



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 02:45 PM EDT

PDB ID : 6IH6
Title : Phosphite Dehydrogenase mutant I151R/P176R/M207A from *Ralstonia* sp. 4506 in complex with non-natural cofactor Nicotinamide Cytosine dinucleotide
Authors : Song, X.; Feng, Y.; Liu, Y.; Zhao, Z.
Deposited on : 2018-09-28
Resolution : 2.49 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

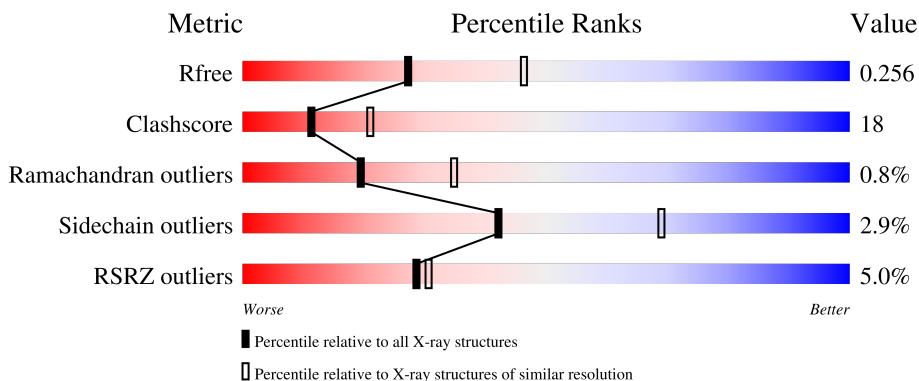
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

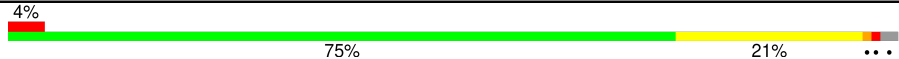



The reported resolution of this entry is 2.49 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	338	
1	B	338	
1	C	338	
1	D	338	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10429 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.

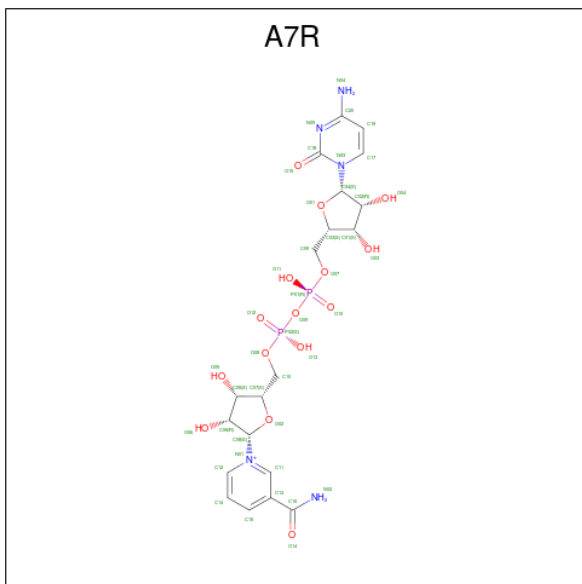
- Molecule 1 is a protein called Phosphite dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2533	1609	442	466	16	0	0	0
1	B	330	2533	1609	442	466	16	0	0	0
1	C	330	2533	1609	442	466	16	0	0	0
1	D	330	2533	1609	442	466	16	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ARG	ILE	engineered mutation	UNP G4XDR8
A	176	ARG	PRO	engineered mutation	UNP G4XDR8
A	207	ALA	MET	engineered mutation	UNP G4XDR8
A	337	LEU	-	expression tag	UNP G4XDR8
A	338	GLU	-	expression tag	UNP G4XDR8
B	151	ARG	ILE	engineered mutation	UNP G4XDR8
B	176	ARG	PRO	engineered mutation	UNP G4XDR8
B	207	ALA	MET	engineered mutation	UNP G4XDR8
B	337	LEU	-	expression tag	UNP G4XDR8
B	338	GLU	-	expression tag	UNP G4XDR8
C	151	ARG	ILE	engineered mutation	UNP G4XDR8
C	176	ARG	PRO	engineered mutation	UNP G4XDR8
C	207	ALA	MET	engineered mutation	UNP G4XDR8
C	337	LEU	-	expression tag	UNP G4XDR8
C	338	GLU	-	expression tag	UNP G4XDR8
D	151	ARG	ILE	engineered mutation	UNP G4XDR8
D	176	ARG	PRO	engineered mutation	UNP G4XDR8
D	207	ALA	MET	engineered mutation	UNP G4XDR8
D	337	LEU	-	expression tag	UNP G4XDR8
D	338	GLU	-	expression tag	UNP G4XDR8

- Molecule 2 is [[(2S,3S,4R,5S)-5-(3-aminocarbonylpyridin-1-ium-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2S,3S,4R,5S)-5-(4-azanyl-2-oxidanylidene-pyrimidin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: A7R) (formula: C₂₀H₂₈N₅O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 42	C 20	N 5	O 15	P 2	0	0
2	B	1	Total 42	C 20	N 5	O 15	P 2	0	0

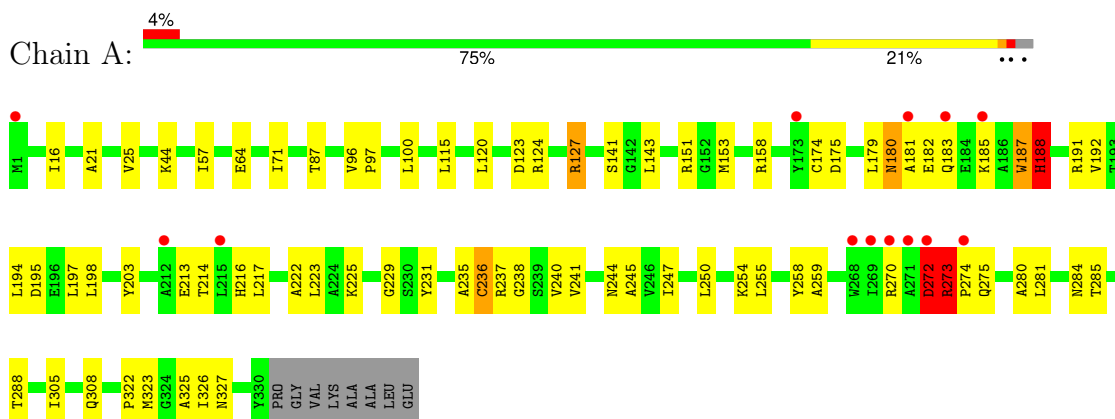
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	49	Total 49	O 49	0	0
3	C	72	Total 72	O 72	0	0
3	D	51	Total 51	O 51	0	0

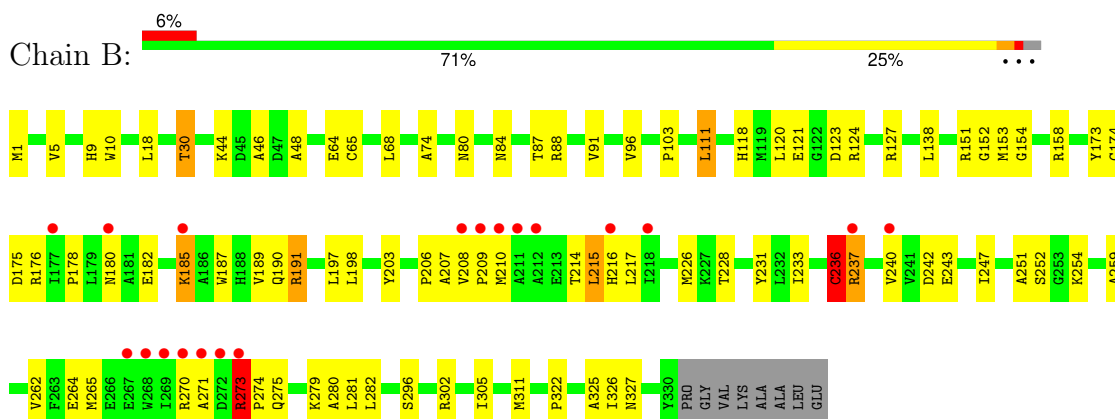
3 Residue-property plots

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.

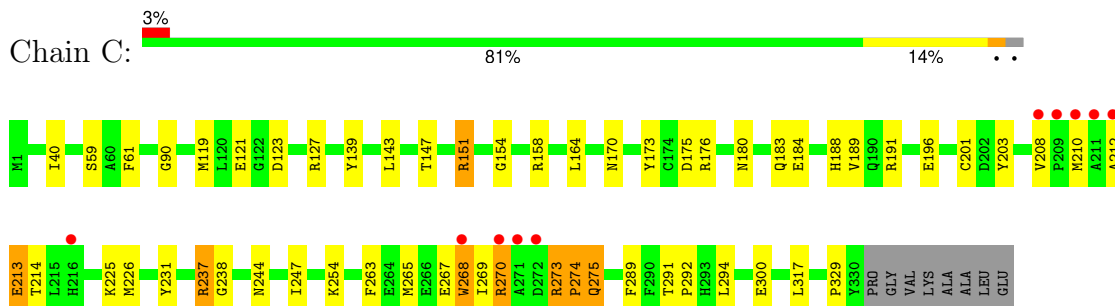
- Molecule 1: Phosphite dehydrogenase



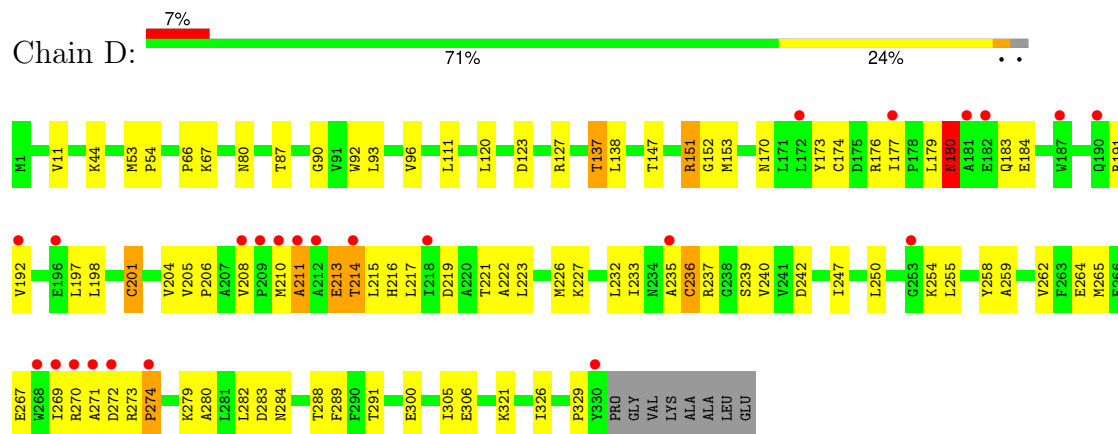
- Molecule 1: Phosphite dehydrogenase



- Molecule 1: Phosphite dehydrogenase



- Molecule 1: Phosphite dehydrogenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.20Å 118.87Å 98.34Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	38.67 – 2.49 45.44 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.3 (38.67-2.49) 96.0 (45.44-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.199 , 0.255 0.203 , 0.256	Depositor DCC
R_{free} test set	2441 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtrriage
Anisotropy	0.439	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 25.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.206 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10429	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A7R

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	0.49	0/2582	0.71	5/3508 (0.1%)
1	B	0.50	0/2582	0.70	3/3508 (0.1%)
1	C	0.51	1/2582 (0.0%)	0.70	2/3508 (0.1%)
1	D	0.50	1/2582 (0.0%)	0.70	3/3508 (0.1%)
All	All	0.50	2/10328 (0.0%)	0.70	13/14032 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	THR	C-N	6.97	1.47	1.34
1	D	291	THR	C-N	5.02	1.43	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	180	ASN	CB-CA-C	-6.86	96.67	110.40
1	B	237	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	120	LEU	CA-CB-CG	-5.93	101.66	115.30
1	C	275	GLN	N-CA-C	-5.61	95.86	111.00
1	D	176	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	100	LEU	CA-CB-CG	5.59	128.16	115.30
1	C	151	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	272	ASP	N-CA-C	-5.54	96.03	111.00
1	B	236	CYS	CA-CB-SG	5.20	123.36	114.00
1	D	236	CYS	N-CA-C	-5.17	97.05	111.00
1	B	273	ARG	C-N-CD	5.06	139.02	128.40
1	A	273	ARG	C-N-CD	5.04	138.97	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2533	0	2578	93	0
1	B	2533	0	2578	98	0
1	C	2533	0	2577	61	0
1	D	2533	0	2578	117	0
2	A	42	0	0	5	0
2	B	42	0	0	8	0
3	A	41	0	0	2	0
3	B	49	0	0	5	0
3	C	72	0	0	4	0
3	D	51	0	0	4	0
All	All	10429	0	10311	365	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 18.

All (365) 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:D:179:LEU:CD2	1:D:180:ASN:ND2	1.94	1.31
1:A:180:ASN:HD21	1:A:183:GLN:CD	1.35	1.29
1:D:210:MET:CA	1:D:215:LEU:HD21	1.72	1.19
1:B:273:ARG:NH2	1:B:275:GLN:HG3	1.55	1.18
1:B:273:ARG:HH22	1:B:275:GLN:CG	1.57	1.18
1:D:179:LEU:HD22	1:D:180:ASN:ND2	1.56	1.18
1:D:210:MET:O	1:D:215:LEU:CD2	1.93	1.15
1:D:210:MET:CB	1:D:215:LEU:HD21	1.77	1.14
1:D:210:MET:C	1:D:215:LEU:HD21	1.68	1.12
1:C:268:TRP:CA	1:C:273:ARG:HE	1.61	1.11
1:D:210:MET:CB	1:D:215:LEU:HD11	1.78	1.11
1:C:268:TRP:HA	1:C:273:ARG:NE	1.62	1.11
1:D:210:MET:HB2	1:D:215:LEU:HD21	1.31	1.08
1:A:179:LEU:HD23	1:A:180:ASN:H	1.08	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HH22	1:A:275:GLN:HA	1.15	1.06
1:C:268:TRP:HA	1:C:273:ARG:HE	0.95	1.06
1:A:180:ASN:ND2	1:A:183:GLN:CD	2.11	1.04
1:D:236:CYS:O	1:D:262:VAL:HG21	1.56	1.04
1:D:210:MET:HB2	1:D:215:LEU:HD11	1.37	1.03
1:C:273:ARG:HG3	1:C:273:ARG:HH11	1.23	1.03
1:B:214:THR:HB	1:B:217:LEU:CD1	1.90	1.02
1:D:179:LEU:HD23	1:D:180:ASN:ND2	1.75	1.00
1:A:179:LEU:HD23	1:A:180:ASN:N	1.76	0.99
1:D:237:ARG:NH1	1:D:267:GLU:OE1	1.95	0.99
1:D:210:MET:C	1:D:215:LEU:CD2	2.34	0.95
1:D:147:THR:HG22	1:D:170:ASN:HB3	1.49	0.95
1:D:210:MET:O	1:D:215:LEU:HD23	1.67	0.95
1:D:210:MET:HB2	1:D:215:LEU:CD2	1.97	0.93
1:D:179:LEU:CD2	1:D:180:ASN:HD22	1.70	0.93
1:D:210:MET:HB3	1:D:215:LEU:HD11	1.51	0.92
1:A:180:ASN:ND2	1:A:183:GLN:NE2	2.18	0.92
1:C:210:MET:H	1:C:237:ARG:NH1	1.46	0.92
1:D:210:MET:HB2	1:D:215:LEU:CD1	2.00	0.91
1:D:137:THR:OG1	3:D:401:HOH:O	1.89	0.89
1:A:179:LEU:HD21	1:A:183:GLN:HB2	1.55	0.88
1:C:210:MET:N	1:C:237:ARG:NH1	2.12	0.88
1:D:273:ARG:NH1	1:D:274:PRO:HD2	1.89	0.88
1:A:273:ARG:NH2	1:A:275:GLN:HA	1.88	0.87
1:C:208:VAL:O	1:C:237:ARG:NH2	2.06	0.87
1:D:210:MET:CA	1:D:215:LEU:CD2	2.52	0.87
1:B:273:ARG:HH22	1:B:275:GLN:HG3	0.75	0.87
1:A:273:ARG:CB	1:A:273:ARG:HH11	1.88	0.86
1:D:179:LEU:HD22	1:D:180:ASN:HD21	1.35	0.86
1:B:176:ARG:HH21	1:B:176:ARG:HG3	1.38	0.86
1:D:179:LEU:CD2	1:D:180:ASN:HD21	1.88	0.86
1:B:151:ARG:HE	1:B:217:LEU:HD21	1.41	0.85
1:A:273:ARG:HH11	1:A:273:ARG:HB3	1.38	0.85
1:B:215:LEU:O	1:B:240:VAL:HA	1.77	0.85
1:B:87:THR:OG1	1:B:327:ASN:OD1	1.94	0.85
1:A:273:ARG:HH22	1:A:275:GLN:CA	1.89	0.84
1:B:9:HIS:O	3:B:501:HOH:O	1.98	0.82
1:B:180:ASN:OD1	1:B:182:GLU:OE1	1.98	0.81
1:A:153:MET:O	1:A:158:ARG:NH1	2.15	0.80
1:B:215:LEU:HG	1:B:216:HIS:H	1.45	0.79
1:D:179:LEU:HD23	1:D:180:ASN:HD22	1.40	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:MET:HB2	1:D:215:LEU:CG	2.11	0.79
1:A:115:LEU:HD13	1:A:259:ALA:HB2	1.66	0.78
1:A:180:ASN:OD1	1:A:182:GLU:N	2.16	0.78
1:D:213:GLU:O	1:D:214:THR:OG1	2.02	0.77
1:A:236:CYS:SG	1:A:240:VAL:HG11	2.24	0.77
1:D:210:MET:CB	1:D:215:LEU:CD1	2.59	0.77
1:A:115:LEU:HD21	1:A:231:TYR:HD2	1.48	0.77
1:C:213:GLU:HG2	1:C:214:THR:N	1.99	0.76
1:C:184:GLU:OE2	3:C:401:HOH:O	2.03	0.75
1:B:214:THR:HB	1:B:217:LEU:HD13	1.67	0.75
1:D:247:ILE:O	3:D:402:HOH:O	2.05	0.75
1:D:273:ARG:CZ	1:D:274:PRO:HD2	2.18	0.74
1:A:180:ASN:ND2	1:A:183:GLN:OE1	2.16	0.74
1:A:270:ARG:HG3	1:A:272:ASP:O	1.87	0.74
1:D:236:CYS:O	1:D:262:VAL:CG2	2.35	0.73
1:B:247:ILE:HD13	1:B:280:ALA:HB3	1.69	0.73
1:C:213:GLU:HG2	1:C:214:THR:OG1	1.88	0.73
1:A:322:PRO:HG2	1:A:325:ALA:HB2	1.70	0.73
1:A:191:ARG:NH1	1:A:192:VAL:O	2.22	0.73
1:C:210:MET:HE3	1:C:237:ARG:HD2	1.72	0.72
1:A:270:ARG:NE	1:A:272:ASP:HB2	2.04	0.72
1:B:322:PRO:HG2	1:B:325:ALA:HB2	1.70	0.72
1:C:147:THR:HG22	1:C:170:ASN:HB3	1.72	0.72
1:B:215:LEU:CD2	1:B:215:LEU:H	2.04	0.70
1:D:210:MET:CB	1:D:215:LEU:CD2	2.60	0.69
1:A:87:THR:OG1	1:A:327:ASN:ND2	2.26	0.69
1:B:215:LEU:CG	1:B:216:HIS:H	2.05	0.69
1:D:179:LEU:HD23	1:D:180:ASN:H	1.58	0.69
1:D:180:ASN:HD22	1:D:180:ASN:N	1.90	0.68
1:B:237:ARG:N	2:B:400:A7R:O06	2.26	0.68
1:C:268:TRP:HB3	1:C:273:ARG:HH21	1.58	0.68
1:A:175:ASP:OD1	2:A:400:A7R:O04	2.11	0.68
1:A:275:GLN:HG3	1:A:275:GLN:O	1.93	0.68
1:D:210:MET:CE	1:D:215:LEU:HG	2.25	0.67
1:B:111:LEU:HG	1:B:259:ALA:HB1	1.78	0.66
1:D:179:LEU:HD22	1:D:180:ASN:HD22	1.37	0.65
1:B:153:MET:H	1:B:175:ASP:HB2	1.60	0.65
1:B:214:THR:HB	1:B:217:LEU:HD12	1.75	0.65
1:A:240:VAL:HG13	1:A:241:VAL:HG23	1.79	0.65
1:D:180:ASN:HD21	1:D:183:GLN:HB2	1.61	0.65
1:A:179:LEU:CD2	1:A:183:GLN:HB2	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ARG:HH11	1:C:273:ARG:CG	2.06	0.64
1:D:152:GLY:HA3	1:D:208:VAL:HG13	1.77	0.64
1:D:279:LYS:HG3	1:D:282:LEU:HB2	1.79	0.64
1:A:273:ARG:HH11	1:A:273:ARG:CG	2.11	0.64
1:D:210:MET:HE2	1:D:215:LEU:CD2	2.28	0.64
1:B:273:ARG:NH2	1:B:275:GLN:CG	2.36	0.64
1:D:210:MET:SD	1:D:211:ALA:N	2.72	0.63
1:D:250:LEU:HD12	1:D:255:LEU:HB2	1.80	0.63
1:B:84:ASN:O	1:B:88:ARG:HG3	1.98	0.63
1:A:124:ARG:NH2	1:A:285:THR:HB	2.13	0.62
1:C:210:MET:CE	1:C:237:ARG:HD2	2.28	0.62
1:D:67:LYS:NZ	3:D:405:HOH:O	2.30	0.62
1:D:210:MET:HE2	1:D:211:ALA:O	2.00	0.62
1:A:273:ARG:HH12	1:A:274:PRO:C	2.02	0.62
1:D:213:GLU:O	1:D:214:THR:CB	2.47	0.62
1:C:269:ILE:HG22	1:C:269:ILE:O	1.99	0.61
1:D:215:LEU:HD12	1:D:239:SER:OG	1.99	0.61
1:C:210:MET:HG2	1:C:237:ARG:CD	2.30	0.61
1:B:236:CYS:SG	1:B:240:VAL:HG21	2.40	0.61
1:C:268:TRP:N	1:C:273:ARG:HE	1.98	0.61
1:D:210:MET:HE2	1:D:215:LEU:HG	1.81	0.61
1:D:180:ASN:ND2	1:D:180:ASN:O	2.33	0.61
1:C:273:ARG:HG3	1:C:273:ARG:NH1	2.03	0.61
1:B:243:GLU:O	1:B:247:ILE:HG13	2.00	0.61
1:C:273:ARG:NH1	1:C:274:PRO:O	2.34	0.60
1:D:198:LEU:HD23	1:D:226:MET:HG3	1.84	0.60
1:A:270:ARG:CZ	1:A:272:ASP:HB2	2.31	0.60
1:B:198:LEU:O	1:B:226:MET:HA	2.01	0.60
1:C:151:ARG:HH12	1:C:208:VAL:HG22	1.66	0.60
1:A:198:LEU:HD22	1:A:225:LYS:HE2	1.84	0.59
1:B:176:ARG:HH21	1:B:176:ARG:CG	2.12	0.59
1:B:214:THR:HG21	2:B:400:A7R:N04	2.18	0.59
1:C:90:GLY:HA2	1:C:329:PRO:HB2	1.85	0.59
1:B:208:VAL:HG23	1:B:240:VAL:HG11	1.83	0.59
1:D:210:MET:HA	1:D:215:LEU:CD2	2.30	0.59
1:B:178:PRO:HB3	1:B:191:ARG:HE	1.68	0.59
1:B:215:LEU:O	1:B:217:LEU:N	2.36	0.59
1:B:151:ARG:HB3	1:B:206:PRO:HA	1.83	0.59
1:B:175:ASP:OD1	1:B:176:ARG:N	2.35	0.58
1:D:179:LEU:HD23	1:D:180:ASN:N	2.19	0.58
1:C:214:THR:HG22	1:C:214:THR:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:MET:H	1:C:237:ARG:HH12	1.43	0.58
1:D:198:LEU:O	1:D:226:MET:HA	2.03	0.57
1:B:176:ARG:HG3	1:B:176:ARG:NH2	2.15	0.57
1:C:238:GLY:HA3	1:C:263:PHE:O	2.04	0.57
1:D:151:ARG:HE	1:D:217:LEU:HD11	1.69	0.57
1:B:215:LEU:H	1:B:215:LEU:HD23	1.69	0.57
1:A:213:GLU:HG3	1:A:214:THR:HG23	1.87	0.57
1:D:213:GLU:O	1:D:214:THR:HG23	2.05	0.56
1:B:18:LEU:HD21	1:B:311:MET:HE3	1.87	0.56
1:A:198:LEU:HD11	1:A:222:ALA:HB1	1.86	0.56
1:A:229:GLY:N	1:A:254:LYS:O	2.35	0.56
1:B:265:MET:HA	1:B:274:PRO:HD2	1.86	0.56
1:A:203:TYR:HD1	1:A:231:TYR:HB2	1.68	0.56
1:D:210:MET:HE2	1:D:215:LEU:CG	2.36	0.56
1:B:176:ARG:HH22	2:B:400:A7R:C19	2.19	0.56
1:A:151:ARG:HH21	1:A:217:LEU:HD11	1.71	0.55
1:A:174:CYS:HA	1:A:191:ARG:NH1	2.22	0.55
1:B:203:TYR:HD1	1:B:231:TYR:HB2	1.71	0.55
1:B:187:TRP:HB2	1:B:189:VAL:HG23	1.88	0.55
1:B:252:SER:O	3:B:502:HOH:O	2.17	0.55
1:A:198:LEU:HD21	1:A:222:ALA:O	2.06	0.55
1:C:226:MET:O	1:C:254:LYS:NZ	2.38	0.55
1:D:216:HIS:NE2	1:D:264:GLU:OE1	2.41	0.54
1:A:115:LEU:HD21	1:A:231:TYR:CD2	2.36	0.54
1:D:239:SER:HA	1:D:264:GLU:HG3	1.90	0.54
1:D:250:LEU:HD23	1:D:284:ASN:ND2	2.23	0.54
1:D:273:ARG:CZ	1:D:274:PRO:CD	2.85	0.54
1:B:151:ARG:HH22	2:B:400:A7R:C19	2.21	0.53
1:B:237:ARG:O	1:B:262:VAL:HG22	2.08	0.53
1:D:267:GLU:O	1:D:273:ARG:HG3	2.09	0.53
1:B:279:LYS:HD2	1:B:282:LEU:HD12	1.90	0.52
1:D:93:LEU:HD23	1:D:326:ILE:HD11	1.91	0.52
1:A:236:CYS:HA	2:A:400:A7R:O05	2.08	0.52
1:C:188:HIS:ND1	3:C:405:HOH:O	2.34	0.52
1:D:232:LEU:HD23	1:D:258:TYR:CE1	2.45	0.52
1:B:121:GLU:OE1	3:B:503:HOH:O	2.19	0.52
1:B:215:LEU:CG	1:B:216:HIS:N	2.73	0.52
1:A:247:ILE:HD11	1:A:280:ALA:HB3	1.91	0.52
1:A:273:ARG:HB3	1:A:273:ARG:NH1	2.17	0.52
1:A:270:ARG:NE	1:A:272:ASP:CB	2.73	0.52
1:C:180:ASN:HB3	1:C:183:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HH21	1:A:275:GLN:NE2	2.08	0.51
1:B:216:HIS:CD2	1:B:242:ASP:HB2	2.45	0.51
1:B:326:ILE:HB	1:D:177:ILE:HD13	1.90	0.51
1:D:87:THR:HA	1:D:329:PRO:HB3	1.93	0.51
1:B:96:VAL:HG21	1:B:305:ILE:HG23	1.93	0.51
1:B:174:CYS:HB2	1:B:197:LEU:HD13	1.92	0.51
1:A:244:ASN:O	1:A:247:ILE:HG22	2.11	0.51
1:C:210:MET:HG2	1:C:237:ARG:HD3	1.91	0.51
1:B:123:ASP:O	1:B:127:ARG:HG2	2.10	0.51
1:C:121:GLU:OE2	3:C:403:HOH:O	2.19	0.51
1:C:196:GLU:OE1	3:C:402:HOH:O	2.19	0.51
1:C:268:TRP:HA	1:C:273:ARG:CD	2.39	0.51
1:B:302:ARG:HG3	1:C:139:TYR:CE1	2.46	0.51
1:C:203:TYR:HD1	1:C:231:TYR:HB2	1.76	0.51
1:A:183:GLN:OE1	1:A:183:GLN:N	2.44	0.51
1:D:205:VAL:HG12	1:D:233:ILE:HB	1.93	0.51
1:D:272:ASP:O	1:D:273:ARG:HD2	2.10	0.50
1:A:188:HIS:ND1	1:A:188:HIS:N	2.59	0.50
1:D:92:TRP:HH2	1:D:321:LYS:HD3	1.77	0.50
1:D:213:GLU:C	1:D:214:THR:HG23	2.30	0.50
1:D:247:ILE:HD13	1:D:280:ALA:HB3	1.93	0.50
1:A:115:LEU:CD2	1:A:231:TYR:HD2	2.22	0.50
1:B:46:ALA:O	1:B:68:LEU:HD23	2.12	0.50
1:B:215:LEU:HD23	1:B:215:LEU:N	2.27	0.50
1:A:180:ASN:OD1	1:A:181:ALA:N	2.44	0.50
1:B:103:PRO:HB2	1:B:296:SER:HA	1.93	0.50
1:B:273:ARG:NH2	1:B:275:GLN:NE2	2.60	0.50
1:C:244:ASN:HA	1:C:247:ILE:HD12	1.94	0.49
1:D:90:GLY:HA2	1:D:329:PRO:HB2	1.94	0.49
1:D:44:LYS:O	1:D:66:PRO:HD2	2.12	0.49
1:D:270:ARG:HD2	1:D:271:ALA:H	1.77	0.49
1:A:195:ASP:CG	1:A:225:LYS:HE3	2.32	0.49
1:D:120:LEU:HD21	1:D:289:PHE:CE1	2.48	0.49
1:A:273:ARG:CG	1:A:273:ARG:NH1	2.71	0.49
1:B:273:ARG:NH2	1:B:275:GLN:CD	2.66	0.49
1:D:223:LEU:HD23	1:D:226:MET:CE	2.43	0.49
1:A:237:ARG:O	1:A:240:VAL:HG12	2.13	0.49
1:B:154:GLY:O	1:B:158:ARG:HG3	2.13	0.49
1:A:123:ASP:O	1:A:127:ARG:HG2	2.13	0.48
1:A:57:ILE:HG21	1:A:71:ILE:HD13	1.95	0.48
1:C:267:GLU:O	1:C:273:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:GLU:O	1:D:214:THR:CG2	2.61	0.48
1:D:259:ALA:HA	1:D:289:PHE:O	2.13	0.48
1:C:210:MET:HB3	1:C:237:ARG:NE	2.28	0.48
1:C:267:GLU:O	1:C:273:ARG:CD	2.61	0.48
1:D:300:GLU:CD	1:D:300:GLU:H	2.17	0.48
1:B:111:LEU:HD13	1:C:119:MET:CE	2.43	0.48
1:D:232:LEU:HD23	1:D:258:TYR:CD1	2.48	0.48
1:B:153:MET:SD	1:B:158:ARG:HG2	2.53	0.48
1:B:206:PRO:HD2	1:B:233:ILE:O	2.14	0.48
1:D:11:VAL:HG12	1:D:306:GLU:HG2	1.96	0.48
1:C:173:TYR:HD1	1:C:189:VAL:HG22	1.79	0.48
1:D:180:ASN:ND2	1:D:180:ASN:N	2.60	0.48
1:D:236:CYS:SG	1:D:237:ARG:N	2.87	0.47
1:A:213:GLU:HG2	1:A:214:THR:H	1.78	0.47
1:A:180:ASN:HD22	1:A:183:GLN:NE2	2.09	0.47
1:C:210:MET:CG	1:C:237:ARG:HD2	2.44	0.47
1:B:270:ARG:HD2	1:B:271:ALA:H	1.80	0.47
1:B:273:ARG:HH21	1:B:275:GLN:NE2	2.13	0.47
1:B:18:LEU:HD21	1:B:311:MET:CE	2.44	0.47
1:D:204:VAL:HG21	1:D:226:MET:SD	2.54	0.47
1:A:195:ASP:OD1	1:A:225:LYS:HE3	2.15	0.47
1:A:213:GLU:HG2	1:A:214:THR:N	2.29	0.47
1:D:210:MET:CE	1:D:215:LEU:CG	2.93	0.47
1:A:270:ARG:HG3	1:A:272:ASP:H	1.78	0.46
1:B:65:CYS:HB3	1:B:68:LEU:HG	1.97	0.46
1:B:236:CYS:HB2	2:B:400:A7R:O05	2.16	0.46
1:A:326:ILE:O	1:A:326:ILE:HG13	2.14	0.46
1:D:258:TYR:O	1:D:288:THR:HA	2.16	0.46
1:A:115:LEU:CD2	1:A:231:TYR:CD2	2.97	0.46
1:B:215:LEU:CD2	1:B:215:LEU:N	2.73	0.46
1:D:197:LEU:O	1:D:201:CYS:HB2	2.16	0.46
1:A:96:VAL:HG21	1:A:305:ILE:HG23	1.98	0.46
1:A:158:ARG:HG2	1:A:187:TRP:CZ3	2.50	0.46
1:B:251:ALA:HB3	3:B:504:HOH:O	2.16	0.46
1:A:223:LEU:HD22	1:A:255:LEU:HD23	1.97	0.46
1:B:151:ARG:NH2	2:B:400:A7R:C19	2.79	0.46
1:C:292:PRO:HD2	1:C:294:LEU:HG	1.97	0.46
1:B:282:LEU:HD22	1:C:127:ARG:HA	1.97	0.46
1:C:154:GLY:O	1:C:158:ARG:HD3	2.16	0.46
1:A:151:ARG:HH12	2:A:400:A7R:C19	2.29	0.46
1:A:258:TYR:O	1:A:288:THR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PRO:HD2	1:A:274:PRO:O	2.16	0.46
1:C:40:ILE:HD11	1:C:61:PHE:CD2	2.50	0.45
1:D:223:LEU:HA	1:D:226:MET:HE2	1.99	0.45
1:C:143:LEU:HD23	1:C:143:LEU:HA	1.71	0.45
1:C:270:ARG:HD2	1:C:270:ARG:HA	1.55	0.45
1:A:179:LEU:CD2	1:A:180:ASN:N	2.65	0.45
1:A:247:ILE:CD1	1:A:281:LEU:HG	2.47	0.45
1:A:273:ARG:HH22	1:A:275:GLN:CB	2.28	0.45
1:B:118:HIS:HB3	1:B:138:LEU:HD22	1.98	0.45
1:D:210:MET:HE3	1:D:215:LEU:HG	1.96	0.45
1:D:180:ASN:ND2	1:D:180:ASN:C	2.68	0.45
1:D:279:LYS:HA	1:D:282:LEU:HB2	1.99	0.45
1:A:21:ALA:HB3	3:A:527:HOH:O	2.16	0.45
1:B:215:LEU:O	1:B:240:VAL:CA	2.57	0.45
1:C:180:ASN:HB3	1:C:183:GLN:CD	2.37	0.45
1:C:265:MET:HB3	1:C:274:PRO:HB2	1.99	0.45
1:D:213:GLU:O	1:D:213:GLU:HG3	2.18	0.44
1:B:215:LEU:HG	1:B:216:HIS:N	2.21	0.44
1:D:236:CYS:SG	1:D:240:VAL:HG21	2.57	0.44
1:A:44:LYS:HG2	1:A:64:GLU:O	2.17	0.44
1:A:308:GLN:HE21	1:A:323:MET:CE	2.30	0.44
1:B:173:TYR:HD1	1:B:189:VAL:HG12	1.82	0.44
1:D:273:ARG:HH12	1:D:274:PRO:HD2	1.74	0.44
1:B:80:ASN:OD1	1:B:80:ASN:N	2.48	0.44
1:B:124:ARG:HB2	1:B:124:ARG:HH11	1.83	0.44
1:C:123:ASP:O	1:C:127:ARG:HG2	2.18	0.44
1:D:210:MET:HA	1:D:215:LEU:HD22	2.00	0.44
1:C:300:GLU:H	1:C:300:GLU:CD	2.21	0.44
1:B:120:LEU:HB3	3:B:503:HOH:O	2.18	0.44
1:B:185:LYS:N	1:B:185:LYS:HD2	2.33	0.44
1:C:210:MET:CG	1:C:237:ARG:CD	2.95	0.44
1:D:80:ASN:OD1	1:D:269:ILE:HD11	2.18	0.44
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.76	0.44
1:B:243:GLU:HG3	1:B:264:GLU:OE1	2.18	0.44
1:B:176:ARG:CG	1:B:176:ARG:NH2	2.73	0.43
1:A:192:VAL:HG13	1:A:197:LEU:HB2	2.00	0.43
1:D:223:LEU:HD23	1:D:226:MET:HE1	2.00	0.43
1:A:237:ARG:HG3	1:A:238:GLY:H	1.82	0.43
1:D:111:LEU:HD12	1:D:235:ALA:HB2	2.00	0.43
1:D:210:MET:O	1:D:215:LEU:HD22	2.05	0.43
1:A:16:ILE:HG23	1:A:25:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ASP:O	1:C:191:ARG:NH2	2.28	0.43
1:D:213:GLU:CD	1:D:214:THR:HG23	2.39	0.43
1:B:210:MET:HB3	1:B:237:ARG:NE	2.33	0.43
1:D:210:MET:O	1:D:214:THR:OG1	2.36	0.43
1:D:219:ASP:OD1	1:D:221:THR:N	2.52	0.43
1:D:279:LYS:HG2	1:D:283:ASP:OD2	2.19	0.43
1:A:235:ALA:O	2:A:400:A7R:N02	2.52	0.43
1:A:237:ARG:N	2:A:400:A7R:O06	2.52	0.42
1:A:270:ARG:CG	1:A:272:ASP:O	2.63	0.42
1:C:267:GLU:C	1:C:269:ILE:N	2.71	0.42
1:B:247:ILE:HD11	1:B:281:LEU:HG	2.02	0.42
1:D:96:VAL:HG21	1:D:305:ILE:HG23	2.02	0.42
1:D:205:VAL:HG23	1:D:205:VAL:O	2.19	0.42
1:D:273:ARG:NH2	1:D:274:PRO:C	2.73	0.42
1:A:194:LEU:O	1:A:198:LEU:HB3	2.20	0.42
1:A:198:LEU:CD2	1:A:225:LYS:HG3	2.50	0.42
1:C:267:GLU:C	1:C:269:ILE:H	2.22	0.42
1:D:272:ASP:O	1:D:273:ARG:HG2	2.19	0.42
1:A:223:LEU:HD12	1:A:245:ALA:HB1	2.00	0.42
1:A:273:ARG:NH2	1:A:275:GLN:CD	2.73	0.42
1:B:68:LEU:O	1:B:91:VAL:HG22	2.19	0.42
1:B:124:ARG:HH11	1:B:124:ARG:CB	2.32	0.42
1:A:97:PRO:HD2	1:A:308:GLN:OE1	2.20	0.42
1:A:192:VAL:CG1	1:A:197:LEU:HB2	2.49	0.42
1:A:250:LEU:HD13	1:A:284:ASN:OD1	2.19	0.41
1:B:176:ARG:NH2	2:B:400:A7R:C19	2.82	0.41
1:D:191:ARG:O	1:D:192:VAL:HG13	2.20	0.41
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.88	0.41
1:A:143:LEU:N	3:A:501:HOH:O	2.17	0.41
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.94	0.41
1:B:210:MET:HB2	1:B:237:ARG:HG2	2.01	0.41
1:B:44:LYS:HG3	1:B:64:GLU:O	2.21	0.41
1:B:210:MET:HB3	1:B:237:ARG:HE	1.85	0.41
1:B:210:MET:CB	1:B:237:ARG:HE	2.34	0.41
1:C:213:GLU:CG	1:C:214:THR:N	2.72	0.41
1:C:210:MET:SD	1:C:237:ARG:HD2	2.61	0.41
1:D:123:ASP:O	1:D:127:ARG:HG2	2.21	0.41
1:C:225:LYS:HE3	1:C:225:LYS:HB2	1.75	0.41
1:A:273:ARG:NH1	1:A:274:PRO:C	2.71	0.41
1:B:74:ALA:HB1	1:B:305:ILE:HG22	2.03	0.41
1:B:215:LEU:H	1:B:215:LEU:HD22	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:HD13	1:C:269:ILE:HA	1.94	0.41
1:D:137:THR:HG23	1:D:138:LEU:HG	2.02	0.41
1:B:228:THR:HA	1:B:254:LYS:HD3	2.03	0.41
1:D:206:PRO:HD2	1:D:233:ILE:O	2.21	0.41
1:A:255:LEU:HD12	1:A:255:LEU:C	2.41	0.40
1:D:153:MET:HE3	1:D:173:TYR:HB2	2.03	0.40
1:B:281:LEU:HA	1:B:281:LEU:HD23	1.80	0.40
1:D:227:LYS:C	1:D:254:LYS:HE3	2.41	0.40
1:D:237:ARG:O	1:D:240:VAL:HG22	2.20	0.40
1:A:179:LEU:CD2	1:A:180:ASN:ND2	2.84	0.40
1:B:5:VAL:HA	1:B:48:ALA:O	2.21	0.40
1:B:152:GLY:O	1:B:207:ALA:HB3	2.21	0.40
1:B:176:ARG:HH22	2:B:400:A7R:C17	2.34	0.40
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.93	0.40
1:D:53:MET:HB3	1:D:54:PRO:HD3	2.03	0.40
1:D:216:HIS:HB3	1:D:242:ASP:HB2	2.04	0.40
1:A:272:ASP:O	1:A:273:ARG:HB2	2.21	0.40
1:B:1:MET:O	1:B:1:MET:CG	2.70	0.40
1:B:10:TRP:HB2	1:B:30:THR:O	2.22	0.40
1:B:173:TYR:CZ	1:B:191:ARG:HD3	2.56	0.40
1:D:184:GLU:OE1	1:D:191:ARG:HG2	2.21	0.40
1:D:198:LEU:HD21	1:D:222:ALA:HB1	2.03	0.40
1:D:306:GLU:OE1	3:D:403:HOH:O	2.22	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	328/338 (97%)	312 (95%)	13 (4%)	3 (1%)	17 31
1	B	328/338 (97%)	312 (95%)	15 (5%)	1 (0%)	41 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	328/338 (97%)	309 (94%)	17 (5%)	2 (1%)	25 43
1	D	328/338 (97%)	303 (92%)	21 (6%)	4 (1%)	13 24
All	All	1312/1352 (97%)	1236 (94%)	66 (5%)	10 (1%)	19 35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	PRO
1	A	188	HIS
1	D	214	THR
1	D	274	PRO
1	D	211	ALA
1	A	180	ASN
1	C	212	ALA
1	A	236	CYS
1	D	265	MET
1	C	274	PRO

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	265/270 (98%)	258 (97%)	7 (3%)	46 72
1	B	265/270 (98%)	257 (97%)	8 (3%)	41 68
1	C	265/270 (98%)	255 (96%)	10 (4%)	33 58
1	D	265/270 (98%)	259 (98%)	6 (2%)	50 76
All	All	1060/1080 (98%)	1029 (97%)	31 (3%)	42 69

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	185	LYS

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Mol	Chain	Res	Type
1	A	187	TRP
1	A	188	HIS
1	A	216	HIS
1	A	272	ASP
1	A	273	ARG
1	B	30	THR
1	B	111	LEU
1	B	185	LYS
1	B	190	GLN
1	B	191	ARG
1	B	215	LEU
1	B	236	CYS
1	B	273	ARG
1	C	59	SER
1	C	176	ARG
1	C	201	CYS
1	C	213	GLU
1	C	237	ARG
1	C	268	TRP
1	C	270	ARG
1	C	273	ARG
1	C	275	GLN
1	C	289	PHE
1	D	137	THR
1	D	151	ARG
1	D	174	CYS
1	D	180	ASN
1	D	201	CYS
1	D	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	287	GLN
1	A	308	GLN
1	A	327	ASN
1	B	180	ASN
1	C	132	GLN
1	D	125	GLN
1	D	180	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

2 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	A7R	B	400	-	43,45,45	3.53	19 (44%)	59,68,68	2.43	23 (38%)
2	A7R	A	400	-	43,45,45	3.54	22 (51%)	59,68,68	2.36	17 (28%)

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	A7R	B	400	-	-	17/30/62/62	0/4/4/4
2	A7R	A	400	-	-	18/30/62/62	0/4/4/4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	A7R	C06-C05	-10.21	1.25	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	A7R	C06-C05	-10.05	1.26	1.53
2	A	400	A7R	C16-N02	7.73	1.47	1.33
2	B	400	A7R	O01-C03	7.72	1.62	1.45
2	A	400	A7R	O01-C03	7.68	1.62	1.45
2	B	400	A7R	C16-N02	7.37	1.46	1.33
2	B	400	A7R	P02-O09	7.21	1.67	1.59
2	A	400	A7R	O02-C08	-6.59	1.32	1.40
2	A	400	A7R	C01-C03	-6.12	1.37	1.53
2	A	400	A7R	P02-O09	6.06	1.66	1.59
2	B	400	A7R	O02-C08	-6.00	1.33	1.40
2	B	400	A7R	C01-C03	-5.95	1.37	1.53
2	A	400	A7R	C20-N04	4.93	1.45	1.33
2	B	400	A7R	C20-N04	4.91	1.45	1.33
2	B	400	A7R	P01-O09	4.84	1.64	1.59
2	B	400	A7R	O01-C04	-4.60	1.31	1.42
2	A	400	A7R	P01-O09	4.57	1.64	1.59
2	A	400	A7R	C13-C16	4.25	1.56	1.50
2	A	400	A7R	O02-C07	4.14	1.54	1.45
2	A	400	A7R	O01-C04	-4.06	1.32	1.42
2	B	400	A7R	C13-C16	4.05	1.56	1.50
2	B	400	A7R	O02-C07	3.99	1.53	1.45
2	A	400	A7R	O05-C05	3.21	1.50	1.43
2	B	400	A7R	O04-C02	-3.20	1.35	1.43
2	A	400	A7R	O04-C02	-3.18	1.35	1.43
2	A	400	A7R	C10-C07	-3.15	1.42	1.51
2	B	400	A7R	O05-C05	2.97	1.50	1.43
2	A	400	A7R	C18-N03	-2.89	1.34	1.40
2	B	400	A7R	C10-C07	-2.85	1.43	1.51
2	A	400	A7R	O15-C18	-2.75	1.18	1.23
2	B	400	A7R	O15-C18	-2.69	1.18	1.23
2	B	400	A7R	O03-C01	2.61	1.49	1.43
2	B	400	A7R	P01-O07	2.44	1.69	1.59
2	A	400	A7R	C02-C04	2.41	1.61	1.53
2	A	400	A7R	P01-O07	2.40	1.68	1.59
2	A	400	A7R	O03-C01	2.39	1.48	1.43
2	B	400	A7R	C11-C13	2.30	1.42	1.39
2	B	400	A7R	C18-N03	-2.18	1.35	1.40
2	A	400	A7R	C18-N05	-2.09	1.32	1.36
2	A	400	A7R	O14-C16	-2.02	1.20	1.24
2	A	400	A7R	C17-N03	-2.02	1.33	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	A7R	C03-O01-C04	-7.35	93.25	109.47
2	A	400	A7R	C03-O01-C04	-6.73	94.60	109.47
2	A	400	A7R	C13-C16-N02	6.16	125.33	117.74
2	B	400	A7R	O01-C04-N03	5.82	121.55	108.36
2	A	400	A7R	O01-C04-N03	5.38	120.54	108.36
2	B	400	A7R	C04-N03-C18	4.84	129.13	118.44
2	B	400	A7R	O15-C18-N05	-4.65	115.01	122.33
2	A	400	A7R	C07-O02-C08	-4.62	105.69	109.92
2	B	400	A7R	C04-N03-C17	-4.50	111.17	120.78
2	A	400	A7R	O14-C16-N02	-4.38	116.29	122.62
2	B	400	A7R	C07-O02-C08	-4.30	105.99	109.92
2	B	400	A7R	O14-C16-N02	-4.13	116.65	122.62
2	B	400	A7R	C13-C16-N02	4.05	122.73	117.74
2	A	400	A7R	O15-C18-N05	-3.99	116.04	122.33
2	A	400	A7R	C04-N03-C18	3.91	127.08	118.44
2	B	400	A7R	C12-N01-C11	-3.60	118.82	121.88
2	A	400	A7R	C12-N01-C11	-3.51	118.89	121.88
2	A	400	A7R	C04-N03-C17	-3.46	113.38	120.78
2	A	400	A7R	C02-C04-N03	3.46	122.88	113.25
2	A	400	A7R	O05-C05-C07	-3.17	101.97	111.08
2	A	400	A7R	O04-C02-C04	3.14	120.91	110.10
2	B	400	A7R	O07-P01-O10	3.11	121.27	108.94
2	A	400	A7R	O07-P01-O10	3.10	121.23	108.94
2	B	400	A7R	C11-N01-C08	3.09	125.96	119.13
2	A	400	A7R	C10-C07-C05	-2.99	104.43	115.21
2	B	400	A7R	C11-C13-C16	2.96	127.99	119.46
2	B	400	A7R	O05-C05-C07	-2.83	102.97	111.08
2	A	400	A7R	C11-C13-C16	2.66	127.12	119.46
2	B	400	A7R	O01-C04-C02	-2.64	100.97	106.62
2	A	400	A7R	C11-N01-C08	2.48	124.60	119.13
2	B	400	A7R	C02-C04-N03	2.48	120.14	113.25
2	B	400	A7R	O08-C10-C07	2.47	117.42	108.99
2	B	400	A7R	C06-C05-C07	2.44	107.33	102.61
2	B	400	A7R	C12-N01-C08	-2.31	115.20	119.73
2	B	400	A7R	C10-C07-C05	-2.28	107.01	115.21
2	B	400	A7R	O04-C02-C04	2.26	117.87	110.10
2	B	400	A7R	O01-C03-C09	2.16	116.27	109.33
2	B	400	A7R	C15-C13-C16	-2.10	115.35	121.06
2	A	400	A7R	C11-C13-C15	-2.01	115.92	118.26
2	B	400	A7R	N03-C18-N05	2.00	122.28	118.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

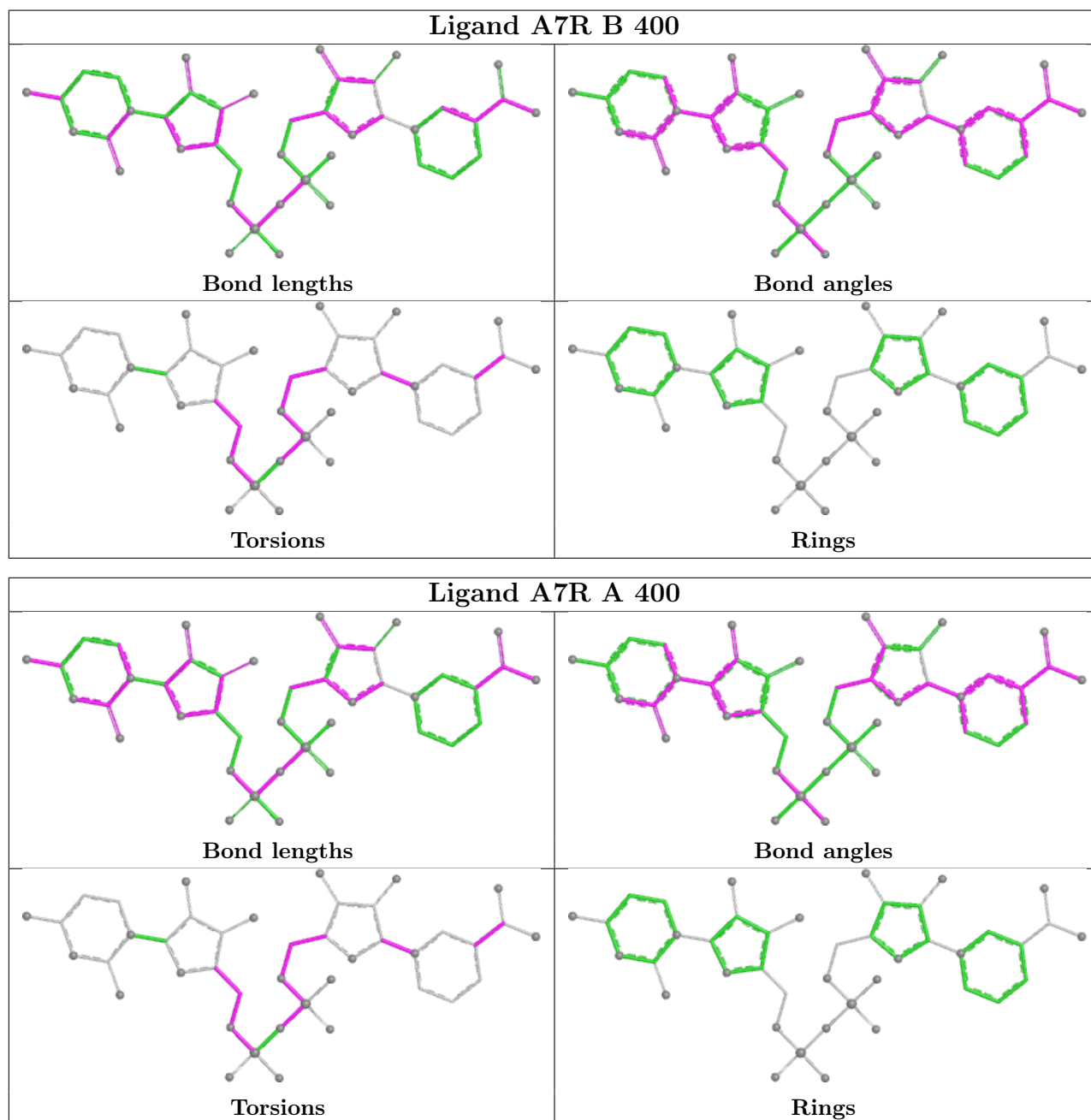
Mol	Chain	Res	Type	Atoms
2	A	400	A7R	O01-C03-C09-O07
2	A	400	A7R	C06-C08-N01-C11
2	A	400	A7R	C06-C08-N01-C12
2	A	400	A7R	C09-O07-P01-O09
2	A	400	A7R	C09-O07-P01-O11
2	A	400	A7R	C10-O08-P02-O09
2	A	400	A7R	C10-O08-P02-O12
2	A	400	A7R	C10-O08-P02-O13
2	B	400	A7R	C01-C03-C09-O07
2	B	400	A7R	C06-C08-N01-C11
2	B	400	A7R	C06-C08-N01-C12
2	B	400	A7R	C09-O07-P01-O09
2	B	400	A7R	C09-O07-P01-O11
2	B	400	A7R	C10-O08-P02-O13
2	A	400	A7R	C01-C03-C09-O07
2	A	400	A7R	C05-C07-C10-O08
2	A	400	A7R	O02-C07-C10-O08
2	B	400	A7R	C05-C07-C10-O08
2	B	400	A7R	O02-C07-C10-O08
2	B	400	A7R	C11-C13-C16-N02
2	B	400	A7R	C11-C13-C16-O14
2	B	400	A7R	C15-C13-C16-N02
2	B	400	A7R	O01-C03-C09-O07
2	B	400	A7R	C15-C13-C16-O14
2	A	400	A7R	C11-C13-C16-O14
2	A	400	A7R	C15-C13-C16-N02
2	A	400	A7R	C11-C13-C16-N02
2	A	400	A7R	C15-C13-C16-O14
2	A	400	A7R	C03-C09-O07-P01
2	B	400	A7R	C07-C10-O08-P02
2	B	400	A7R	C10-O08-P02-O12
2	B	400	A7R	C03-C09-O07-P01
2	A	400	A7R	C07-C10-O08-P02
2	B	400	A7R	P01-O09-P02-O13
2	A	400	A7R	P01-O09-P02-O13

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	A7R	8	0
2	A	400	A7R	5	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 than 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.



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, 95th 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	330/338 (97%)	0.10	13 (3%) 39 42	28, 51, 93, 128	0
1	B	330/338 (97%)	0.11	19 (5%) 23 24	30, 51, 90, 125	0
1	C	330/338 (97%)	0.01	10 (3%) 50 53	28, 43, 83, 118	0
1	D	330/338 (97%)	0.29	24 (7%) 15 15	29, 51, 98, 122	0
All	All	1320/1352 (97%)	0.13	66 (5%) 28 30	28, 49, 94, 128	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	ALA	11.4
1	D	211	ALA	10.0
1	C	268	TRP	9.7
1	D	212	ALA	9.1
1	C	208	VAL	8.7
1	C	271	ALA	7.7
1	D	269	ILE	7.3
1	B	269	ILE	7.1
1	D	214	THR	6.9
1	B	271	ALA	6.7
1	C	209	PRO	6.4
1	D	271	ALA	6.4
1	C	211	ALA	5.9
1	D	268	TRP	5.8
1	C	210	MET	5.2
1	B	208	VAL	5.2
1	D	181	ALA	5.2
1	C	270	ARG	5.1
1	D	210	MET	5.0
1	A	270	ARG	4.8
1	D	274	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	183	GLN	4.5
1	A	268	TRP	4.4
1	A	269	ILE	4.3
1	D	182	GLU	4.0
1	A	215	LEU	4.0
1	B	209	PRO	4.0
1	D	208	VAL	3.9
1	D	209	PRO	3.8
1	B	185	LYS	3.8
1	A	212	ALA	3.6
1	B	268	TRP	3.5
1	D	253	GLY	3.3
1	D	272	ASP	3.3
1	D	172	LEU	3.2
1	D	330	TYR	3.2
1	D	196	GLU	3.1
1	B	272	ASP	3.1
1	B	273	ARG	3.1
1	D	270	ARG	3.0
1	C	272	ASP	2.9
1	A	185	LYS	2.8
1	B	212	ALA	2.8
1	D	187	TRP	2.7
1	B	211	ALA	2.7
1	A	272	ASP	2.6
1	B	177	ILE	2.5
1	A	271	ALA	2.5
1	A	1	MET	2.5
1	B	270	ARG	2.4
1	A	173	TYR	2.4
1	D	218	ILE	2.4
1	D	192	VAL	2.4
1	A	274	PRO	2.4
1	B	216	HIS	2.4
1	D	235	ALA	2.3
1	D	190	GLN	2.3
1	B	180	ASN	2.2
1	A	181	ALA	2.2
1	D	177	ILE	2.2
1	B	240	VAL	2.2
1	C	216	HIS	2.1
1	B	210	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	218	ILE	2.0
1	B	237	ARG	2.0
1	B	267	GLU	2.0

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](#)

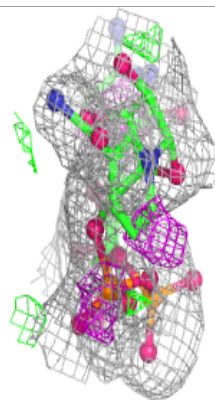
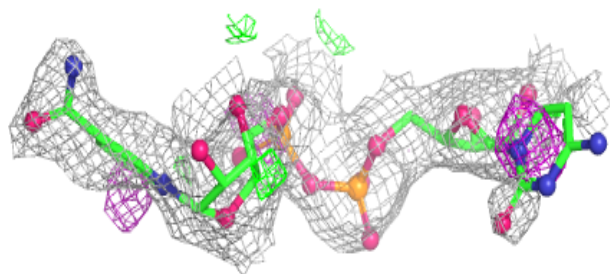
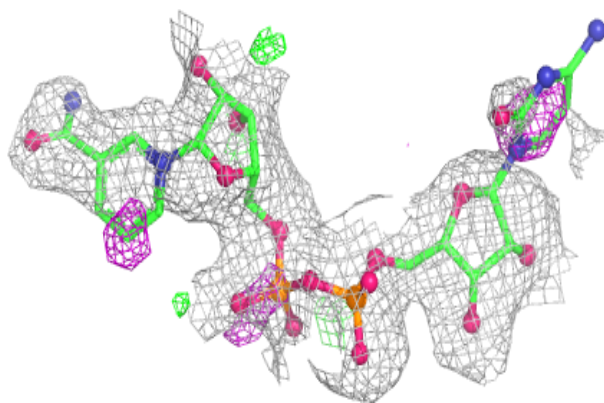
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A7R	B	400	42/42	0.74	0.25	55,85,97,100	0
2	A7R	A	400	42/42	0.82	0.20	53,83,90,93	0

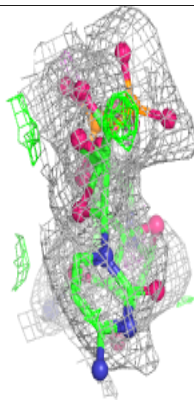
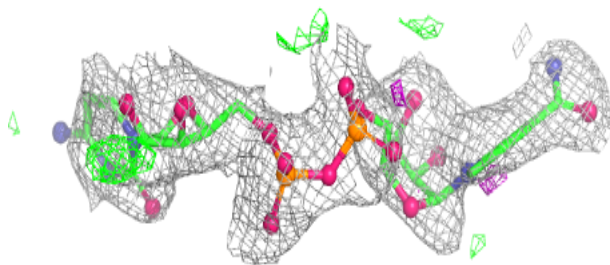
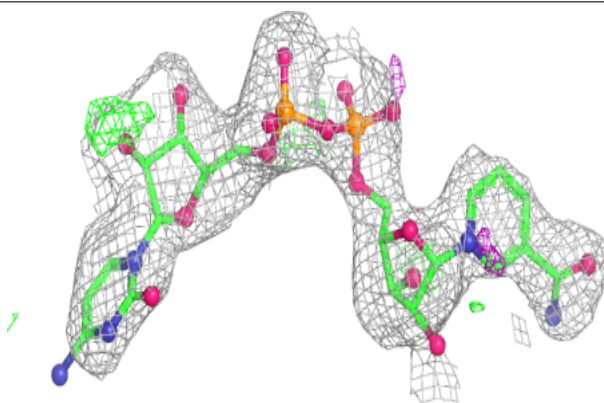
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A7R B 400:

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

**Electron density around A7R A 400:**

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



6.5 Other polymers

There are no such residues in this entry.