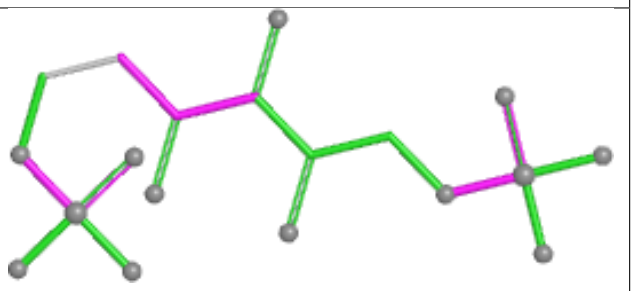


Rings

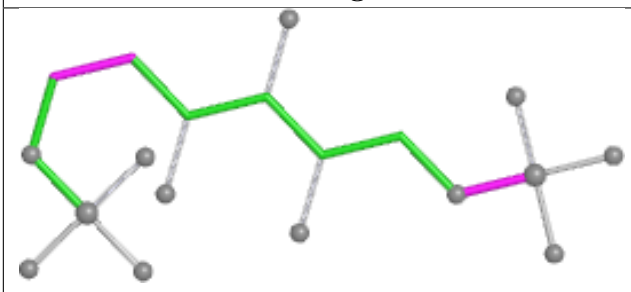
Ligand F2P I 501



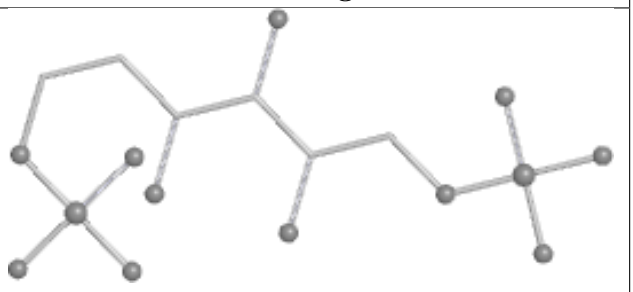
Bond lengths



Bond angles

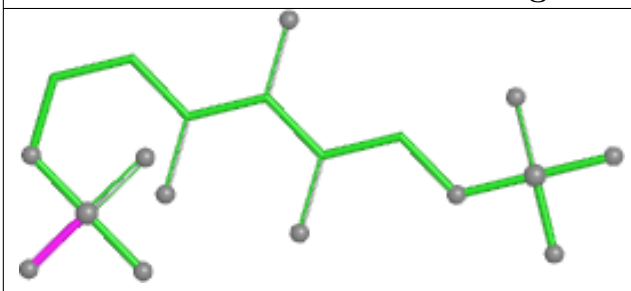


Torsions

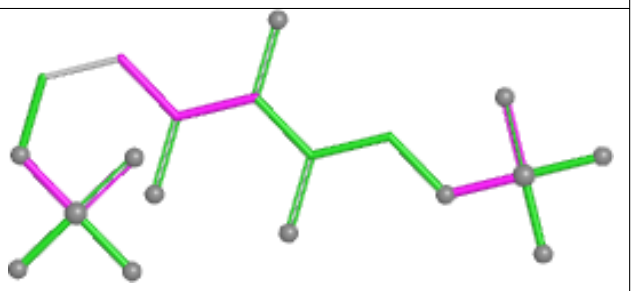


Rings

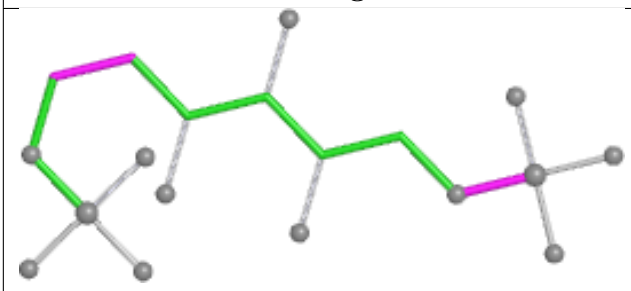
Ligand F2P B 501



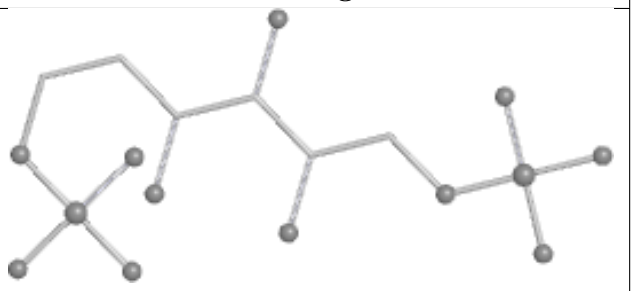
Bond lengths



Bond angles

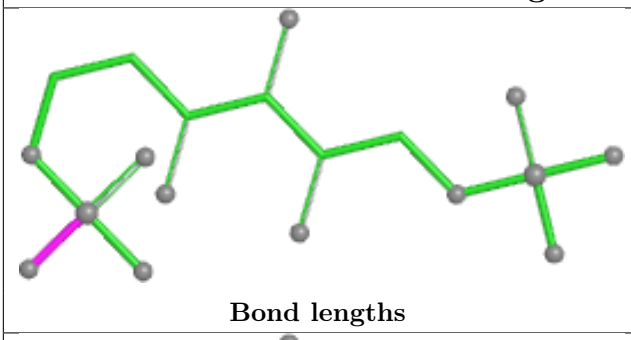


Torsions

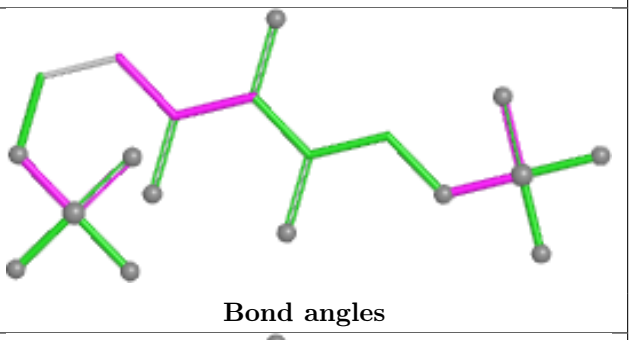


Rings

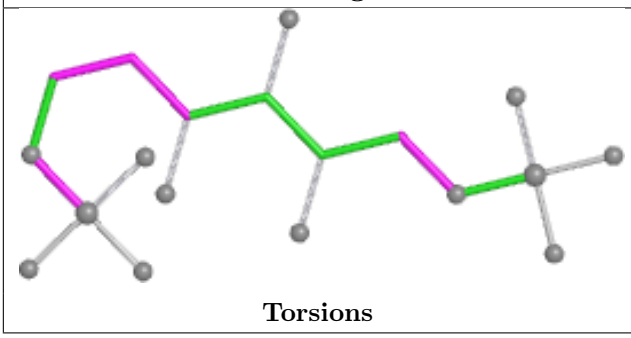
Ligand F2P G 501



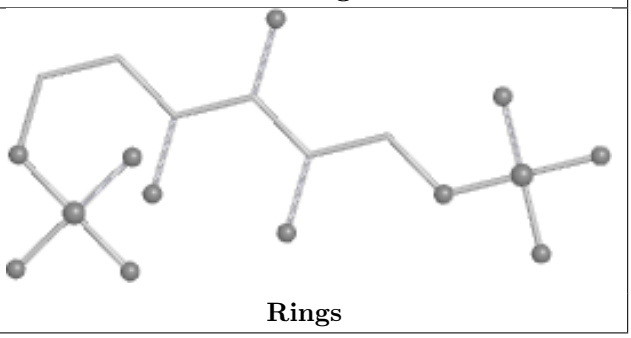
Bond lengths



Bond angles

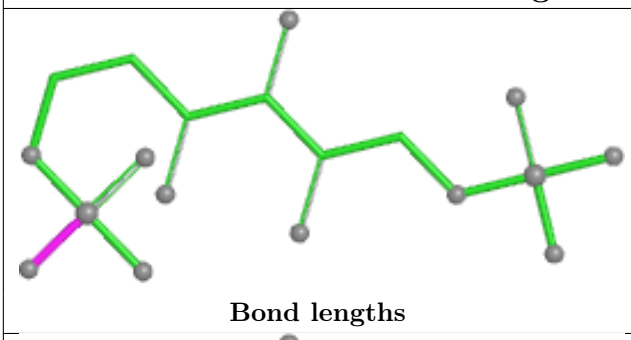


Torsions

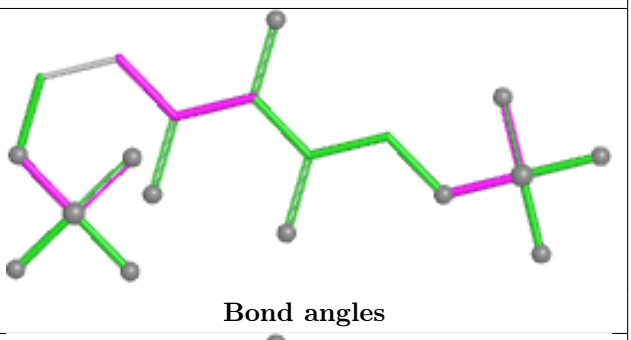


Rings

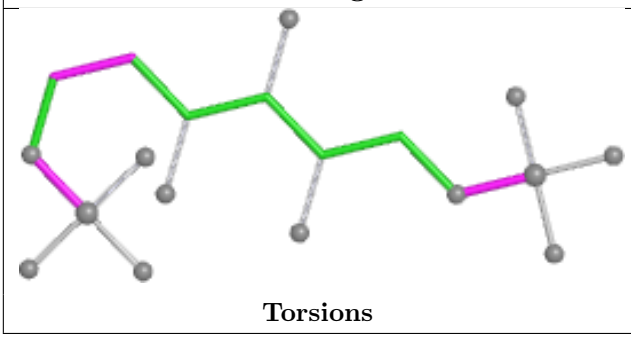
Ligand F2P S 501



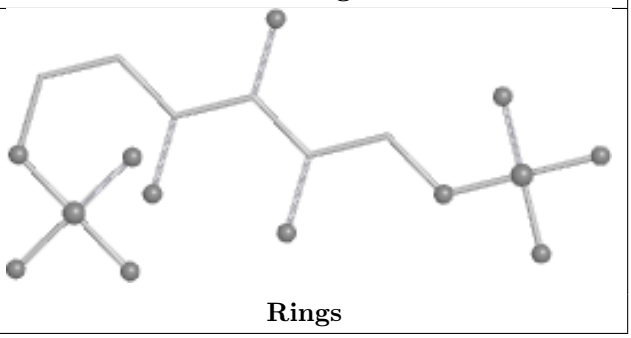
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	272/273 (99%)	-0.40	4 (1%)	73	70	19, 37, 69, 100	0
1	B	268/273 (98%)	-0.51	1 (0%)	92	91	20, 34, 69, 115	0
1	C	262/273 (95%)	-0.29	2 (0%)	86	84	16, 38, 68, 107	0
1	D	267/273 (97%)	-0.43	2 (0%)	87	86	18, 36, 64, 96	0
1	E	268/273 (98%)	-0.48	0	100	100	19, 36, 70, 95	0
1	F	263/273 (96%)	-0.41	0	100	100	19, 36, 64, 85	0
1	G	268/273 (98%)	-0.37	1 (0%)	92	91	18, 35, 71, 96	0
1	H	267/273 (97%)	-0.50	1 (0%)	92	91	16, 33, 65, 109	0
1	I	265/273 (97%)	-0.46	1 (0%)	92	91	16, 37, 69, 84	0
1	J	269/273 (98%)	-0.29	3 (1%)	80	78	18, 40, 76, 96	0
1	K	266/273 (97%)	-0.29	4 (1%)	73	70	23, 43, 75, 117	0
1	L	269/273 (98%)	-0.46	0	100	100	20, 36, 71, 100	0
1	M	265/273 (97%)	-0.33	7 (2%)	56	50	20, 39, 72, 96	0
1	N	265/273 (97%)	-0.43	0	100	100	17, 39, 66, 88	0
1	O	266/273 (97%)	-0.39	0	100	100	15, 39, 68, 98	0
1	P	268/273 (98%)	-0.30	1 (0%)	92	91	21, 41, 70, 109	0
1	Q	272/273 (99%)	-0.45	2 (0%)	87	86	18, 36, 76, 118	0
1	R	269/273 (98%)	-0.42	3 (1%)	80	78	19, 39, 80, 101	0
1	S	264/273 (96%)	-0.26	2 (0%)	86	84	23, 43, 72, 91	0
1	T	267/273 (97%)	-0.29	2 (0%)	87	86	19, 40, 69, 106	0
All	All	5340/5460 (97%)	-0.39	36 (0%)	87	86	15, 38, 72, 118	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	272	LYS	4.6
1	T	73	HIS	4.2
1	J	73	HIS	3.6
1	A	77	GLY	3.3
1	J	271	ARG	3.2
1	B	77	GLY	2.9
1	K	72	GLY	2.9
1	T	214	ASN	2.8
1	P	73	HIS	2.8
1	Q	79	ASP	2.8
1	K	272	LYS	2.8
1	M	267	LEU	2.7
1	M	270	ILE	2.7
1	S	261	ALA	2.6
1	K	268	LYS	2.6
1	Q	77	GLY	2.5
1	M	56	GLU	2.4
1	S	271	ARG	2.4
1	D	72	GLY	2.3
1	A	75	GLY	2.3
1	J	272	LYS	2.3
1	A	76	TYR	2.3
1	M	217	GLU	2.3
1	H	74	ARG	2.2
1	A	72	GLY	2.2
1	K	52	ASN	2.2
1	R	79	ASP	2.2
1	G	214	ASN	2.1
1	C	270	ILE	2.1
1	M	268	LYS	2.1
1	R	251	ARG	2.1
1	R	266	ALA	2.1
1	M	251	ARG	2.1
1	I	214	ASN	2.1
1	D	1	MET	2.1
1	M	216	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

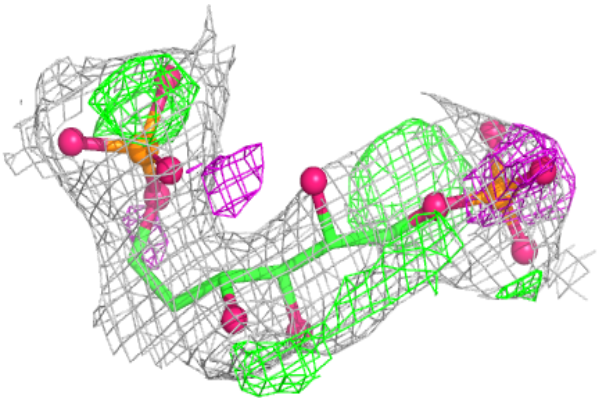
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

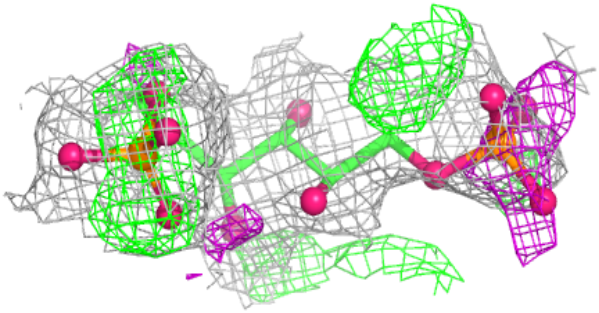
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F2P	H	501	19/20	0.82	0.31	53,63,82,82	0
2	F2P	S	501	19/20	0.83	0.27	62,75,96,97	0
2	F2P	O	501	19/20	0.84	0.21	62,72,90,90	0
2	F2P	B	501	19/20	0.84	0.24	47,65,78,79	0
2	F2P	D	501	19/20	0.84	0.31	48,65,88,88	0
2	F2P	C	501	19/20	0.85	0.23	55,63,87,87	0
2	F2P	N	501	19/20	0.86	0.21	48,64,88,88	0
2	F2P	G	501	19/20	0.86	0.23	44,58,88,88	0
2	F2P	P	501	19/20	0.87	0.23	50,68,81,81	0
2	F2P	R	501	19/20	0.87	0.21	59,64,82,82	0
2	F2P	K	501	19/20	0.87	0.23	56,65,89,90	0
2	F2P	A	501	19/20	0.88	0.22	53,63,87,88	0
2	F2P	J	501	19/20	0.89	0.24	50,70,91,91	0
2	F2P	F	501	19/20	0.89	0.20	55,65,82,83	0
2	F2P	E	501	19/20	0.90	0.20	43,57,79,80	0
2	F2P	Q	501	19/20	0.90	0.20	28,50,87,88	0
2	F2P	I	501	19/20	0.90	0.19	48,63,82,83	0
2	F2P	M	501	19/20	0.90	0.19	56,72,95,95	0
2	F2P	L	501	19/20	0.91	0.21	51,62,83,83	0
2	F2P	T	501	19/20	0.92	0.20	44,57,79,79	0

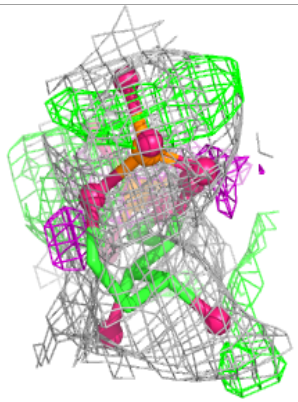
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F2P H 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

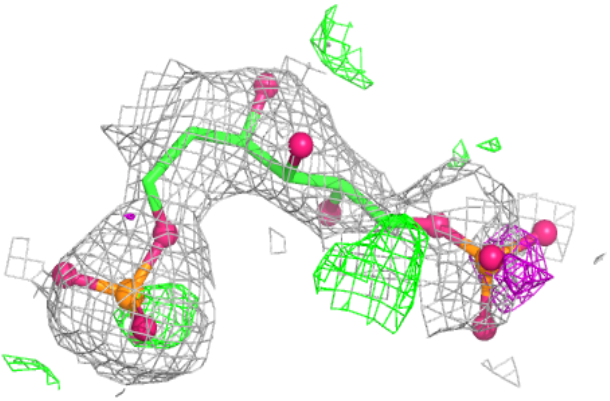


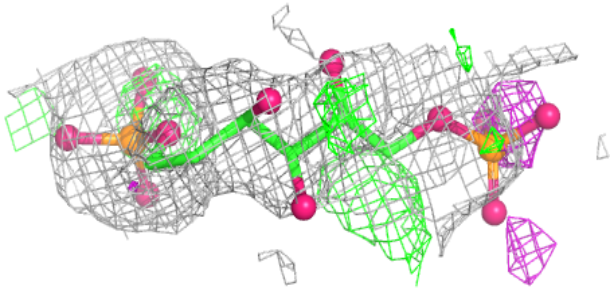


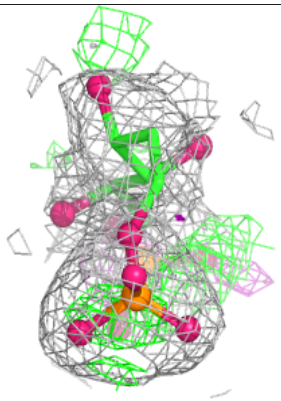


Electron density around F2P S 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

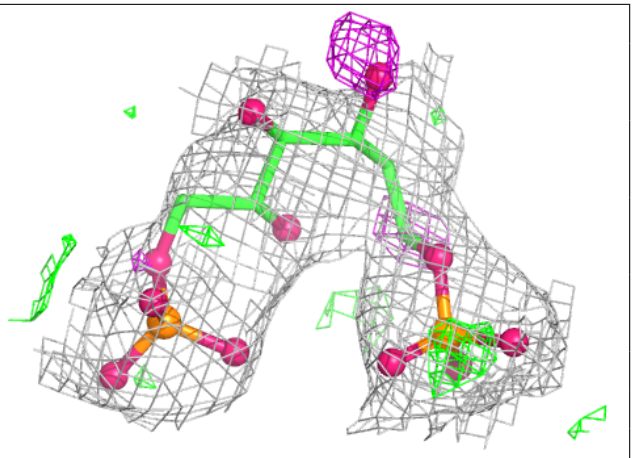


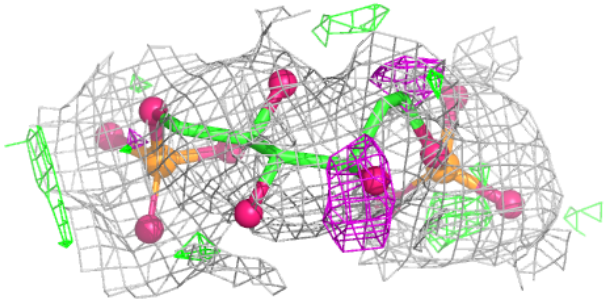


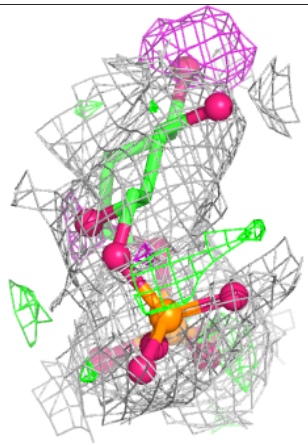


Electron density around F2P O 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

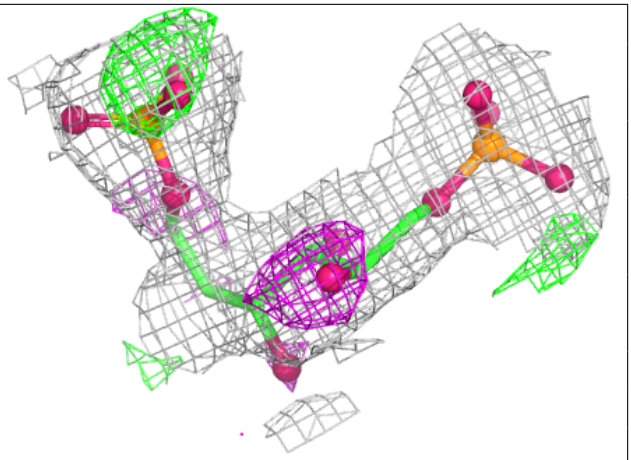


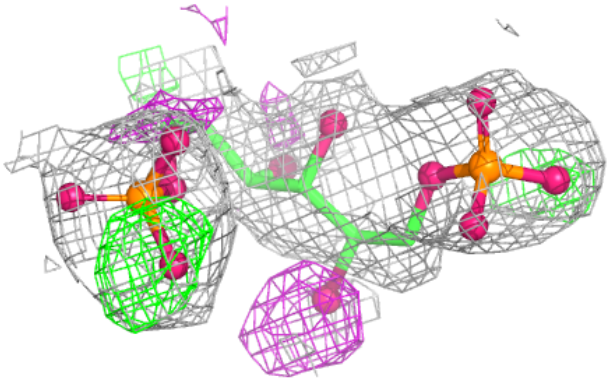


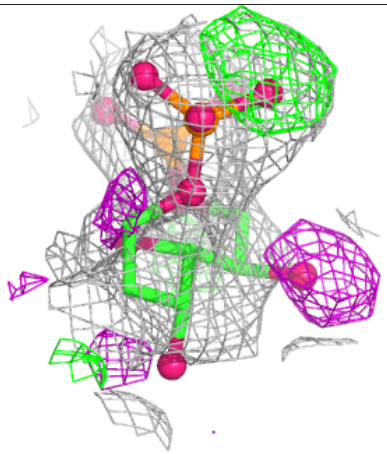


Electron density around F2P B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

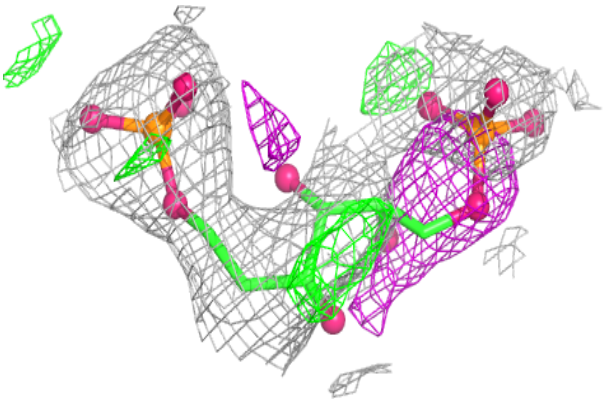


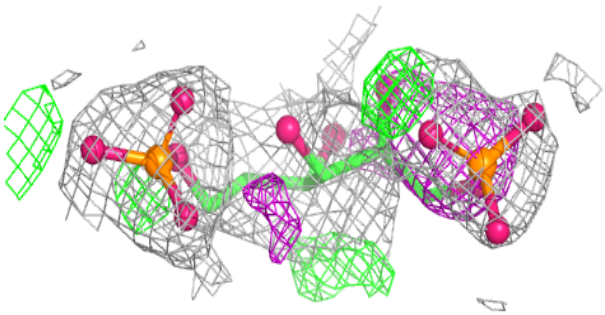




Electron density around F2P D 501:

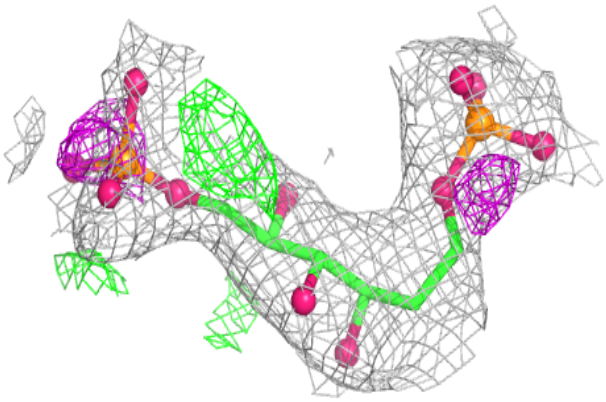
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

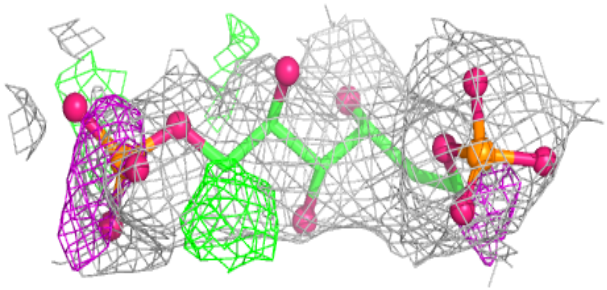


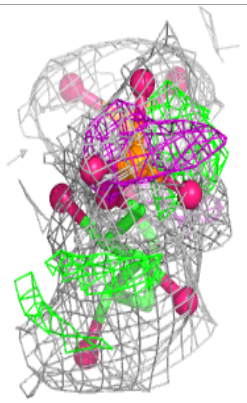


Electron density around F2P C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

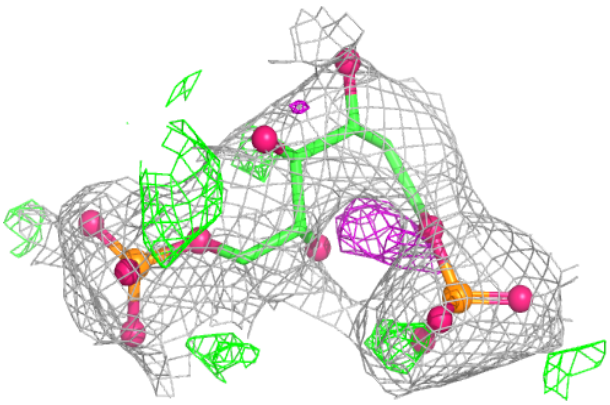


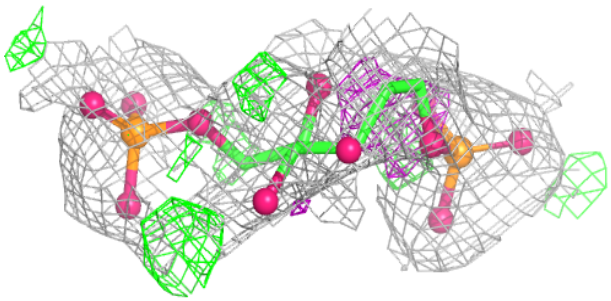


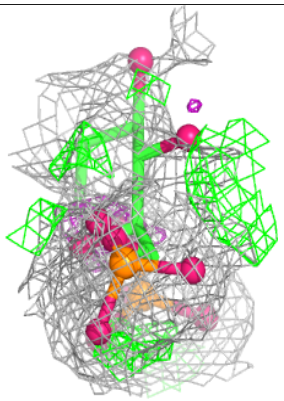


Electron density around F2P N 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

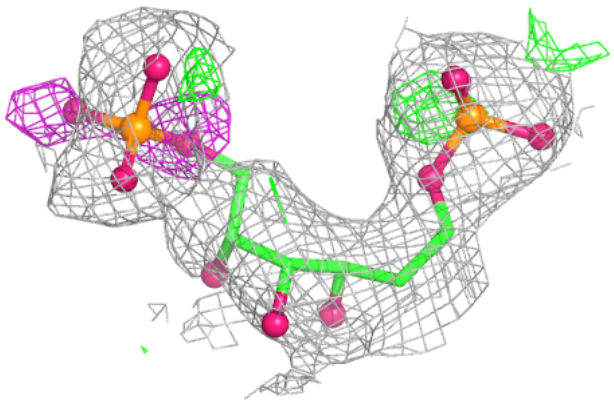


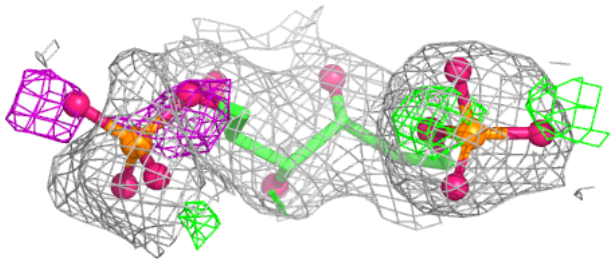


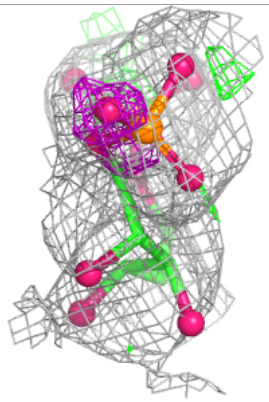


Electron density around F2P G 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

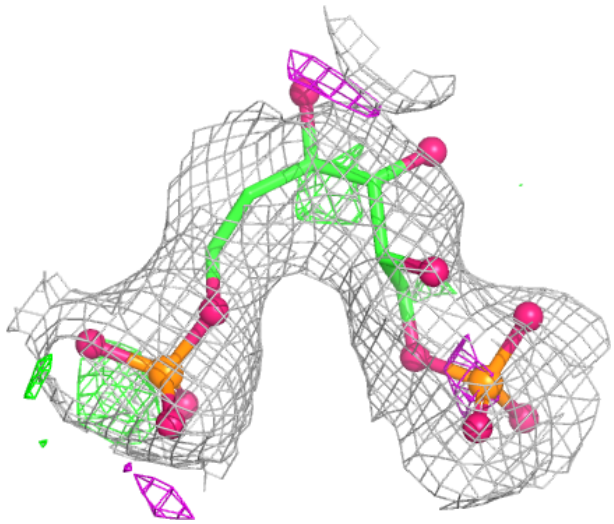


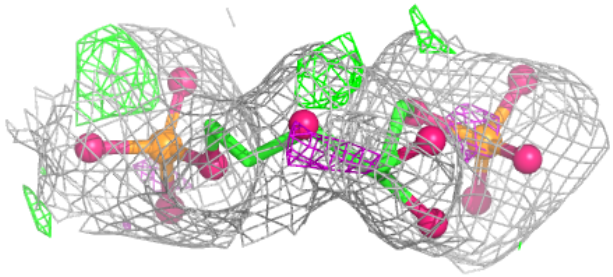


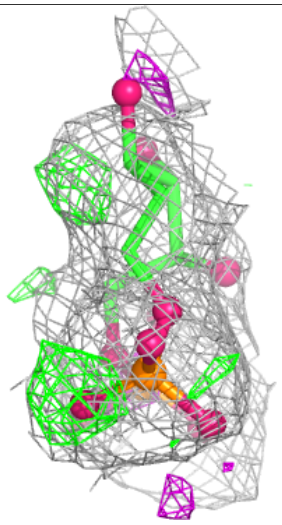


Electron density around F2P P 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

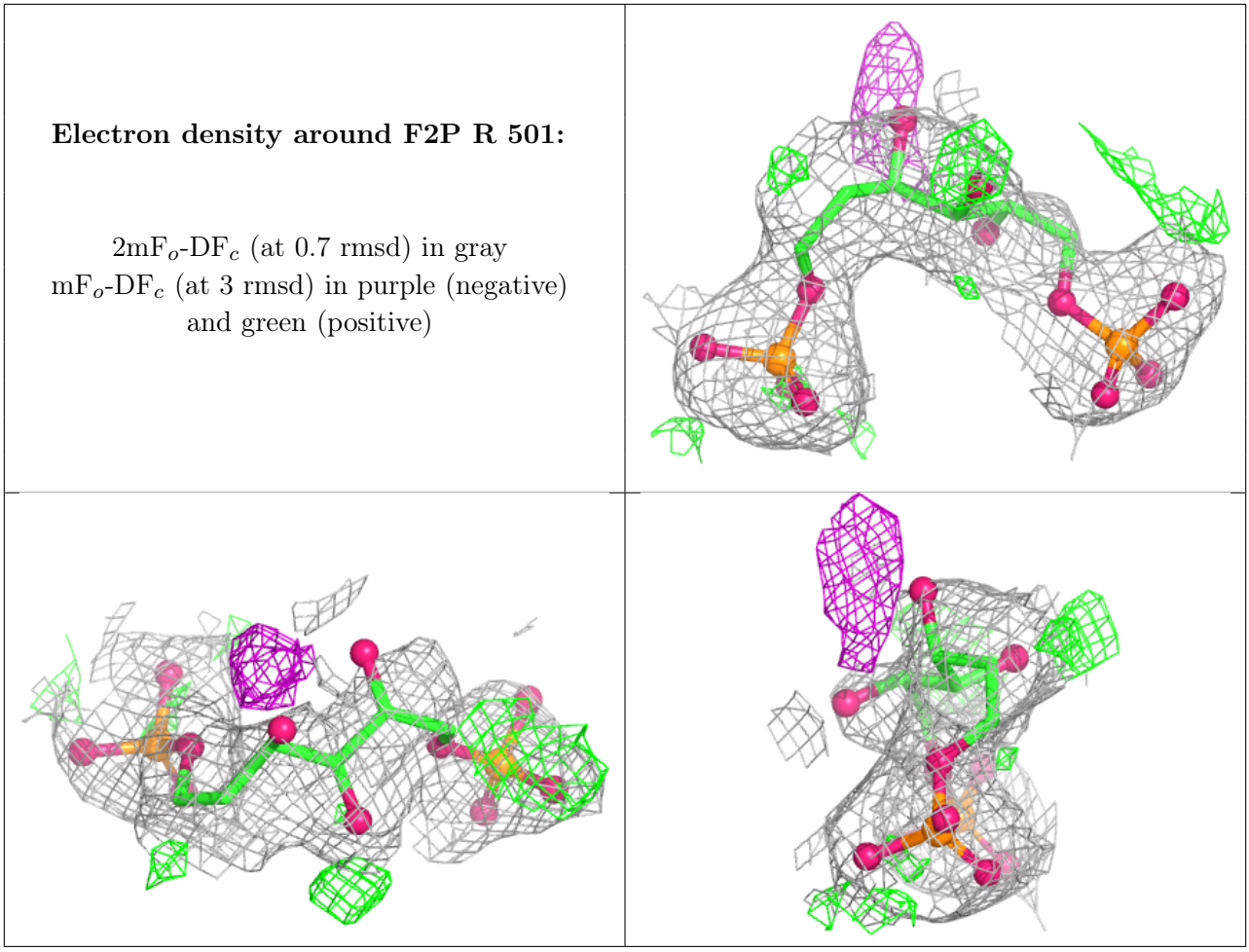






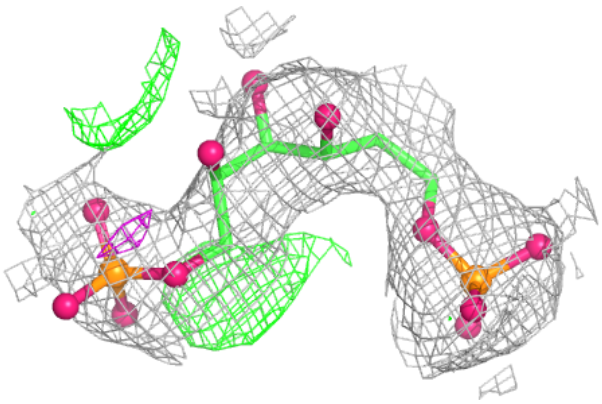
Electron density around F2P R 501:

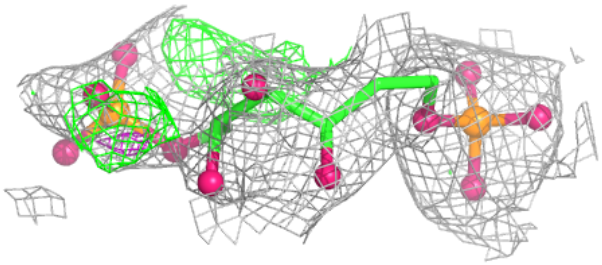
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

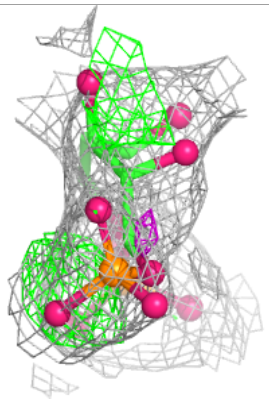


Electron density around F2P K 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

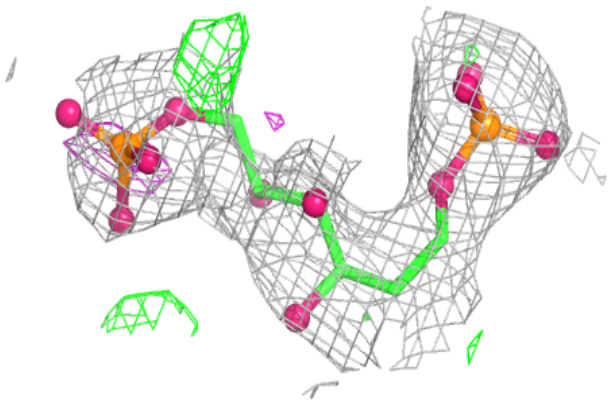


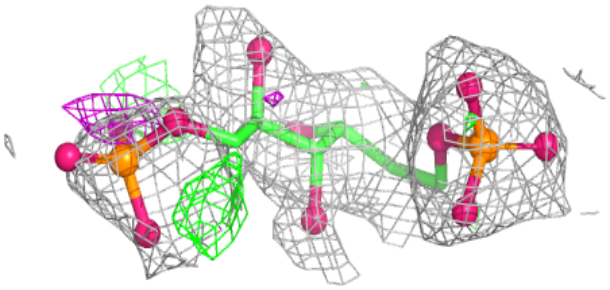


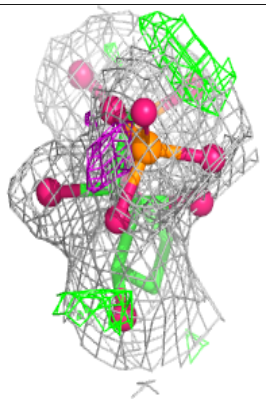


Electron density around F2P A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

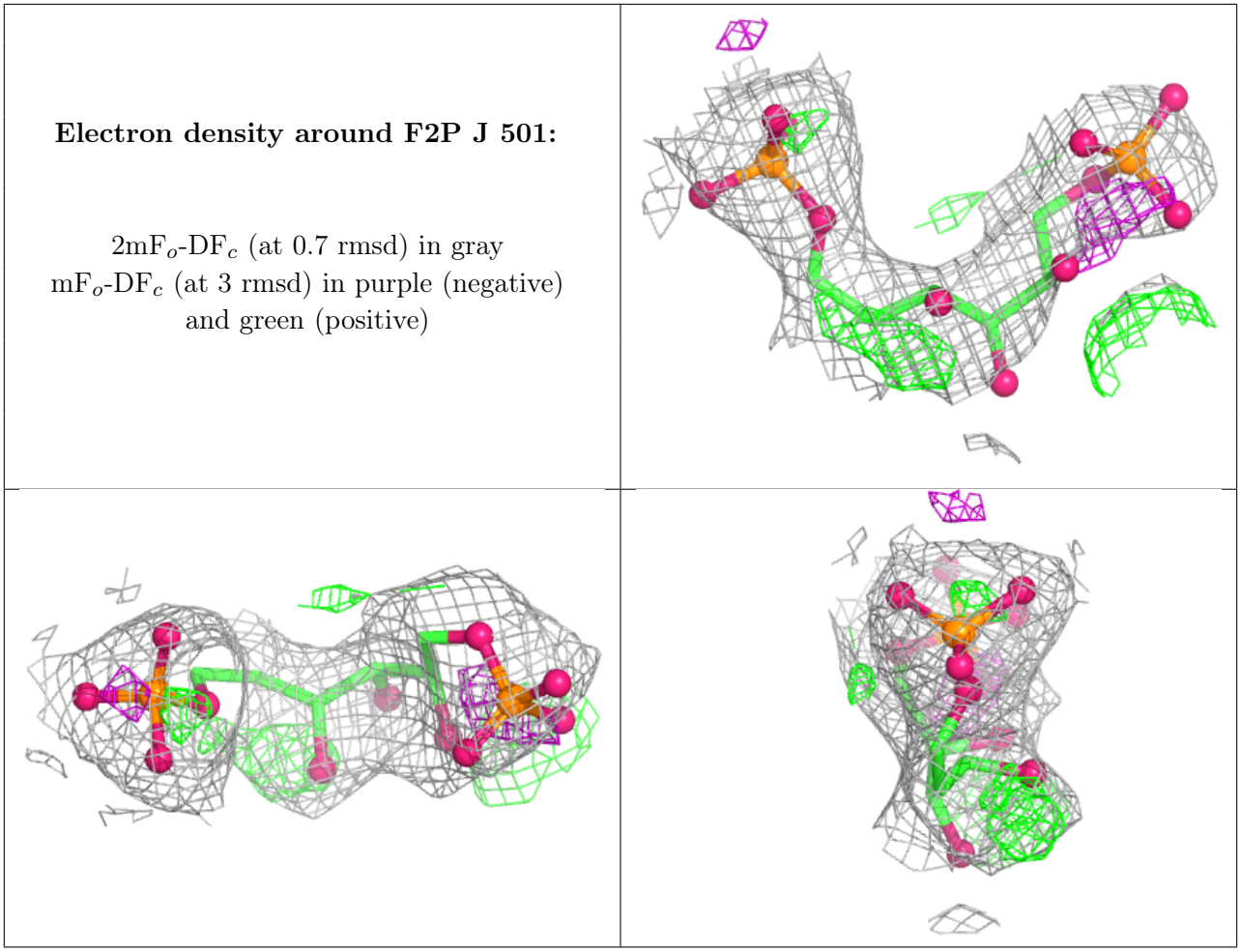






Electron density around F2P J 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around F2P F 501:

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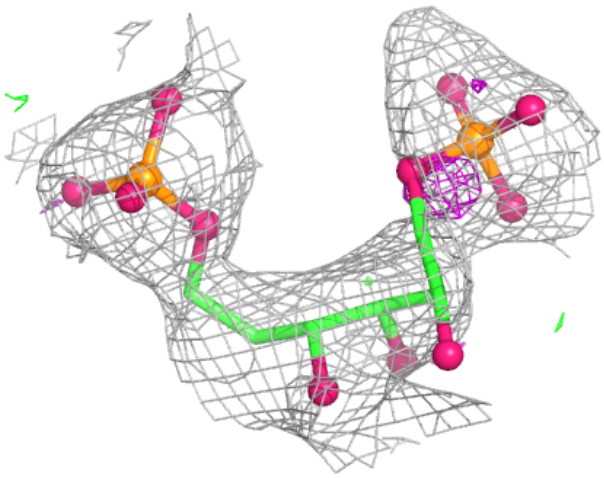
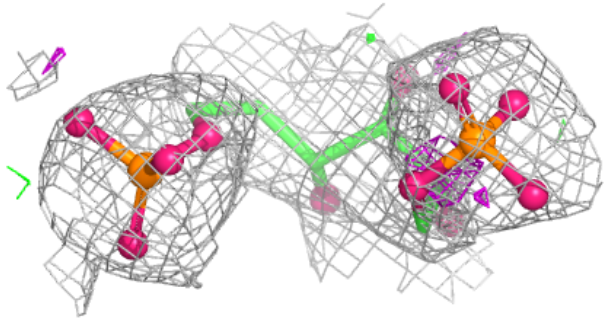
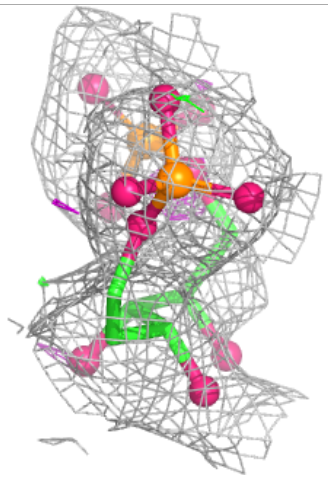
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

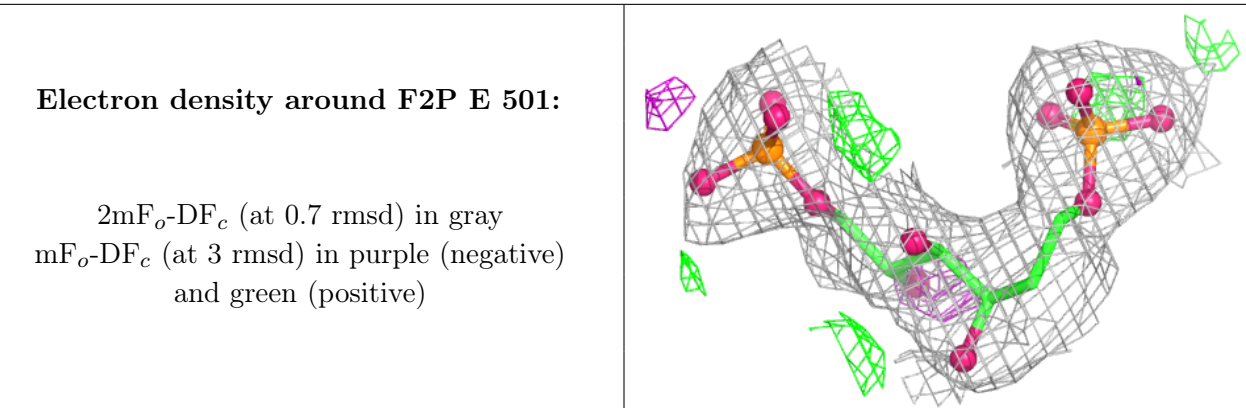


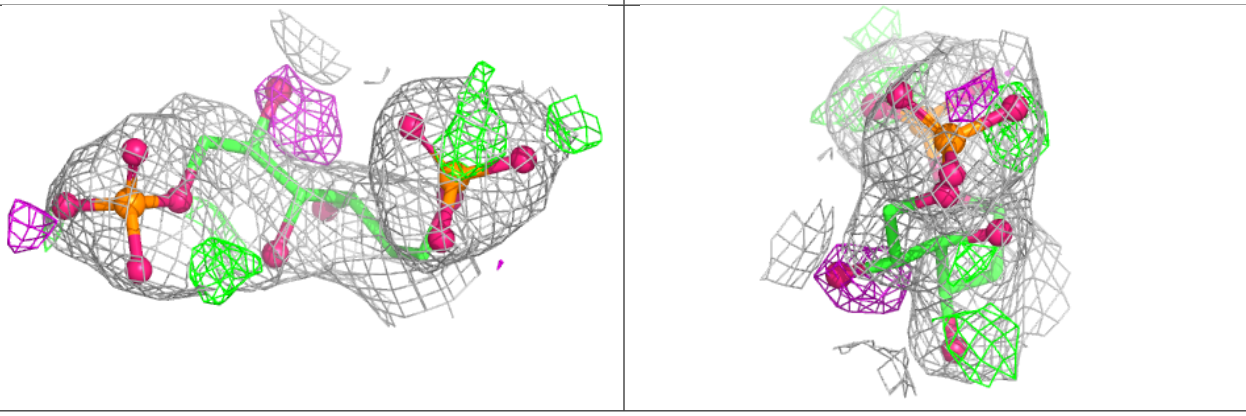




Electron density around F2P E 501:

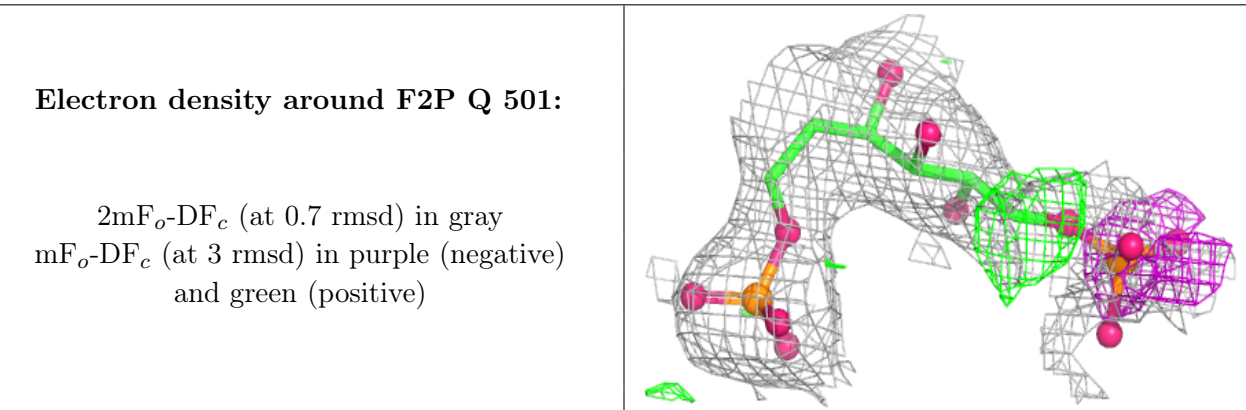
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

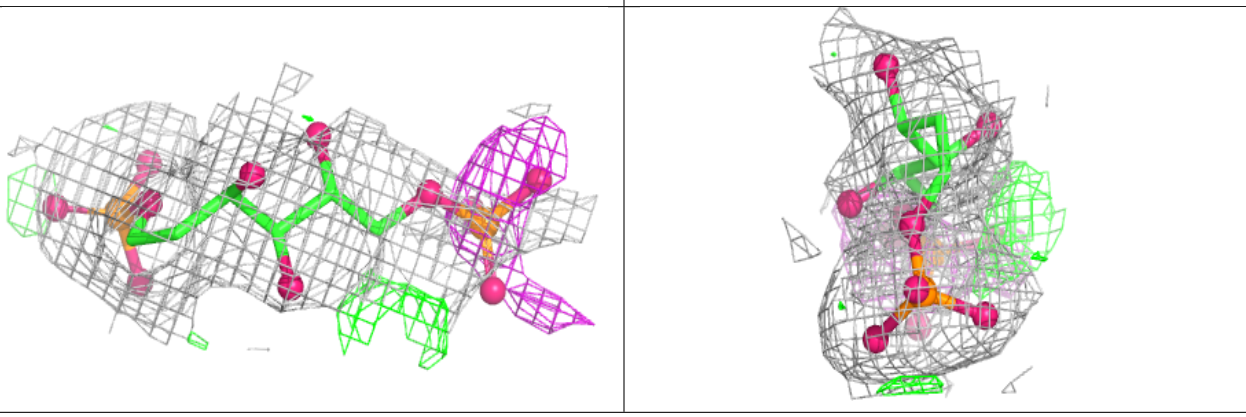




Electron density around F2P Q 501:

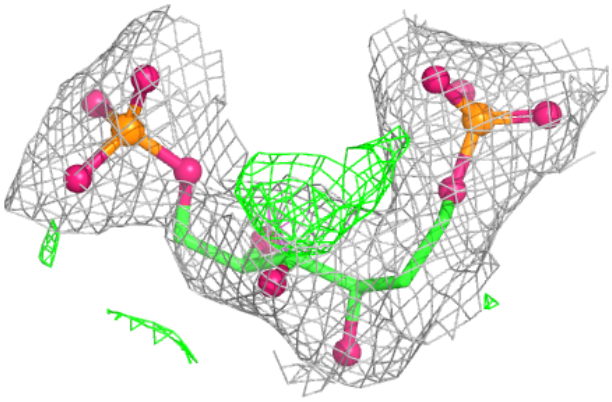
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

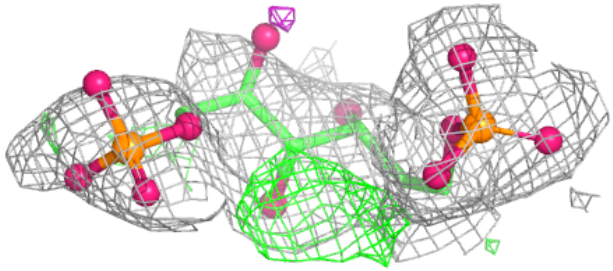


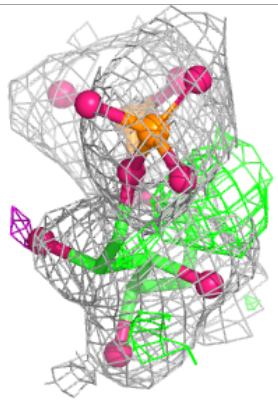


Electron density around F2P I 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

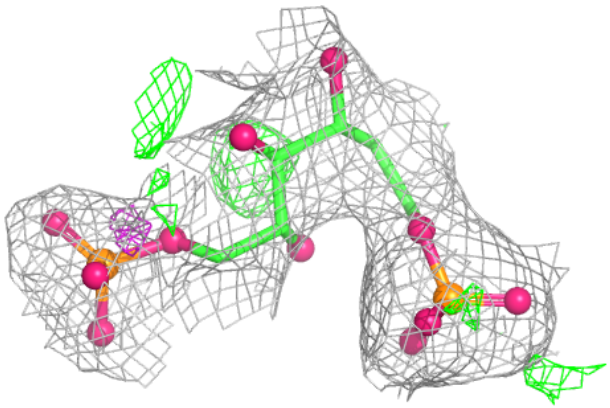


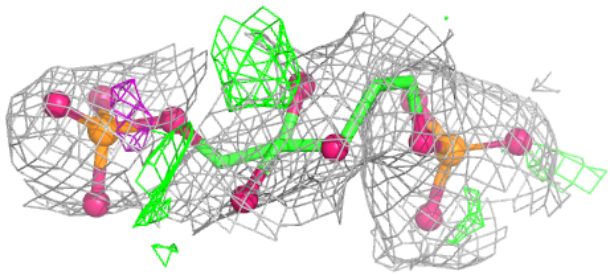




Electron density around F2P M 501:

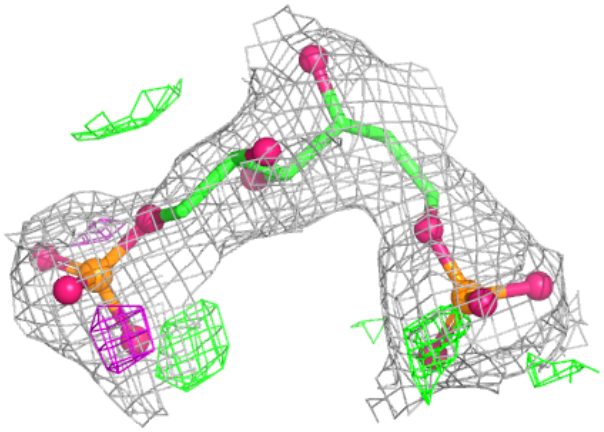
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

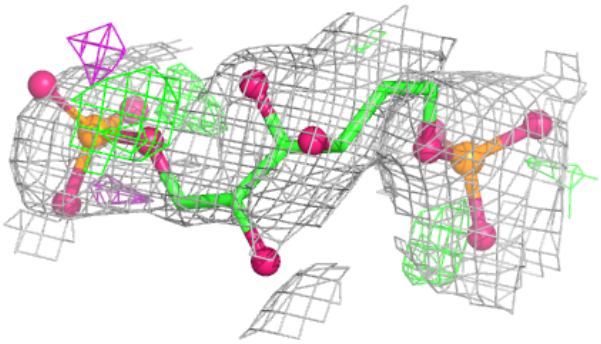


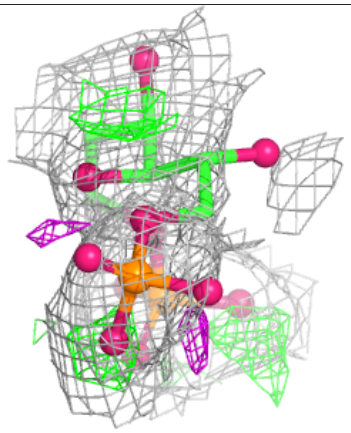


Electron density around F2P L 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

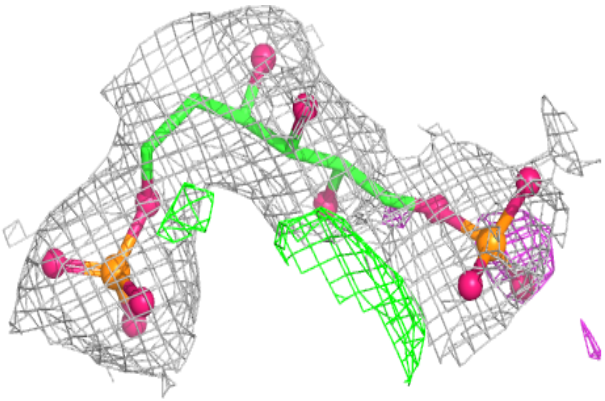


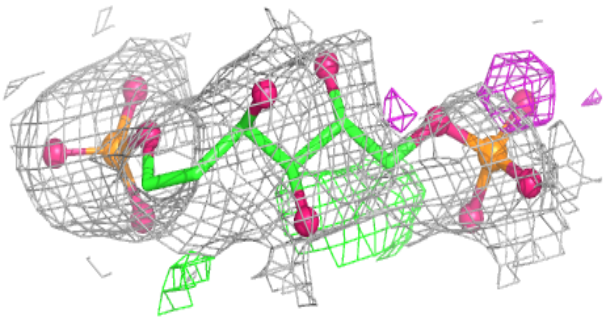




Electron density around F2P T 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.