Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 06:20 AM EDT

PDB ID	:	1IQP
Title	:	Crystal Structure of the Clamp Loader Small Subunit from Pyrococcus furiosus
Authors	:	Oyama, T.; Ishino, Y.; Cann, I.K.O.; Ishino, S.; Morikawa, K.
Deposited on	:	2001-07-24
Resolution	:	2.80 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:

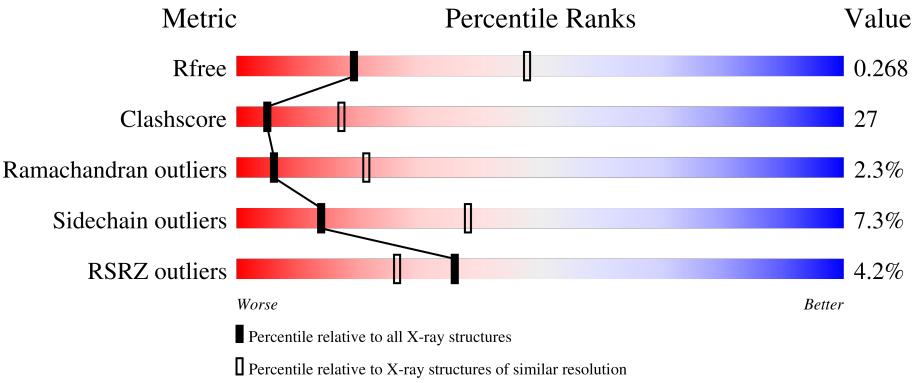
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	327	59% 37%
1	B	327	57% 37% 6%
1	C	327	11% 47% 46% 5%
1	D	327	9% 48% 47% 5%
1	E	327	2% 51% 42% 6%

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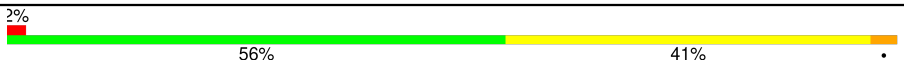
Mol	Chain	Length	Quality of chain
1	F	327	

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	ADP	A	401	-	-	X	X
2	ADP	B	402	-	-	X	-
2	ADP	E	404	-	-	X	-

2 Entry composition (i)

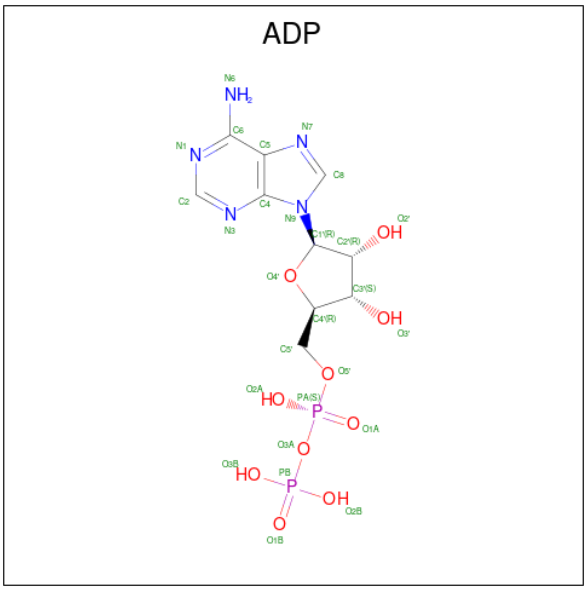
There are 3 unique types of molecules in this entry. The entry contains 16031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RFCS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2623	1670	466	477	10			
1	B	326	Total	C	N	O	S	0	0	0
			2623	1670	466	477	10			
1	C	319	Total	C	N	O	S	0	0	0
			2564	1635	456	463	10			
1	D	326	Total	C	N	O	S	0	0	0
			2623	1670	466	477	10			
1	E	326	Total	C	N	O	S	0	0	0
			2623	1670	466	477	10			
1	F	326	Total	C	N	O	S	0	0	0
			2623	1670	466	477	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

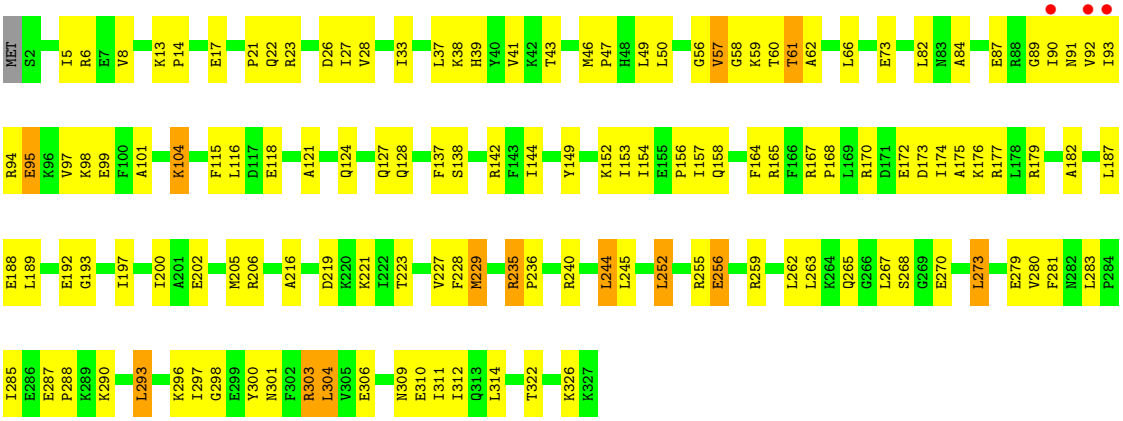
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	60	Total	O	0	0
			60	60		
3	C	25	Total	O	0	0
			25	25		
3	D	13	Total	O	0	0
			13	13		
3	E	33	Total	O	0	0
			33	33		
3	F	36	Total	O	0	0
			36	36		

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.

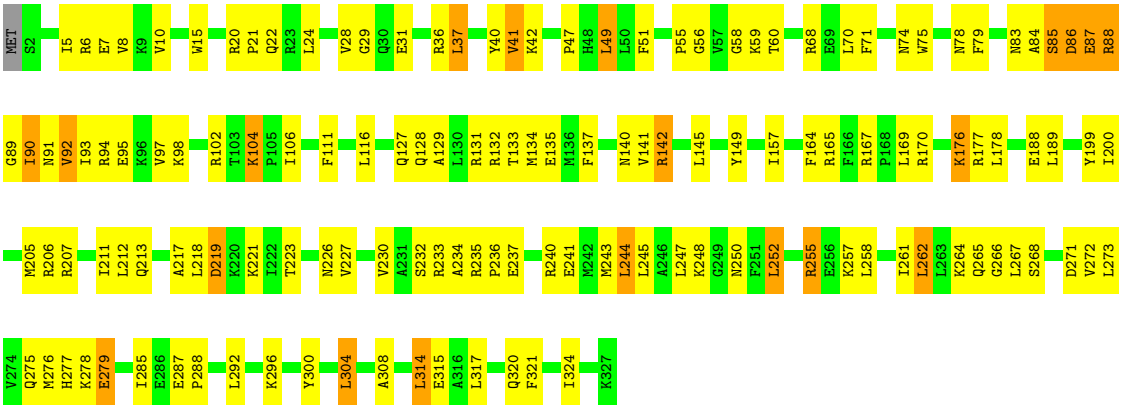
• Molecule 1: RFCS

Chain A:



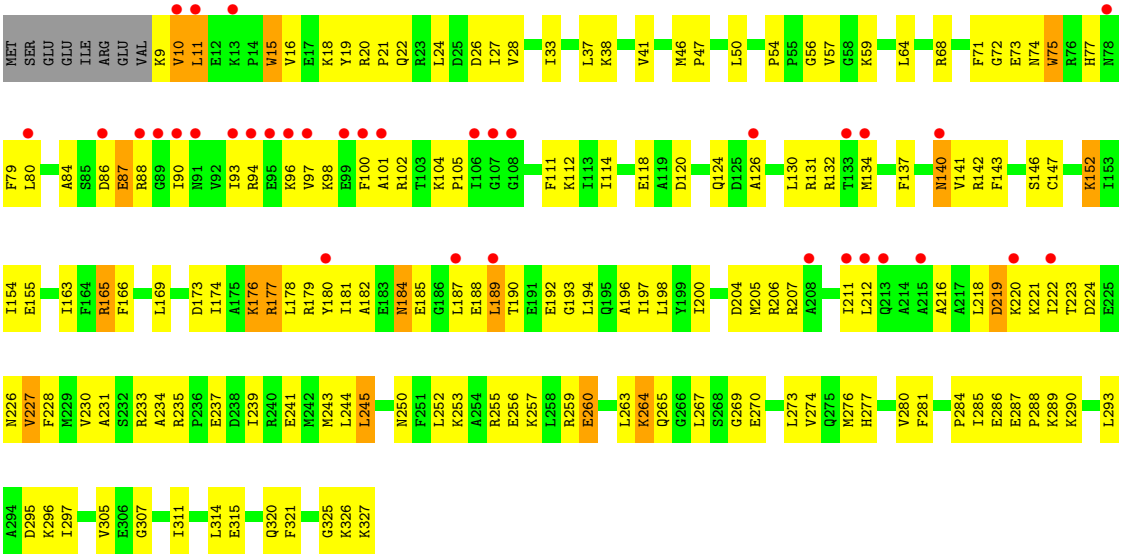
• Molecule 1: RFCS

Chain B:



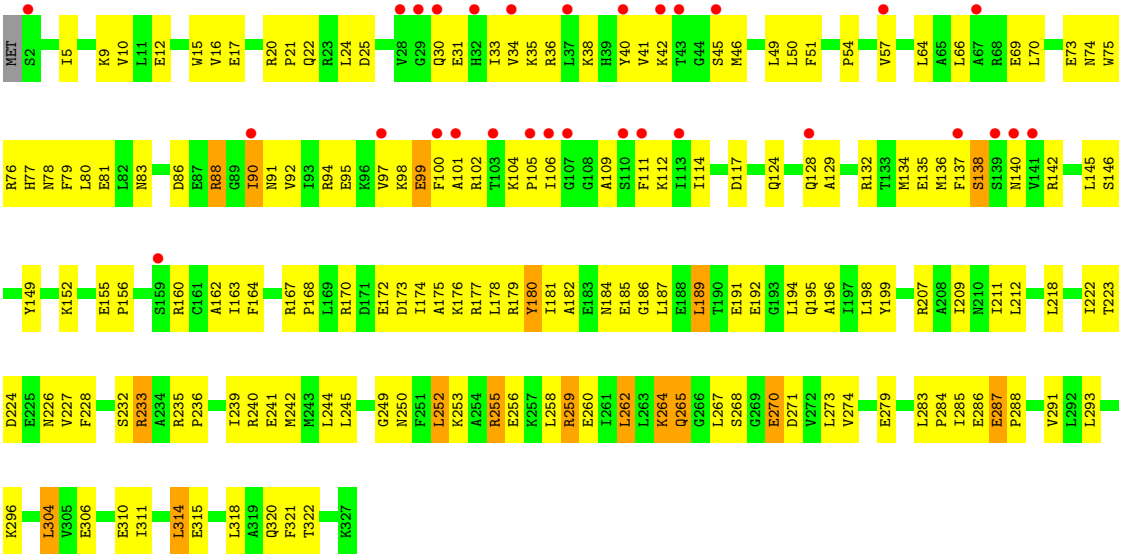
• Molecule 1: RFCS

Chain C:



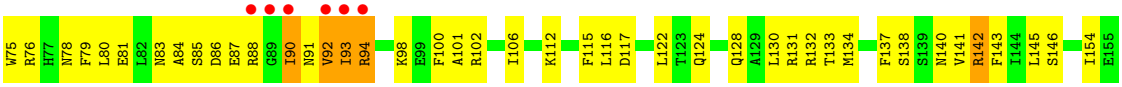
• Molecule 1: RFCS

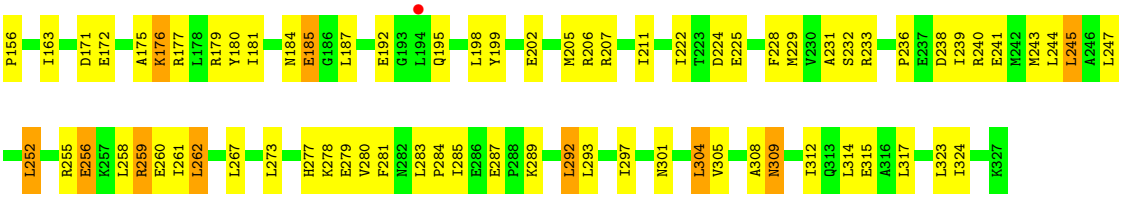
Chain D:



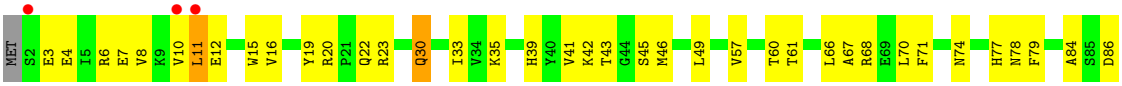
• Molecule 1: RFCS

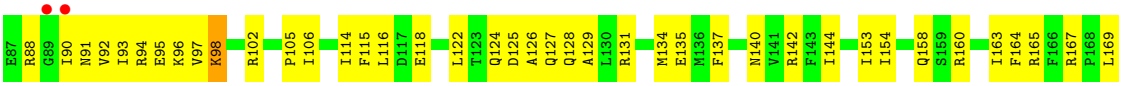
Chain E:

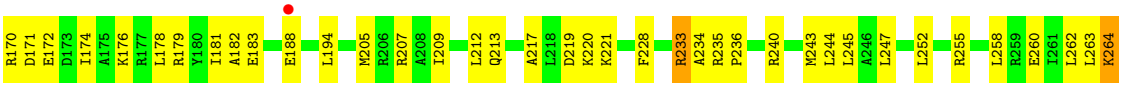


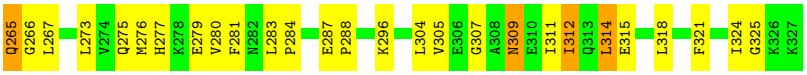


• Molecule 1: RFCS









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.36Å 105.61Å 316.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 65.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.80) 93.0 (65.53-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 2.81Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.224 , 0.277 0.218 , 0.268	Depositor DCC
R_{free} test set	3848 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16031	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: ADP

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	0.41	0/2663	0.61	0/3576
1	B	0.41	0/2663	0.61	0/3576
1	C	0.36	0/2604	0.57	0/3497
1	D	0.36	0/2663	0.53	0/3576
1	E	0.34	0/2663	0.58	0/3576
1	F	0.35	0/2663	0.55	0/3576
All	All	0.37	0/15919	0.58	0/21377

There are no bond length outliers.

There are no bond angle outliers.

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	2623	0	2711	119	0
1	B	2623	0	2711	136	0
1	C	2564	0	2655	179	0
1	D	2623	0	2711	170	0
1	E	2623	0	2711	153	0
1	F	2623	0	2711	146	0
2	A	27	0	12	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	11	0
2	C	27	0	12	7	0
2	E	27	0	12	13	0
3	A	77	0	0	3	0
3	B	60	0	0	1	0
3	C	25	0	0	0	0
3	D	13	0	0	1	0
3	E	33	0	0	0	0
3	F	36	0	0	0	0
All	All	16031	0	16258	867	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 27.

All (867) 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:A:174:ILE:HA	1:A:205:MET:HE1	1.22	1.17
1:D:101:ALA:HA	1:D:112:LYS:HZ1	1.22	1.04
1:F:3:GLU:HB2	1:F:7:GLU:HG3	1.43	1.00
1:E:252:LEU:HD22	1:F:287:GLU:HG3	1.45	0.99
1:A:28:VAL:H	2:A:401:ADP:HN62	0.96	0.96
1:D:105:PRO:HD3	1:D:140:ASN:HD21	1.26	0.96
1:A:28:VAL:H	2:A:401:ADP:N6	1.63	0.95
1:C:105:PRO:HG3	1:C:112:LYS:HG3	1.47	0.95
1:C:177:ARG:HH11	1:C:177:ARG:HB3	1.31	0.94
1:D:170:ARG:HB3	1:D:170:ARG:NH1	1.81	0.94
1:E:87:GLU:HG3	1:E:92:VAL:HG22	1.48	0.94
1:C:28:VAL:H	2:C:403:ADP:HN62	1.08	0.94
1:F:127:GLN:HE22	1:F:154:ILE:H	1.16	0.94
1:F:94:ARG:HD3	1:F:129:ALA:HB1	1.51	0.93
1:D:105:PRO:HG3	1:D:112:LYS:HG3	1.48	0.92
1:D:170:ARG:HB2	1:D:173:ASP:HB2	1.49	0.91
1:B:83:ASN:HD21	1:B:85:SER:HB3	1.35	0.91
1:F:3:GLU:HB3	1:F:6:ARG:HB2	1.54	0.88
1:D:252:LEU:HD22	1:E:287:GLU:HG3	1.54	0.87
1:F:233:ARG:HG3	1:F:233:ARG:HH11	1.38	0.87
1:D:41:VAL:HA	1:D:70:LEU:HD21	1.55	0.87
1:C:177:ARG:HB3	1:C:177:ARG:NH1	1.89	0.85
1:D:30:GLN:HB3	1:D:33:ILE:HD12	1.58	0.85
1:F:20:ARG:HE	1:F:61:THR:HG22	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:N	2:A:401:ADP:HN62	1.75	0.84
1:E:56:GLY:HA2	2:E:404:ADP:H5'1	1.58	0.83
1:F:20:ARG:NE	1:F:61:THR:HG22	1.93	0.83
1:E:28:VAL:H	2:E:404:ADP:HN62	1.23	0.83
1:A:27:ILE:HD11	1:A:62:ALA:HA	1.59	0.83
1:C:90:ILE:HD13	1:C:126:ALA:HA	1.59	0.83
1:B:56:GLY:HA2	2:B:402:ADP:H5'1	1.61	0.83
1:E:60:THR:HG22	1:E:115:PHE:HZ	1.45	0.82
1:F:127:GLN:NE2	1:F:154:ILE:H	1.78	0.82
1:D:9:LYS:O	1:D:12:GLU:HG2	1.81	0.81
1:D:223:THR:O	1:D:227:VAL:HG13	1.81	0.81
1:D:170:ARG:HB3	1:D:170:ARG:HH11	1.45	0.81
1:D:105:PRO:HB2	1:D:109:ALA:HB3	1.62	0.81
1:A:56:GLY:HA2	2:A:401:ADP:H5'1	1.63	0.80
1:E:78:ASN:HD21	1:E:106:ILE:HG12	1.47	0.80
1:F:219:ASP:OD1	1:F:221:LYS:HG2	1.81	0.80
1:B:78:ASN:HD21	1:B:106:ILE:H	1.30	0.79
1:B:83:ASN:ND2	1:B:85:SER:HB3	1.96	0.79
1:E:84:ALA:HB2	1:E:116:LEU:HD11	1.65	0.79
1:C:192:GLU:HG3	1:C:224:ASP:H	1.48	0.78
1:F:46:MET:HE3	1:F:66:LEU:HD21	1.64	0.77
1:C:252:LEU:H	1:C:252:LEU:HD22	1.49	0.77
1:F:135:GLU:HB2	1:F:160:ARG:HH12	1.49	0.77
1:A:46:MET:O	1:A:142:ARG:HD3	1.85	0.77
1:E:131:ARG:HH12	1:E:132:ARG:HG3	1.48	0.76
1:E:131:ARG:HH11	1:E:131:ARG:HB3	1.51	0.75
1:F:3:GLU:OE2	1:F:220:LYS:HG2	1.85	0.75
1:D:112:LYS:HB2	1:D:112:LYS:NZ	2.00	0.75
1:C:169:LEU:HD12	1:C:205:MET:HB2	1.68	0.75
1:D:232:SER:C	1:D:233:ARG:HD2	2.07	0.75
1:E:131:ARG:HB3	1:E:131:ARG:NH1	2.02	0.75
1:F:11:LEU:HD23	1:F:217:ALA:HB1	1.67	0.75
1:F:6:ARG:O	1:F:10:VAL:HG22	1.86	0.74
1:D:54:PRO:HG2	1:D:168:PRO:HG3	1.69	0.74
1:D:105:PRO:CD	1:D:140:ASN:HD21	1.99	0.74
1:C:182:ALA:HA	1:C:187:LEU:HD12	1.68	0.74
1:F:88:ARG:HE	1:F:92:VAL:HG11	1.52	0.74
1:C:165:ARG:HG2	1:C:165:ARG:HH11	1.53	0.73
1:D:196:ALA:CB	1:D:227:VAL:HG21	2.18	0.73
1:F:169:LEU:HB2	1:F:174:ILE:HD11	1.70	0.73
1:B:116:LEU:HB2	1:B:145:LEU:HD23	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ARG:HH21	1:D:129:ALA:HB1	1.53	0.73
1:A:59:LYS:HB2	2:A:401:ADP:O2B	1.86	0.73
1:D:244:LEU:HD13	1:D:283:LEU:HD22	1.70	0.73
1:C:22:GLN:HG2	1:C:68:ARG:HH12	1.53	0.73
1:C:50:LEU:HD23	1:C:163:ILE:HD12	1.69	0.73
1:F:6:ARG:HB3	1:F:220:LYS:NZ	2.03	0.73
1:D:196:ALA:HB1	1:D:227:VAL:HG21	1.71	0.73
1:A:244:LEU:HD13	1:A:283:LEU:HD22	1.71	0.72
1:F:41:VAL:HA	1:F:70:LEU:HD21	1.71	0.72
1:C:311:ILE:O	1:C:315:GLU:HG3	1.89	0.72
1:E:21:PRO:HB3	1:E:26:ASP:HB2	1.70	0.72
1:A:98:LYS:HB3	1:A:98:LYS:NZ	2.04	0.72
1:E:4:GLU:HB3	1:E:8:VAL:CG1	2.20	0.72
1:C:22:GLN:HG2	1:C:68:ARG:NH1	2.04	0.72
1:C:28:VAL:N	2:C:403:ADP:HN62	1.85	0.72
1:B:91:ASN:C	1:B:93:ILE:H	1.93	0.72
1:B:273:LEU:HD23	1:B:276:MET:HE1	1.71	0.71
1:D:41:VAL:HG23	1:D:69:GLU:O	1.91	0.71
1:A:309:ASN:HD22	1:A:312:ILE:H	1.35	0.71
1:F:233:ARG:HG3	1:F:233:ARG:NH1	2.03	0.71
1:E:10:VAL:HG23	1:E:15:TRP:CZ2	2.26	0.71
1:B:15:TRP:H	1:B:213:GLN:HE22	1.39	0.71
1:C:255:ARG:NH1	1:C:259:ARG:HH21	1.89	0.70
1:D:100:PHE:O	1:D:112:LYS:HE2	1.90	0.70
1:B:15:TRP:H	1:B:213:GLN:NE2	1.88	0.70
1:A:170:ARG:HG3	1:A:172:GLU:OE1	1.90	0.70
1:D:101:ALA:HA	1:D:112:LYS:NZ	2.04	0.70
1:C:276:MET:O	1:C:280:VAL:HG23	1.92	0.70
1:D:97:VAL:HG22	1:D:114:ILE:HD13	1.74	0.70
1:B:86:ASP:C	1:B:88:ARG:H	1.93	0.70
1:F:46:MET:CE	1:F:66:LEU:HD21	2.22	0.70
1:B:252:LEU:HD22	1:C:287:GLU:HG3	1.74	0.69
1:C:28:VAL:H	2:C:403:ADP:N6	1.87	0.69
1:C:187:LEU:HA	1:C:220:LYS:HB2	1.74	0.69
1:C:260:GLU:HB3	1:C:264:LYS:HE3	1.74	0.69
1:F:169:LEU:HD12	1:F:205:MET:HB2	1.74	0.69
1:E:292:LEU:HB3	1:E:324:ILE:HD13	1.74	0.69
1:E:81:GLU:HG2	1:E:115:PHE:HD2	1.56	0.69
1:F:276:MET:O	1:F:280:VAL:HG23	1.93	0.69
1:C:114:ILE:HG13	1:C:141:VAL:HG21	1.74	0.69
1:B:51:PHE:HB3	1:B:59:LYS:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ASN:OD1	1:E:94:ARG:HD3	1.92	0.69
1:D:175:ALA:HB1	1:D:179:ARG:HH12	1.57	0.69
1:A:89:GLY:HA2	1:A:92:VAL:HG12	1.73	0.69
1:F:30:GLN:HA	1:F:30:GLN:HE21	1.58	0.69
1:D:112:LYS:HB2	1:D:112:LYS:HZ2	1.57	0.68
1:E:134:MET:HG3	1:E:143:PHE:CD1	2.28	0.68
1:D:74:ASN:ND2	1:D:106:ILE:HD13	2.09	0.68
1:D:135:GLU:HB3	1:D:160:ARG:NH1	2.07	0.68
1:D:256:GLU:O	1:D:260:GLU:HG3	1.93	0.68
1:D:74:ASN:HD22	1:D:106:ILE:HD13	1.59	0.68
1:D:135:GLU:HB3	1:D:160:ARG:HH12	1.58	0.68
1:D:224:ASP:O	1:D:227:VAL:HG22	1.94	0.68
1:F:243:MET:HE1	1:F:279:GLU:HB2	1.76	0.68
1:F:127:GLN:NE2	1:F:154:ILE:HG23	2.09	0.68
1:C:307:GLY:HA3	1:F:307:GLY:HA3	1.75	0.67
1:C:320:GLN:NE2	1:F:296:LYS:HE2	2.08	0.67
1:A:229:MET:HE2	1:B:165:ARG:HE	1.58	0.67
1:D:98:LYS:O	1:D:102:ARG:HB2	1.93	0.67
1:A:173:ASP:O	1:A:176:LYS:HG2	1.94	0.67
1:A:13:LYS:HG3	1:A:14:PRO:HD2	1.74	0.67
1:C:192:GLU:HG3	1:C:224:ASP:OD1	1.95	0.67
1:A:93:ILE:O	1:A:97:VAL:HG23	1.94	0.67
1:D:38:LYS:HA	1:D:41:VAL:HG12	1.76	0.67
1:F:60:THR:HG22	1:F:115:PHE:CE2	2.30	0.67
1:D:265:GLN:HB3	1:D:267:LEU:CD1	2.25	0.67
1:C:64:LEU:O	1:C:68:ARG:HG3	1.95	0.67
1:F:88:ARG:H	1:F:88:ARG:HD3	1.59	0.66
1:D:175:ALA:HA	1:D:178:LEU:HD12	1.77	0.66
1:D:182:ALA:HA	1:D:187:LEU:HD12	1.77	0.66
1:E:4:GLU:H	1:E:9:LYS:HE3	1.60	0.66
1:E:176:LYS:HE2	1:E:176:LYS:HA	1.78	0.66
1:B:88:ARG:HG2	1:B:92:VAL:HG11	1.77	0.66
1:E:315:GLU:OE2	1:F:277:HIS:HE1	1.78	0.66
1:F:88:ARG:HB2	1:F:92:VAL:HG21	1.78	0.66
1:B:273:LEU:HD23	1:B:276:MET:CE	2.26	0.66
1:B:218:LEU:O	1:B:219:ASP:HB2	1.95	0.66
1:C:216:ALA:HB2	1:C:222:ILE:HD11	1.77	0.66
1:A:27:ILE:CD1	1:A:62:ALA:HA	2.26	0.66
1:C:56:GLY:HA2	2:C:403:ADP:H5'1	1.79	0.66
1:D:306:GLU:HG2	1:F:312:ILE:HD11	1.77	0.65
1:E:308:ALA:HA	1:F:305:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:HIS:HD2	1:F:106:ILE:HG13	1.60	0.65
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.60	0.65
1:B:60:THR:HB	2:B:402:ADP:O1A	1.97	0.65
1:C:280:VAL:HG13	1:C:293:LEU:HD23	1.77	0.65
1:E:3:GLU:HB3	1:E:9:LYS:NZ	2.10	0.65
1:C:192:GLU:HG2	1:C:193:GLY:N	2.11	0.65
1:D:104:LYS:HG3	1:D:105:PRO:HD2	1.78	0.65
1:D:124:GLN:O	1:D:128:GLN:HG2	1.96	0.65
1:F:60:THR:HG22	1:F:115:PHE:HE2	1.62	0.65
1:D:46:MET:SD	1:D:66:LEU:HD21	2.37	0.64
1:B:308:ALA:HA	1:C:305:VAL:HG21	1.79	0.64
1:A:90:ILE:HG23	1:A:91:ASN:ND2	2.13	0.64
1:C:200:ILE:HG23	1:C:233:ARG:HG3	1.78	0.64
1:C:252:LEU:HD22	1:C:252:LEU:N	2.11	0.64
1:D:64:LEU:HD22	1:D:75:TRP:HZ3	1.61	0.64
1:D:232:SER:O	1:D:233:ARG:HD2	1.97	0.64
1:A:188:GLU:HB3	1:A:221:LYS:HA	1.79	0.64
1:F:98:LYS:HG2	1:F:102:ARG:HH21	1.61	0.64
1:A:38:LYS:O	1:A:41:VAL:HG22	1.98	0.64
1:B:21:PRO:HG2	2:B:402:ADP:C2	2.33	0.64
1:C:101:ALA:HB1	1:C:137:PHE:HB3	1.80	0.64
1:E:98:LYS:O	1:E:102:ARG:HG3	1.98	0.64
1:F:170:ARG:HH12	1:F:172:GLU:HB2	1.63	0.64
1:D:24:LEU:HD23	1:D:69:GLU:CD	2.19	0.63
1:A:104:LYS:CE	1:A:104:LYS:H	2.11	0.63
1:E:21:PRO:HB3	1:E:26:ASP:CB	2.27	0.63
1:C:270:GLU:OE2	1:C:273:LEU:HD23	1.98	0.63
1:D:31:GLU:O	1:D:35:LYS:HD3	1.98	0.63
1:E:46:MET:CE	1:E:142:ARG:HG2	2.29	0.63
1:F:169:LEU:CD1	1:F:205:MET:HB2	2.29	0.63
1:E:229:MET:SD	1:F:165:ARG:HD2	2.38	0.63
1:A:28:VAL:HG12	2:A:401:ADP:N6	2.13	0.63
1:A:138:SER:O	1:A:142:ARG:NH2	2.30	0.63
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.63	0.63
1:C:84:ALA:HB3	1:C:118:GLU:O	1.99	0.62
1:F:22:GLN:HB3	1:F:68:ARG:HE	1.63	0.62
1:A:192:GLU:CD	1:A:192:GLU:H	2.01	0.62
1:C:253:LYS:O	1:C:256:GLU:HB3	1.99	0.62
1:B:265:GLN:HB2	1:B:267:LEU:CD1	2.30	0.62
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.63	0.62
1:B:21:PRO:HG2	2:B:402:ADP:H2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ARG:O	1:D:211:ILE:HG13	2.00	0.62
1:D:77:HIS:ND1	1:D:106:ILE:HD12	2.14	0.62
1:C:269:GLY:O	1:C:273:LEU:HB2	2.00	0.62
1:D:191:GLU:O	1:D:195:GLN:HG3	1.99	0.62
1:A:98:LYS:HB3	1:A:98:LYS:HZ3	1.65	0.61
1:B:255:ARG:HD3	1:B:315:GLU:CD	2.20	0.61
1:A:104:LYS:H	1:A:104:LYS:HE3	1.65	0.61
1:A:236:PRO:O	1:A:240:ARG:HG3	1.99	0.61
1:C:152:LYS:HB2	1:C:152:LYS:NZ	2.14	0.61
1:C:188:GLU:HB3	1:C:221:LYS:HA	1.82	0.61
1:C:197:ILE:HG12	1:C:211:ILE:HG22	1.82	0.61
1:C:204:ASP:OD1	1:C:206:ARG:HG2	2.01	0.61
1:C:255:ARG:HD3	1:C:259:ARG:HE	1.65	0.61
1:F:311:ILE:O	1:F:315:GLU:HG3	2.01	0.61
1:D:170:ARG:HH11	1:D:170:ARG:CB	2.12	0.61
1:F:265:GLN:HG3	1:F:267:LEU:HD21	1.82	0.61
1:D:40:TYR:HB3	1:D:46:MET:HB2	1.82	0.61
1:E:236:PRO:O	1:E:240:ARG:HG3	2.00	0.61
1:C:174:ILE:HA	1:C:205:MET:CE	2.31	0.61
1:D:88:ARG:HB2	1:D:92:VAL:HG11	1.82	0.61
1:A:33:ILE:HG23	1:A:164:PHE:HD2	1.66	0.61
1:F:262:LEU:O	1:F:266:GLY:HA2	2.01	0.61
1:D:33:ILE:HG23	1:D:164:PHE:HD2	1.65	0.60
1:A:229:MET:CE	1:B:165:ARG:HE	2.12	0.60
1:D:86:ASP:HA	1:E:124:GLN:HE22	1.64	0.60
1:E:22:GLN:HG3	1:E:68:ARG:NH1	2.16	0.60
1:F:46:MET:HG3	1:F:142:ARG:HG2	1.84	0.60
1:B:272:VAL:HG12	1:B:276:MET:CE	2.31	0.60
1:C:315:GLU:OE2	1:F:255:ARG:HG3	2.01	0.60
1:F:205:MET:HE2	1:F:209:ILE:HD11	1.84	0.60
1:B:84:ALA:O	1:B:86:ASP:N	2.26	0.60
1:A:104:LYS:H	1:A:104:LYS:CD	2.13	0.60
1:D:296:LYS:HE2	1:D:320:GLN:OE1	2.01	0.60
1:E:68:ARG:HG2	1:E:68:ARG:HH11	1.67	0.60
1:E:207:ARG:HH11	1:E:207:ARG:HG2	1.67	0.60
1:F:124:GLN:O	1:F:128:GLN:HG2	2.02	0.59
1:D:15:TRP:CZ2	1:D:185:GLU:HG2	2.37	0.59
1:C:10:VAL:HG13	1:C:11:LEU:H	1.67	0.59
1:E:60:THR:HG22	1:E:115:PHE:CZ	2.32	0.59
1:C:19:TYR:CD2	1:C:181:ILE:HG12	2.36	0.59
1:D:240:ARG:HD3	1:D:279:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LEU:HD22	1:F:287:GLU:CG	2.25	0.59
1:D:30:GLN:O	1:D:34:VAL:HG23	2.03	0.59
1:E:137:PHE:O	1:E:141:VAL:HG12	2.01	0.59
1:F:84:ALA:HB3	1:F:118:GLU:O	2.03	0.59
1:F:94:ARG:CD	1:F:129:ALA:HB1	2.30	0.59
1:B:20:ARG:NH1	2:B:402:ADP:H3'	2.17	0.59
1:C:141:VAL:HG22	1:C:142:ARG:N	2.18	0.59
1:C:176:LYS:HD2	1:C:177:ARG:N	2.18	0.59
1:D:30:GLN:HE22	1:D:167:ARG:HG3	1.67	0.59
1:B:252:LEU:HD22	1:C:287:GLU:OE2	2.01	0.59
1:C:192:GLU:CG	1:C:224:ASP:H	2.15	0.59
1:F:6:ARG:HB3	1:F:220:LYS:HZ1	1.68	0.59
1:A:309:ASN:HD21	1:A:311:ILE:HG22	1.67	0.59
1:C:165:ARG:HH11	1:C:165:ARG:CG	2.14	0.59
1:C:227:VAL:O	1:C:230:VAL:HG22	2.03	0.59
1:D:86:ASP:HA	1:E:124:GLN:NE2	2.17	0.59
1:E:46:MET:O	1:E:142:ARG:HD3	2.03	0.59
1:D:99:GLU:HG3	1:D:102:ARG:NH1	2.17	0.59
1:D:286:GLU:HB2	1:D:288:PRO:HD2	1.84	0.59
1:E:4:GLU:HB3	1:E:8:VAL:HG11	1.84	0.58
1:A:223:THR:O	1:A:227:VAL:HG23	2.03	0.58
1:F:15:TRP:H	1:F:213:GLN:HE22	1.50	0.58
1:A:101:ALA:HB1	1:A:137:PHE:CD2	2.38	0.58
1:F:153:ILE:O	1:F:158:GLN:NE2	2.35	0.58
1:D:105:PRO:HD3	1:D:140:ASN:ND2	2.09	0.58
1:D:259:ARG:HG2	1:D:259:ARG:HH11	1.68	0.58
1:F:11:LEU:HD23	1:F:217:ALA:CB	2.33	0.58
1:E:172:GLU:CD	1:E:172:GLU:H	2.07	0.58
1:F:90:ILE:HD13	1:F:126:ALA:HA	1.86	0.58
1:E:285:ILE:CG2	1:E:289:LYS:HB2	2.34	0.58
1:C:72:GLY:O	1:C:75:TRP:HE3	1.87	0.58
1:B:252:LEU:HD22	1:C:287:GLU:CG	2.34	0.57
1:A:270:GLU:HG2	1:A:301:ASN:HD21	1.69	0.57
1:B:177:ARG:HH22	2:B:402:ADP:H2	1.52	0.57
1:C:87:GLU:H	1:C:87:GLU:CD	2.07	0.57
1:A:173:ASP:HA	1:A:176:LYS:NZ	2.19	0.57
1:C:252:LEU:H	1:C:252:LEU:CD2	2.14	0.57
1:D:54:PRO:CG	1:D:168:PRO:HG3	2.34	0.57
1:E:41:VAL:HA	1:E:70:LEU:CD1	2.34	0.57
1:F:33:ILE:HG23	1:F:164:PHE:HD2	1.69	0.57
1:C:90:ILE:O	1:C:93:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:PHE:HD1	1:D:164:PHE:HB2	1.69	0.57
1:C:257:LYS:O	1:C:260:GLU:HB2	2.04	0.57
1:D:180:TYR:HD1	1:D:181:ILE:N	2.02	0.57
1:A:56:GLY:N	2:A:401:ADP:O1B	2.37	0.57
1:B:241:GLU:OE2	1:B:257:LYS:HE2	2.05	0.57
1:D:50:LEU:HD12	1:D:163:ILE:HD12	1.86	0.57
1:E:124:GLN:O	1:E:128:GLN:HG2	2.04	0.57
1:C:10:VAL:HG13	1:C:11:LEU:N	2.19	0.57
1:E:224:ASP:OD2	1:E:225:GLU:N	2.37	0.57
1:E:83:ASN:HB3	1:E:86:ASP:OD1	2.05	0.57
1:E:255:ARG:NH2	1:F:281:PHE:CG	2.73	0.57
1:B:199:TYR:OH	1:B:279:GLU:OE2	2.23	0.57
1:D:264:LYS:HB3	1:D:265:GLN:NE2	2.20	0.57
1:A:23:ARG:O	1:A:26:ASP:HB2	2.05	0.56
1:A:60:THR:N	2:A:401:ADP:O1A	2.39	0.56
1:B:199:TYR:CZ	1:B:278:LYS:HE2	2.39	0.56
1:E:24:LEU:HD12	1:E:65:ALA:HB1	1.87	0.56
1:E:116:LEU:HD21	1:E:122:LEU:HD11	1.87	0.56
1:F:88:ARG:NE	1:F:92:VAL:HG11	2.19	0.56
1:E:21:PRO:HG2	2:E:404:ADP:C2	2.40	0.56
1:E:259:ARG:HG2	1:E:259:ARG:HH11	1.70	0.56
1:E:259:ARG:HG2	1:E:259:ARG:NH1	2.19	0.56
1:A:149:TYR:HB2	1:A:152:LYS:HG3	1.86	0.56
1:B:8:VAL:HG22	1:C:47:PRO:HD3	1.87	0.56
1:D:244:LEU:CD1	1:D:283:LEU:HD22	2.35	0.56
1:D:265:GLN:HB3	1:D:267:LEU:HD13	1.87	0.56
1:E:309:ASN:ND2	1:E:312:ILE:H	2.03	0.56
1:F:309:ASN:C	1:F:309:ASN:HD22	2.09	0.56
1:B:234:ALA:HB2	1:B:261:ILE:HG23	1.86	0.56
1:E:131:ARG:HH22	1:E:132:ARG:HG2	1.71	0.56
1:F:236:PRO:O	1:F:240:ARG:HG3	2.05	0.56
1:A:39:HIS:O	1:A:43:THR:HG23	2.05	0.56
1:B:178:LEU:HD22	1:B:212:LEU:HD22	1.88	0.56
1:E:93:ILE:HG22	1:E:93:ILE:O	2.05	0.56
1:F:179:ARG:O	1:F:182:ALA:HB3	2.05	0.56
1:D:170:ARG:O	1:D:173:ASP:HB3	2.06	0.56
1:B:315:GLU:OE2	1:C:277:HIS:HE1	1.88	0.56
1:D:95:GLU:HA	1:D:98:LYS:HZ2	1.71	0.56
1:B:288:PRO:O	1:B:292:LEU:HD22	2.06	0.56
1:D:105:PRO:CB	1:D:109:ALA:HB3	2.34	0.56
1:E:24:LEU:HD11	1:E:66:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLN:O	1:A:157:ILE:HD11	2.06	0.55
1:C:177:ARG:HH11	1:C:177:ARG:CB	2.13	0.55
1:F:188:GLU:HB2	1:F:221:LYS:HA	1.87	0.55
1:A:33:ILE:HG23	1:A:164:PHE:CD2	2.41	0.55
1:B:268:SER:H	1:B:271:ASP:HB2	1.71	0.55
1:E:231:ALA:O	1:E:233:ARG:N	2.38	0.55
1:E:301:ASN:O	1:E:305:VAL:HG23	2.06	0.55
1:F:33:ILE:HD12	1:F:33:ILE:N	2.20	0.55
1:F:41:VAL:HG23	1:F:70:LEU:HD23	1.89	0.55
1:F:127:GLN:HE22	1:F:154:ILE:N	1.94	0.55
1:F:42:LYS:O	1:F:42:LYS:HG2	2.06	0.55
1:E:4:GLU:N	1:E:9:LYS:HE3	2.21	0.55
1:D:80:LEU:HD23	1:D:114:ILE:HG12	1.86	0.55
1:F:68:ARG:HG3	1:F:68:ARG:HH11	1.71	0.55
1:C:9:LYS:HE3	1:C:18:LYS:NZ	2.21	0.55
1:B:131:ARG:CZ	1:B:132:ARG:HG3	2.37	0.55
1:E:131:ARG:NH1	1:E:132:ARG:HG3	2.20	0.55
1:D:174:ILE:O	1:D:178:LEU:HG	2.07	0.55
1:D:223:THR:HG23	1:D:226:ASN:H	1.72	0.55
1:A:263:LEU:O	1:B:167:ARG:NH2	2.40	0.55
1:D:240:ARG:HG2	1:D:279:GLU:HB3	1.87	0.55
1:D:241:GLU:O	1:D:245:LEU:HB2	2.07	0.55
1:F:228:PHE:CD1	1:F:235:ARG:HG2	2.41	0.55
1:B:98:LYS:O	1:B:102:ARG:HG2	2.07	0.54
1:C:114:ILE:HD12	1:C:143:PHE:CE1	2.42	0.54
1:C:235:ARG:HD2	1:C:237:GLU:OE1	2.07	0.54
1:C:325:GLY:O	1:C:327:LYS:N	2.38	0.54
1:E:177:ARG:HH22	2:E:404:ADP:H2	1.55	0.54
1:E:75:TRP:CG	1:E:76:ARG:N	2.74	0.54
1:F:22:GLN:HB3	1:F:68:ARG:NE	2.21	0.54
1:F:49:LEU:HB2	1:F:144:ILE:HG12	1.90	0.54
1:F:287:GLU:HB3	1:F:288:PRO:HD3	1.89	0.54
1:C:20:ARG:HD3	1:C:64:LEU:HD12	1.88	0.54
1:C:71:PHE:HB2	1:C:75:TRP:CB	2.38	0.54
1:C:265:GLN:HB2	1:C:267:LEU:HG	1.88	0.54
1:C:293:LEU:O	1:C:297:ILE:HG12	2.07	0.54
1:C:94:ARG:O	1:C:98:LYS:HB2	2.07	0.54
1:D:98:LYS:HZ2	1:D:98:LYS:HB2	1.72	0.54
1:E:13:LYS:HD2	1:E:14:PRO:HD2	1.89	0.54
1:A:309:ASN:ND2	1:A:312:ILE:H	2.06	0.54
1:B:5:ILE:HG13	1:B:8:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:HG22	1:B:142:ARG:N	2.23	0.54
1:C:281:PHE:HA	1:C:290:LYS:HD3	1.89	0.54
1:D:41:VAL:HG13	1:D:42:LYS:HG2	1.89	0.54
1:A:57:VAL:HG21	1:A:168:PRO:HA	1.90	0.54
1:F:179:ARG:O	1:F:183:GLU:HG3	2.08	0.54
1:B:55:PRO:HA	2:B:402:ADP:O3B	2.07	0.54
1:D:49:LEU:CD2	1:D:162:ALA:HB3	2.37	0.54
1:A:8:VAL:HG22	1:B:47:PRO:HD3	1.90	0.53
1:D:245:LEU:HD21	1:D:253:LYS:HB3	1.90	0.53
1:A:90:ILE:HA	1:A:93:ILE:HG22	1.89	0.53
1:C:33:ILE:O	1:C:37:LEU:HD13	2.08	0.53
1:B:60:THR:N	2:B:402:ADP:O1A	2.42	0.53
1:A:280:VAL:HG21	1:A:293:LEU:HB3	1.89	0.53
1:F:258:LEU:O	1:F:262:LEU:HD23	2.08	0.53
1:E:5:ILE:HG13	1:E:8:VAL:HG12	1.91	0.53
1:B:116:LEU:HD12	1:B:145:LEU:CD2	2.39	0.53
1:E:28:VAL:N	2:E:404:ADP:HN62	2.00	0.53
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.73	0.53
1:C:230:VAL:HG23	1:C:231:ALA:N	2.23	0.53
1:F:176:LYS:HD3	1:F:176:LYS:C	2.29	0.53
1:A:174:ILE:CA	1:A:205:MET:HE1	2.16	0.53
1:F:16:VAL:O	1:F:20:ARG:HB2	2.09	0.53
1:D:10:VAL:HG23	1:D:15:TRP:CZ2	2.44	0.52
1:E:4:GLU:HB3	1:E:8:VAL:HG13	1.89	0.52
1:E:137:PHE:HB2	1:E:141:VAL:HG12	1.91	0.52
1:F:8:VAL:O	1:F:12:GLU:HB3	2.09	0.52
1:A:95:GLU:OE1	1:A:95:GLU:HA	2.08	0.52
1:B:90:ILE:HG23	1:B:91:ASN:H	1.73	0.52
1:C:187:LEU:HD23	1:C:220:LYS:HA	1.90	0.52
1:A:326:LYS:HG2	3:A:413:HOH:O	2.09	0.52
1:E:93:ILE:O	1:E:94:ARG:HD2	2.10	0.52
1:E:130:LEU:O	1:E:134:MET:HB2	2.09	0.52
1:F:127:GLN:HE21	1:F:154:ILE:HG12	1.73	0.52
1:B:86:ASP:HB2	1:B:89:GLY:CA	2.39	0.52
1:C:185:GLU:HA	1:C:185:GLU:OE1	2.09	0.52
1:F:6:ARG:HB3	1:F:220:LYS:HZ3	1.73	0.52
1:F:15:TRP:H	1:F:213:GLN:NE2	2.06	0.52
1:F:97:VAL:CG1	1:F:114:ILE:HD13	2.39	0.52
1:B:94:ARG:HD3	1:B:133:THR:OG1	2.10	0.52
1:D:212:LEU:HD11	1:D:222:ILE:HG13	1.92	0.52
1:A:104:LYS:H	1:A:104:LYS:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LYS:HB2	1:C:96:LYS:NZ	2.25	0.52
1:C:255:ARG:HH11	1:C:259:ARG:HH21	1.58	0.52
1:D:189:LEU:HA	1:D:222:ILE:HB	1.90	0.52
1:E:30:GLN:HE21	1:E:30:GLN:HA	1.75	0.52
1:E:93:ILE:C	1:E:94:ARG:HD2	2.29	0.52
1:C:9:LYS:NZ	1:C:9:LYS:HB3	2.25	0.52
1:C:71:PHE:HB3	1:C:74:ASN:O	2.09	0.52
1:D:74:ASN:C	1:D:76:ARG:H	2.11	0.52
1:A:255:ARG:O	1:A:259:ARG:HG2	2.10	0.52
1:C:190:THR:HB	1:C:192:GLU:OE1	2.09	0.52
1:C:194:LEU:O	1:C:198:LEU:HD13	2.10	0.52
1:F:170:ARG:NH1	1:F:172:GLU:HB2	2.24	0.52
1:E:38:LYS:O	1:E:41:VAL:HG12	2.11	0.51
1:E:171:ASP:OD2	1:E:198:LEU:HB3	2.10	0.51
1:F:122:LEU:HD22	1:F:126:ALA:HB1	1.92	0.51
1:B:255:ARG:HD3	1:B:315:GLU:OE1	2.10	0.51
1:D:228:PHE:CE1	1:D:235:ARG:HG2	2.45	0.51
1:E:55:PRO:HA	2:E:404:ADP:O3B	2.11	0.51
1:A:182:ALA:HA	1:A:187:LEU:HD12	1.92	0.51
1:D:22:GLN:HE21	1:D:22:GLN:HA	1.75	0.51
1:F:260:GLU:O	1:F:263:LEU:HB3	2.10	0.51
1:B:94:ARG:O	1:B:97:VAL:HG22	2.11	0.51
1:F:30:GLN:HA	1:F:30:GLN:NE2	2.24	0.51
1:A:99:GLU:HA	1:A:99:GLU:OE1	2.09	0.51
1:A:235:ARG:HG3	1:A:235:ARG:NH1	2.25	0.51
1:E:128:GLN:HA	1:E:128:GLN:NE2	2.25	0.51
1:E:46:MET:HE3	1:E:142:ARG:HG2	1.91	0.51
1:A:87:GLU:O	1:A:90:ILE:HG22	2.10	0.51
1:B:7:GLU:HG3	1:B:217:ALA:O	2.11	0.51
1:D:111:PHE:CG	1:D:142:ARG:HD3	2.45	0.51
1:E:51:PHE:HB3	1:E:59:LYS:HG2	1.92	0.51
1:B:272:VAL:O	1:B:276:MET:HG3	2.10	0.51
1:E:181:ILE:O	1:E:185:GLU:HB2	2.11	0.51
1:B:137:PHE:HB2	1:B:141:VAL:HG12	1.93	0.51
1:A:175:ALA:O	1:A:179:ARG:HG3	2.10	0.51
1:B:176:LYS:HB2	1:B:176:LYS:NZ	2.26	0.51
1:C:54:PRO:O	1:C:57:VAL:HG22	2.11	0.51
1:D:51:PHE:CD1	1:D:164:PHE:HB2	2.46	0.51
1:A:200:ILE:HD11	1:A:228:PHE:CD2	2.45	0.50
1:B:248:LYS:HE2	1:B:250:ASN:HD21	1.76	0.50
1:C:90:ILE:CD1	1:C:126:ALA:HA	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:O	1:A:197:ILE:HG13	2.11	0.50
1:D:94:ARG:NH2	1:D:129:ALA:HB1	2.23	0.50
1:D:170:ARG:HB3	1:D:170:ARG:CZ	2.39	0.50
1:B:127:GLN:O	1:B:157:ILE:HD11	2.12	0.50
1:B:247:LEU:HD12	1:B:321:PHE:O	2.11	0.50
1:E:30:GLN:O	1:E:33:ILE:N	2.44	0.50
1:E:38:LYS:HA	1:E:41:VAL:HG12	1.94	0.50
1:E:46:MET:HE3	1:E:47:PRO:O	2.12	0.50
1:C:179:ARG:C	1:C:181:ILE:H	2.14	0.50
1:D:38:LYS:HA	1:D:41:VAL:CG1	2.40	0.50
1:D:117:ASP:HA	1:D:146:SER:HB3	1.92	0.50
1:D:304:LEU:HD11	1:D:310:GLU:HA	1.92	0.50
1:F:33:ILE:HG23	1:F:164:PHE:CD2	2.47	0.50
1:C:219:ASP:OD2	1:C:221:LYS:HB3	2.11	0.50
1:D:100:PHE:CZ	1:D:112:LYS:HD2	2.46	0.50
1:E:101:ALA:HB1	1:E:137:PHE:CD2	2.47	0.50
1:F:90:ILE:O	1:F:93:ILE:HB	2.12	0.50
1:C:56:GLY:HA3	1:C:206:ARG:HG2	1.93	0.50
1:D:180:TYR:CD1	1:D:181:ILE:N	2.80	0.50
1:D:195:GLN:HA	1:D:198:LEU:HD12	1.93	0.50
1:E:32:HIS:CE1	1:E:36:ARG:HD2	2.46	0.50
1:C:218:LEU:O	1:C:219:ASP:HB3	2.11	0.50
1:A:5:ILE:HD12	1:A:6:ARG:H	1.76	0.50
1:B:92:VAL:HG22	1:B:92:VAL:O	2.12	0.50
1:F:131:ARG:HD3	1:F:131:ARG:C	2.32	0.50
1:A:91:ASN:ND2	1:A:94:ARG:HH21	2.10	0.50
1:A:268:SER:HB3	1:B:149:TYR:CD2	2.46	0.50
1:D:77:HIS:HB3	1:D:106:ILE:HG21	1.94	0.50
1:C:173:ASP:O	1:C:176:LYS:HG3	2.12	0.49
1:E:163:ILE:HD12	1:E:163:ILE:N	2.27	0.49
1:A:304:LEU:HD11	1:A:310:GLU:HA	1.94	0.49
1:B:41:VAL:HG12	1:B:70:LEU:HD13	1.93	0.49
1:E:46:MET:HE2	1:E:142:ARG:HG2	1.93	0.49
1:E:117:ASP:HA	1:E:146:SER:HB3	1.93	0.49
1:C:274:VAL:O	1:C:277:HIS:HB3	2.12	0.49
1:C:321:PHE:O	1:C:325:GLY:N	2.41	0.49
1:D:255:ARG:HD3	1:D:315:GLU:CD	2.33	0.49
1:E:116:LEU:HB3	1:E:145:LEU:HD23	1.94	0.49
1:E:280:VAL:HG13	1:E:281:PHE:CD1	2.47	0.49
1:A:13:LYS:HG3	1:A:14:PRO:CD	2.41	0.49
1:C:38:LYS:HA	1:C:41:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HB2	1:C:224:ASP:HB3	1.94	0.49
1:F:176:LYS:HD3	1:F:176:LYS:O	2.13	0.49
1:A:104:LYS:HD2	1:A:104:LYS:N	2.28	0.49
1:E:60:THR:N	2:E:404:ADP:O1A	2.45	0.49
1:F:234:ALA:N	1:F:275:GLN:OE1	2.43	0.49
1:B:265:GLN:HB2	1:B:267:LEU:HD12	1.95	0.49
1:A:153:ILE:HG22	1:A:158:GLN:HG3	1.93	0.49
1:C:241:GLU:HG3	1:C:245:LEU:CD2	2.42	0.49
1:D:176:LYS:C	1:D:178:LEU:H	2.15	0.49
1:E:28:VAL:H	2:E:404:ADP:N6	2.02	0.49
1:B:236:PRO:O	1:B:240:ARG:HG3	2.13	0.49
1:C:16:VAL:HG13	2:C:403:ADP:H4'	1.94	0.49
1:C:80:LEU:HB2	1:C:100:PHE:CE1	2.47	0.49
1:C:177:ARG:O	1:C:181:ILE:HG13	2.12	0.49
1:C:226:ASN:O	1:C:230:VAL:HG13	2.12	0.49
1:D:135:GLU:HA	1:D:138:SER:HB3	1.94	0.49
1:E:84:ALA:HB1	1:E:122:LEU:HD21	1.93	0.49
1:D:265:GLN:CB	1:D:267:LEU:HD13	2.42	0.49
1:C:197:ILE:HG12	1:C:211:ILE:CG2	2.43	0.49
1:F:95:GLU:O	1:F:98:LYS:HE3	2.13	0.49
1:D:17:GLU:HG2	1:D:20:ARG:NH1	2.27	0.48
1:E:222:ILE:HD12	1:E:222:ILE:N	2.28	0.48
1:F:71:PHE:O	1:F:74:ASN:HB2	2.13	0.48
1:B:90:ILE:HG23	1:B:91:ASN:N	2.28	0.48
1:E:256:GLU:O	1:E:260:GLU:HG3	2.13	0.48
1:B:86:ASP:HB2	1:B:89:GLY:HA2	1.94	0.48
1:C:255:ARG:O	1:C:259:ARG:HG2	2.12	0.48
1:D:49:LEU:HD22	1:D:162:ALA:HB3	1.93	0.48
1:C:98:LYS:HA	1:C:137:PHE:CE2	2.48	0.48
1:D:194:LEU:O	1:D:198:LEU:HG	2.13	0.48
1:A:61:THR:HG22	1:A:62:ALA:N	2.28	0.48
1:A:252:LEU:HD22	1:B:287:GLU:CD	2.34	0.48
1:B:89:GLY:O	1:B:92:VAL:HG12	2.14	0.48
1:C:239:ILE:HG23	1:C:243:MET:HE2	1.96	0.48
1:D:104:LYS:CG	1:D:105:PRO:HD2	2.42	0.48
1:E:199:TYR:O	1:E:202:GLU:HG3	2.14	0.48
1:E:309:ASN:HD22	1:E:312:ILE:H	1.62	0.48
1:B:42:LYS:O	1:B:42:LYS:HG2	2.14	0.48
1:B:104:LYS:NZ	1:B:104:LYS:HB3	2.29	0.48
1:C:130:LEU:O	1:C:134:MET:HB2	2.14	0.48
1:D:78:ASN:HA	1:D:112:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ARG:HG2	1:E:177:ARG:HH11	1.77	0.48
1:A:273:LEU:HG	1:A:297:ILE:HG23	1.96	0.48
1:B:47:PRO:O	1:B:49:LEU:HD13	2.14	0.48
1:C:120:ASP:HB3	1:C:147:CYS:HB2	1.96	0.48
1:E:232:SER:O	1:E:233:ARG:HD2	2.13	0.48
1:C:280:VAL:HG13	1:C:293:LEU:CD2	2.43	0.48
1:E:60:THR:HG23	2:E:404:ADP:O1B	2.13	0.48
1:E:241:GLU:HG2	1:E:245:LEU:HD22	1.95	0.48
1:F:7:GLU:O	1:F:11:LEU:HD11	2.13	0.48
1:F:178:LEU:HG	1:F:212:LEU:HD22	1.96	0.48
1:F:264:LYS:HD3	1:F:265:GLN:NE2	2.29	0.48
1:F:273:LEU:HD12	1:F:273:LEU:HA	1.70	0.48
1:B:320:GLN:NE2	1:C:295:ASP:OD1	2.46	0.47
1:C:21:PRO:HB3	1:C:26:ASP:HB2	1.96	0.47
1:C:165:ARG:CG	1:C:165:ARG:NH1	2.76	0.47
1:D:196:ALA:HB3	1:D:227:VAL:HG21	1.93	0.47
1:D:244:LEU:HD11	1:D:284:PRO:HD2	1.95	0.47
1:E:78:ASN:ND2	1:E:106:ILE:HG12	2.22	0.47
1:B:71:PHE:O	1:B:74:ASN:HB2	2.15	0.47
1:B:272:VAL:HG12	1:B:276:MET:HE3	1.95	0.47
1:C:68:ARG:HG2	1:C:75:TRP:CE2	2.49	0.47
1:C:112:LYS:O	1:C:141:VAL:HG23	2.14	0.47
1:D:268:SER:H	1:D:271:ASP:HB2	1.78	0.47
1:E:128:GLN:HA	1:E:128:GLN:HE21	1.79	0.47
1:F:35:LYS:HD3	1:F:35:LYS:C	2.34	0.47
1:B:188:GLU:HB3	1:B:221:LYS:HA	1.95	0.47
1:B:206:ARG:HH21	1:C:155:GLU:CB	2.26	0.47
1:C:104:LYS:HD2	1:C:104:LYS:N	2.29	0.47
1:E:5:ILE:CG1	1:E:8:VAL:HG12	2.43	0.47
1:C:9:LYS:HE3	1:C:18:LYS:HZ3	1.79	0.47
1:C:206:ARG:HG3	1:C:206:ARG:NH1	2.29	0.47
1:D:90:ILE:HD12	1:D:91:ASN:OD1	2.13	0.47
1:A:240:ARG:NE	1:A:279:GLU:OE1	2.47	0.47
1:B:5:ILE:CG1	1:B:8:VAL:HG23	2.45	0.47
1:B:135:GLU:HA	1:B:135:GLU:OE1	2.15	0.47
1:B:267:LEU:HD12	1:B:267:LEU:H	1.79	0.47
1:D:95:GLU:HA	1:D:98:LYS:NZ	2.29	0.47
1:E:309:ASN:HD22	1:E:309:ASN:C	2.18	0.47
1:A:121:ALA:O	1:F:284:PRO:HG2	2.15	0.47
1:A:154:ILE:HB	1:A:156:PRO:HD2	1.96	0.47
1:B:258:LEU:HG	1:B:262:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TRP:CZ2	1:C:185:GLU:HG2	2.50	0.47
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.79	0.47
1:C:289:LYS:O	1:C:293:LEU:HD13	2.15	0.47
1:E:273:LEU:HD22	1:E:304:LEU:HD22	1.95	0.47
1:A:170:ARG:HA	1:A:170:ARG:HD2	1.68	0.47
1:B:87:GLU:O	1:B:88:ARG:HB2	2.15	0.47
1:B:287:GLU:HB3	1:B:288:PRO:HD3	1.96	0.47
1:C:120:ASP:HB2	1:C:152:LYS:HG2	1.97	0.47
1:F:57:VAL:HG21	1:F:167:ARG:O	2.15	0.47
1:B:86:ASP:C	1:B:88:ARG:N	2.61	0.47
1:D:184:ASN:OD1	1:D:184:ASN:O	2.33	0.47
1:E:23:ARG:C	1:E:25:ASP:H	2.17	0.47
1:C:27:ILE:HG23	2:C:403:ADP:N6	2.30	0.47
1:C:255:ARG:CD	1:C:259:ARG:HE	2.27	0.47
1:E:79:PHE:HE1	1:E:81:GLU:HB2	1.80	0.47
1:F:95:GLU:OE1	1:F:98:LYS:HE2	2.15	0.47
1:F:10:VAL:HG11	1:F:220:LYS:HE3	1.97	0.46
1:A:91:ASN:ND2	1:A:94:ARG:NH2	2.63	0.46
1:C:176:LYS:CE	1:C:177:ARG:HG2	2.45	0.46
1:C:206:ARG:HG3	1:C:207:ARG:N	2.30	0.46
1:C:130:LEU:HD11	1:C:143:PHE:CE2	2.50	0.46
1:A:104:LYS:CD	1:A:104:LYS:N	2.79	0.46
1:B:91:ASN:C	1:B:93:ILE:N	2.62	0.46
1:C:105:PRO:HG2	1:C:111:PHE:C	2.35	0.46
1:D:135:GLU:HG3	1:D:136:MET:N	2.31	0.46
1:C:77:HIS:C	1:C:79:PHE:H	2.18	0.46
1:D:249:GLY:HA2	1:D:322:THR:HG23	1.98	0.46
1:E:12:GLU:HG3	1:E:13:LYS:N	2.30	0.46
1:A:58:GLY:N	2:A:401:ADP:O2A	2.49	0.46
1:B:199:TYR:CE2	1:B:236:PRO:HG3	2.51	0.46
1:C:22:GLN:O	1:C:68:ARG:HD2	2.15	0.46
1:E:78:ASN:HD21	1:E:106:ILE:CG1	2.24	0.46
1:D:270:GLU:O	1:D:274:VAL:HG23	2.16	0.46
1:B:74:ASN:OD1	1:B:106:ILE:HG22	2.15	0.46
1:B:296:LYS:HE2	3:B:415:HOH:O	2.15	0.46
1:F:3:GLU:OE2	1:F:220:LYS:NZ	2.49	0.46
1:F:39:HIS:O	1:F:43:THR:HG23	2.15	0.46
1:C:102:ARG:HD2	1:C:102:ARG:HA	1.85	0.46
1:E:4:GLU:HG3	1:F:45:SER:HB2	1.98	0.46
1:A:84:ALA:HB3	1:A:118:GLU:O	2.16	0.45
1:A:124:GLN:O	1:A:128:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:HA3	3:A:417:HOH:O	2.16	0.45
1:B:272:VAL:HG12	1:B:276:MET:HE2	1.98	0.45
1:C:101:ALA:CB	1:C:137:PHE:HB3	2.46	0.45
1:C:234:ALA:HB2	1:C:265:GLN:HG3	1.97	0.45
1:A:268:SER:HB3	1:B:149:TYR:CG	2.50	0.45
1:D:233:ARG:HD2	1:D:233:ARG:N	2.27	0.45
1:D:318:LEU:O	1:D:321:PHE:HB2	2.17	0.45
1:E:18:LYS:HD2	1:E:19:TYR:CE1	2.51	0.45
1:F:22:GLN:O	1:F:68:ARG:HD3	2.16	0.45
1:F:88:ARG:HH21	1:F:92:VAL:HG13	1.79	0.45
1:B:288:PRO:O	1:B:292:LEU:CD2	2.64	0.45
1:C:84:ALA:C	1:C:86:ASP:H	2.20	0.45
1:D:64:LEU:HD22	1:D:75:TRP:CZ3	2.47	0.45
1:E:4:GLU:HB2	1:E:9:LYS:HE3	1.98	0.45
1:E:34:VAL:HG13	1:E:35:LYS:N	2.31	0.45
1:F:97:VAL:HG12	1:F:114:ILE:HD13	1.98	0.45
1:C:71:PHE:HB2	1:C:75:TRP:HB2	1.98	0.45
1:C:90:ILE:HG21	1:C:126:ALA:HB1	1.99	0.45
1:D:98:LYS:HB2	1:D:98:LYS:NZ	2.32	0.45
1:F:243:MET:CE	1:F:279:GLU:HB2	2.45	0.45
1:B:6:ARG:O	1:B:10:VAL:HG23	2.17	0.45
1:B:84:ALA:C	1:B:86:ASP:H	2.16	0.45
1:C:285:ILE:HD12	1:C:289:LYS:HB2	1.99	0.45
1:D:112:LYS:NZ	1:D:112:LYS:CB	2.75	0.45
1:E:101:ALA:O	1:E:140:ASN:ND2	2.49	0.45
1:E:192:GLU:CD	1:E:192:GLU:H	2.20	0.45
1:A:300:TYR:HA	1:A:303:ARG:HG3	1.97	0.45
1:B:232:SER:O	1:B:233:ARG:NH1	2.47	0.45
1:D:41:VAL:HG21	1:D:69:GLU:HB3	1.98	0.45
1:F:6:ARG:C	1:F:8:VAL:H	2.20	0.45
1:F:244:LEU:HD13	1:F:283:LEU:HD22	1.98	0.45
1:A:206:ARG:NH2	3:A:412:HOH:O	2.50	0.45
1:C:24:LEU:HD12	1:C:38:LYS:HG2	1.98	0.45
1:C:200:ILE:HD11	1:C:228:PHE:CD2	2.52	0.45
1:D:155:GLU:HB3	1:D:156:PRO:HD3	1.98	0.45
1:E:3:GLU:HB3	1:E:9:LYS:HZ2	1.82	0.45
1:E:205:MET:HG2	2:E:404:ADP:H1'	1.98	0.45
1:B:28:VAL:HG22	1:B:29:GLY:N	2.32	0.45
1:C:21:PRO:HB3	1:C:26:ASP:CB	2.47	0.45
1:C:189:LEU:HD22	1:C:194:LEU:HB2	1.98	0.45
1:C:255:ARG:NH1	1:C:259:ARG:NH2	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:THR:HG22	1:E:133:THR:O	2.16	0.45
1:B:296:LYS:O	1:B:300:TYR:HD1	1.99	0.44
1:C:104:LYS:HE3	1:C:140:ASN:ND2	2.32	0.44
1:D:240:ARG:CG	1:D:279:GLU:HB3	2.48	0.44
1:D:288:PRO:O	1:D:291:VAL:HG12	2.17	0.44
1:E:228:PHE:O	1:E:231:ALA:O	2.35	0.44
1:E:255:ARG:HD3	1:E:315:GLU:CD	2.37	0.44
1:E:304:LEU:HD12	1:E:304:LEU:HA	1.83	0.44
1:D:5:ILE:HG12	1:E:45:SER:OG	2.17	0.44
1:D:64:LEU:HD23	1:D:79:PHE:CZ	2.52	0.44
1:F:19:TYR:CD2	1:F:181:ILE:HG12	2.53	0.44
1:B:206:ARG:HH21	1:C:155:GLU:HB3	1.83	0.44
1:E:176:LYS:HE2	1:E:176:LYS:CA	2.47	0.44
1:B:58:GLY:N	2:B:402:ADP:O2A	2.50	0.44
1:B:86:ASP:O	1:B:88:ARG:N	2.50	0.44
1:B:169:LEU:HD22	1:B:205:MET:HB2	2.00	0.44
1:C:28:VAL:O	2:C:403:ADP:N6	2.51	0.44
1:D:258:LEU:HG	1:D:262:LEU:HD22	2.00	0.44
1:A:306:GLU:HA	1:A:306:GLU:OE1	2.18	0.44
1:C:223:THR:O	1:C:227:VAL:HG23	2.17	0.44
1:C:226:ASN:N	1:C:226:ASN:HD22	2.15	0.44
1:B:75:TRP:O	1:B:79:PHE:HB3	2.18	0.44
1:B:90:ILE:O	1:B:93:ILE:HB	2.18	0.44
1:B:91:ASN:O	1:B:93:ILE:N	2.51	0.44
1:D:170:ARG:HH12	1:D:172:GLU:HB2	1.83	0.44
1:F:98:LYS:C	1:F:98:LYS:HD2	2.38	0.44
1:F:314:LEU:HD12	1:F:314:LEU:HA	1.88	0.44
1:E:180:TYR:CD1	1:E:180:TYR:C	2.91	0.44
1:F:3:GLU:CD	1:F:220:LYS:NZ	2.71	0.44
1:D:38:LYS:CA	1:D:41:VAL:HG12	2.45	0.43
1:D:245:LEU:O	1:D:250:ASN:HB2	2.18	0.43
1:D:134:MET:SD	1:D:145:LEU:HD11	2.57	0.43
1:E:132:ARG:C	1:E:134:MET:H	2.22	0.43
1:E:206:ARG:NH2	2:E:404:ADP:O3B	2.52	0.43
1:F:116:LEU:HD23	1:F:116:LEU:HA	1.81	0.43
1:A:244:LEU:HA	1:A:244:LEU:HD12	1.71	0.43
1:B:131:ARG:HD2	1:B:131:ARG:O	2.18	0.43
1:C:24:LEU:CD1	1:C:38:LYS:HG2	2.48	0.43
1:D:17:GLU:HG2	1:D:20:ARG:HH12	1.83	0.43
1:D:132:ARG:HD2	1:D:132:ARG:O	2.18	0.43
1:D:256:GLU:OE1	1:D:256:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:GLY:N	2:E:404:ADP:O2A	2.51	0.43
1:E:184:ASN:O	1:E:185:GLU:HG2	2.18	0.43
1:F:67:ALA:HB2	1:F:79:PHE:CD2	2.53	0.43
1:A:5:ILE:HG13	1:A:6:ARG:N	2.33	0.43
1:A:115:PHE:HD1	1:A:144:ILE:HB	1.83	0.43
1:C:178:LEU:HG	1:C:212:LEU:HD22	2.00	0.43
1:B:134:MET:HB2	1:B:134:MET:HE3	1.85	0.43
1:D:140:ASN:ND2	1:D:140:ASN:O	2.52	0.43
1:E:13:LYS:HA	1:E:14:PRO:HD3	1.85	0.43
1:A:82:LEU:HD13	1:A:90:ILE:CD1	2.49	0.43
1:A:172:GLU:N	1:A:172:GLU:CD	2.72	0.43
1:D:259:ARG:HH11	1:D:259:ARG:CG	2.31	0.43
1:E:32:HIS:HE1	1:E:36:ARG:HD2	1.83	0.43
1:E:132:ARG:C	1:E:134:MET:N	2.72	0.43
1:E:238:ASP:HB3	1:E:261:ILE:HD11	2.01	0.43
1:E:255:ARG:HD3	1:E:315:GLU:OE1	2.19	0.43
1:A:21:PRO:HD3	2:A:401:ADP:C2	2.54	0.43
1:B:131:ARG:NH2	1:B:132:ARG:HG3	2.33	0.43
1:B:267:LEU:HD12	1:B:267:LEU:N	2.33	0.43
1:E:273:LEU:HD22	1:E:304:LEU:CD2	2.49	0.43
1:A:13:LYS:NZ	1:A:17:GLU:CG	2.82	0.43
1:A:283:LEU:O	1:A:285:ILE:N	2.44	0.43
1:C:101:ALA:HB3	1:C:137:PHE:CG	2.54	0.43
1:C:120:ASP:HB2	1:C:152:LYS:HB3	2.01	0.43
1:C:154:ILE:O	1:C:154:ILE:HG13	2.19	0.43
1:F:23:ARG:HG3	1:F:23:ARG:HH11	1.83	0.43
1:A:90:ILE:HG23	1:A:91:ASN:HD22	1.84	0.43
1:B:84:ALA:C	1:B:86:ASP:N	2.71	0.43
1:B:226:ASN:O	1:B:230:VAL:HG22	2.19	0.43
1:C:59:LYS:HE2	1:C:146:SER:OG	2.19	0.43
1:D:78:ASN:OD1	1:D:105:PRO:HB3	2.18	0.43
1:D:104:LYS:CD	1:D:105:PRO:HD2	2.49	0.43
1:D:283:LEU:O	1:D:285:ILE:N	2.48	0.43
1:E:84:ALA:HB1	1:E:122:LEU:CD2	2.49	0.43
1:E:207:ARG:O	1:E:211:ILE:HG13	2.19	0.43
1:F:318:LEU:O	1:F:321:PHE:HB2	2.18	0.43
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.84	0.43
1:B:20:ARG:HH12	2:B:402:ADP:H3'	1.83	0.43
1:B:91:ASN:ND2	1:B:94:ARG:HH21	2.17	0.43
1:C:98:LYS:HZ2	1:C:98:LYS:HB3	1.83	0.43
1:E:258:LEU:O	1:E:262:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:CD	1:A:172:GLU:H	2.22	0.42
1:B:240:ARG:O	1:B:244:LEU:HD22	2.19	0.42
1:B:243:MET:O	1:B:247:LEU:HB2	2.19	0.42
1:C:182:ALA:HB1	1:C:187:LEU:HB2	2.00	0.42
1:D:233:ARG:HG2	1:D:233:ARG:HH11	1.83	0.42
1:D:239:ILE:O	1:D:242:MET:HB3	2.20	0.42
1:F:35:LYS:HD3	1:F:35:LYS:O	2.19	0.42
1:F:125:ASP:O	1:F:128:GLN:HB2	2.19	0.42
1:B:292:LEU:HB3	1:B:324:ILE:HD13	2.02	0.42
1:C:243:MET:HE1	1:C:276:MET:HA	2.01	0.42
1:C:286:GLU:HG3	1:C:289:LYS:HG2	2.01	0.42
1:C:287:GLU:HB3	1:C:288:PRO:HD3	2.01	0.42
1:D:104:LYS:HG3	1:D:105:PRO:CD	2.48	0.42
1:D:287:GLU:OE1	1:D:288:PRO:N	2.52	0.42
1:E:100:PHE:CZ	1:E:112:LYS:HD3	2.54	0.42
1:E:100:PHE:CE2	1:E:112:LYS:HD3	2.54	0.42
1:A:46:MET:CE	1:A:142:ARG:HG2	2.49	0.42
1:B:200:ILE:HD12	1:B:227:VAL:HG12	2.00	0.42
1:B:211:ILE:HG21	1:B:227:VAL:HG13	2.01	0.42
1:B:262:LEU:O	1:B:266:GLY:HA2	2.20	0.42
1:C:174:ILE:HG23	1:C:205:MET:SD	2.57	0.42
1:D:97:VAL:HG22	1:D:114:ILE:CD1	2.45	0.42
1:A:89:GLY:CA	1:A:92:VAL:HG12	2.47	0.42
1:B:41:VAL:HA	1:B:70:LEU:CD1	2.50	0.42
1:B:141:VAL:CG2	1:B:142:ARG:N	2.82	0.42
1:C:152:LYS:HB2	1:C:152:LYS:HZ2	1.82	0.42
1:C:207:ARG:HG2	1:C:207:ARG:NH1	2.33	0.42
1:D:97:VAL:HG13	1:D:114:ILE:CD1	2.49	0.42
1:E:61:THR:N	2:E:404:ADP:O1A	2.51	0.42
1:E:138:SER:O	1:E:142:ARG:NH2	2.46	0.42
1:E:154:ILE:HG13	1:E:156:PRO:HD2	2.00	0.42
1:F:11:LEU:CD2	1:F:217:ALA:HB1	2.45	0.42
1:F:33:ILE:HD12	1:F:33:ILE:H	1.84	0.42
1:F:90:ILE:H	1:F:90:ILE:HG13	1.59	0.42
1:F:95:GLU:O	1:F:98:LYS:HB3	2.19	0.42
1:A:256:GLU:O	1:A:259:ARG:HB2	2.20	0.42
1:B:28:VAL:O	2:B:402:ADP:N6	2.52	0.42
1:B:137:PHE:HB2	1:B:141:VAL:CG1	2.49	0.42
1:E:92:VAL:C	1:E:93:ILE:HG13	2.40	0.42
1:F:134:MET:CB	1:F:160:ARG:HH22	2.32	0.42
1:A:47:PRO:O	1:A:49:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ARG:HB2	1:B:164:PHE:HE2	1.84	0.42
1:B:94:ARG:CZ	1:B:129:ALA:HB1	2.49	0.42
1:B:170:ARG:NH1	1:B:170:ARG:HG3	2.34	0.42
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.85	0.42
1:D:180:TYR:CD1	1:D:180:TYR:C	2.93	0.42
1:F:95:GLU:OE1	1:F:95:GLU:HA	2.19	0.42
1:B:128:GLN:O	1:B:132:ARG:HD3	2.18	0.42
1:C:176:LYS:NZ	1:C:177:ARG:HG2	2.35	0.42
1:E:175:ALA:O	1:E:179:ARG:HG3	2.19	0.42
1:E:277:HIS:HB2	1:E:297:ILE:HG21	2.00	0.42
1:D:192:GLU:OE1	1:D:192:GLU:N	2.44	0.42
1:E:185:GLU:HB3	1:E:187:LEU:HD13	2.02	0.42
1:F:134:MET:HB2	1:F:160:ARG:HH22	1.85	0.42
1:F:283:LEU:HA	1:F:284:PRO:HD3	1.75	0.42
1:A:216:ALA:HA	1:A:219:ASP:O	2.20	0.42
1:A:287:GLU:HB3	1:A:288:PRO:HD3	2.01	0.42
1:C:120:ASP:HB2	1:C:152:LYS:CG	2.50	0.42
1:C:285:ILE:HD12	1:C:289:LYS:CB	2.50	0.42
1:D:24:LEU:O	1:D:34:VAL:HG11	2.20	0.42
1:D:310:GLU:O	1:D:314:LEU:HB2	2.20	0.42
1:F:22:GLN:HB3	1:F:68:ARG:CD	2.50	0.42
1:F:92:VAL:O	1:F:96:LYS:HG3	2.20	0.42
1:A:61:THR:N	2:A:401:ADP:O1A	2.41	0.42
1:B:106:ILE:N	1:B:106:ILE:HD12	2.35	0.42
1:C:141:VAL:CG2	1:C:142:ARG:N	2.82	0.42
1:A:273:LEU:HD12	1:A:273:LEU:HA	1.69	0.41
1:D:175:ALA:O	1:D:178:LEU:HB2	2.20	0.41
1:E:24:LEU:O	1:E:34:VAL:HG21	2.20	0.41
1:E:91:ASN:OD1	1:E:94:ARG:HB2	2.19	0.41
1:E:239:ILE:HG22	1:E:243:MET:HE2	2.01	0.41
1:F:137:PHE:CD1	1:F:137:PHE:N	2.87	0.41
1:C:33:ILE:HD13	1:C:166:PHE:CD1	2.54	0.41
1:C:235:ARG:HG3	1:C:237:GLU:OE1	2.20	0.41
1:D:54:PRO:HB2	1:D:57:VAL:HG21	2.02	0.41
1:D:83:ASN:HB3	1:D:86:ASP:HB2	2.02	0.41
1:C:193:GLY:O	1:C:196:ALA:HB3	2.21	0.41
1:D:22:GLN:HA	1:D:22:GLN:NE2	2.34	0.41
1:D:306:GLU:HG2	1:F:312:ILE:CD1	2.46	0.41
1:A:177:ARG:HH11	1:A:177:ARG:HA	1.86	0.41
1:A:281:PHE:HA	1:A:290:LYS:HD3	2.02	0.41
1:C:94:ARG:HA	1:C:97:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LEU:HD12	1:F:324:ILE:HG21	2.01	0.41
1:A:91:ASN:HD22	1:A:91:ASN:N	2.17	0.41
1:C:15:TRP:HE3	1:C:15:TRP:N	2.17	0.41
1:D:25:ASP:OD2	1:D:38:LYS:HD3	2.20	0.41
1:D:74:ASN:C	1:D:76:ARG:N	2.73	0.41
1:D:311:ILE:HG22	3:D:332:HOH:O	2.19	0.41
1:E:309:ASN:ND2	1:E:309:ASN:C	2.74	0.41
1:F:91:ASN:O	1:F:95:GLU:HB2	2.20	0.41
1:F:94:ARG:HD3	1:F:129:ALA:CB	2.36	0.41
1:F:135:GLU:HB2	1:F:160:ARG:NH1	2.25	0.41
1:A:174:ILE:HG12	1:A:205:MET:CE	2.50	0.41
1:B:111:PHE:HB2	1:B:140:ASN:O	2.21	0.41
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.94	0.41
1:C:46:MET:HG2	1:C:111:PHE:CZ	2.56	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.92	0.41
1:D:149:TYR:CD1	1:D:152:LYS:HE3	2.55	0.41
1:F:127:GLN:O	1:F:131:ARG:HB2	2.21	0.41
1:A:167:ARG:HG3	1:A:167:ARG:NH1	2.30	0.41
1:B:37:LEU:HA	1:B:40:TYR:CD2	2.55	0.41
1:D:16:VAL:HG12	1:D:209:ILE:HB	2.03	0.41
1:E:31:GLU:O	1:E:34:VAL:HG12	2.20	0.41
1:E:240:ARG:HG2	1:E:279:GLU:HB3	2.02	0.41
1:A:50:LEU:HD23	1:A:50:LEU:C	2.40	0.41
1:A:174:ILE:HG12	1:A:205:MET:HE2	2.02	0.41
1:A:200:ILE:HD12	1:A:227:VAL:HG12	2.03	0.41
1:B:22:GLN:OE1	1:B:68:ARG:CZ	2.68	0.41
1:B:86:ASP:HB2	1:B:89:GLY:N	2.36	0.41
1:C:182:ALA:HA	1:C:187:LEU:HB2	2.02	0.41
1:C:216:ALA:C	1:C:218:LEU:H	2.25	0.41
1:D:199:TYR:CE2	1:D:236:PRO:HG2	2.56	0.41
1:D:304:LEU:HD12	1:D:304:LEU:HA	1.75	0.41
1:E:245:LEU:HD12	1:E:245:LEU:HA	1.93	0.41
1:F:71:PHE:CD1	1:F:78:ASN:HB2	2.56	0.41
1:A:252:LEU:HD22	1:B:287:GLU:CG	2.51	0.41
1:B:314:LEU:HD12	1:B:314:LEU:HA	1.87	0.41
1:D:98:LYS:HG2	1:D:137:PHE:CZ	2.56	0.41
1:A:270:GLU:HG2	1:A:301:ASN:ND2	2.34	0.40
1:C:182:ALA:CA	1:C:187:LEU:HB2	2.51	0.40
1:C:253:LYS:HA	1:C:253:LYS:HD2	1.87	0.40
1:E:199:TYR:CZ	1:E:278:LYS:HE2	2.56	0.40
1:F:163:ILE:HD12	1:F:163:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:HA	1:B:240:ARG:HH11	1.86	0.40
1:C:174:ILE:HA	1:C:205:MET:HE1	2.02	0.40
1:C:296:LYS:HD3	1:C:296:LYS:HA	1.84	0.40
1:D:135:GLU:CB	1:D:160:ARG:HH12	2.30	0.40
1:D:262:LEU:HD12	1:D:262:LEU:HA	1.92	0.40
1:F:11:LEU:HD13	1:F:11:LEU:O	2.22	0.40
1:F:20:ARG:CZ	1:F:61:THR:HG22	2.51	0.40
1:A:92:VAL:HG22	1:A:92:VAL:O	2.21	0.40
1:B:104:LYS:HB3	1:B:104:LYS:HZ2	1.85	0.40
1:C:141:VAL:HG22	1:C:142:ARG:H	1.84	0.40
1:D:40:TYR:HD1	1:D:45:SER:O	2.04	0.40
1:A:296:LYS:HA	1:A:296:LYS:HD3	1.85	0.40
1:B:223:THR:HG23	1:B:226:ASN:H	1.87	0.40
1:C:315:GLU:OE2	1:F:255:ARG:CG	2.69	0.40
1:D:173:ASP:O	1:D:176:LYS:HB2	2.22	0.40
1:D:287:GLU:N	1:D:288:PRO:CD	2.85	0.40
1:E:22:GLN:HE21	1:E:22:GLN:HB2	1.69	0.40
1:E:283:LEU:HA	1:E:284:PRO:HD3	1.77	0.40
1:F:30:GLN:NE2	1:F:30:GLN:CA	2.83	0.40
1:D:36:ARG:HB2	1:D:164:PHE:HE2	1.87	0.40
1:F:46:MET:HG3	1:F:46:MET:O	2.21	0.40
1:F:71:PHE:O	1:F:74:ASN:N	2.55	0.40
1:F:174:ILE:O	1:F:178:LEU:HD13	2.21	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	324/327 (99%)	306 (94%)	17 (5%)	1 (0%)	41 72
1	B	324/327 (99%)	303 (94%)	12 (4%)	9 (3%)	5 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	317/327 (97%)	271 (86%)	34 (11%)	12 (4%)	3 10
1	D	324/327 (99%)	287 (89%)	27 (8%)	10 (3%)	4 14
1	E	324/327 (99%)	298 (92%)	17 (5%)	9 (3%)	5 17
1	F	324/327 (99%)	285 (88%)	35 (11%)	4 (1%)	13 39
All	All	1937/1962 (99%)	1750 (90%)	142 (7%)	45 (2%)	6 21

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	88	ARG
1	C	10	VAL
1	C	11	LEU
1	C	88	ARG
1	D	189	LEU
1	E	31	GLU
1	E	85	SER
1	B	31	GLU
1	B	86	ASP
1	B	264	LYS
1	C	219	ASP
1	D	138	SER
1	D	264	LYS
1	E	24	LEU
1	E	59	LYS
1	E	90	ILE
1	E	92	VAL
1	F	264	LYS
1	B	85	SER
1	B	87	GLU
1	B	90	ILE
1	B	92	VAL
1	B	219	ASP
1	C	87	GLU
1	C	326	LYS
1	D	88	ARG
1	F	4	GLU
1	C	180	TYR
1	C	184	ASN
1	C	264	LYS
1	C	284	PRO
1	D	265	GLN

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Mol	Chain	Res	Type
1	E	93	ILE
1	E	185	GLU
1	A	202	GLU
1	C	260	GLU
1	D	180	TYR
1	F	325	GLY
1	D	177	ARG
1	D	21	PRO
1	D	90	ILE
1	F	105	PRO
1	C	227	VAL
1	D	186	GLY
1	E	47	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	278/279 (100%)	254 (91%)	24 (9%)	10 30
1	B	278/279 (100%)	256 (92%)	22 (8%)	12 34
1	C	271/279 (97%)	254 (94%)	17 (6%)	18 46
1	D	278/279 (100%)	263 (95%)	15 (5%)	22 53
1	E	278/279 (100%)	251 (90%)	27 (10%)	8 24
1	F	278/279 (100%)	261 (94%)	17 (6%)	18 48
All	All	1661/1674 (99%)	1539 (93%)	122 (7%)	14 38

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	37	LEU
1	A	57	VAL
1	A	61	THR
1	A	66	LEU

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Mol	Chain	Res	Type
1	A	73	GLU
1	A	95	GLU
1	A	104	LYS
1	A	189	LEU
1	A	229	MET
1	A	235	ARG
1	A	244	LEU
1	A	245	LEU
1	A	252	LEU
1	A	256	GLU
1	A	262	LEU
1	A	265	GLN
1	A	267	LEU
1	A	273	LEU
1	A	293	LEU
1	A	303	ARG
1	A	304	LEU
1	A	314	LEU
1	A	322	THR
1	B	24	LEU
1	B	37	LEU
1	B	41	VAL
1	B	49	LEU
1	B	95	GLU
1	B	104	LYS
1	B	142	ARG
1	B	176	LYS
1	B	189	LEU
1	B	235	ARG
1	B	244	LEU
1	B	245	LEU
1	B	252	LEU
1	B	255	ARG
1	B	262	LEU
1	B	275	GLN
1	B	277	HIS
1	B	279	GLU
1	B	285	ILE
1	B	304	LEU
1	B	314	LEU
1	B	317	LEU
1	C	15	TRP

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Mol	Chain	Res	Type
1	C	73	GLU
1	C	75	TRP
1	C	124	GLN
1	C	131	ARG
1	C	140	ASN
1	C	152	LYS
1	C	165	ARG
1	C	176	LYS
1	C	177	ARG
1	C	184	ASN
1	C	189	LEU
1	C	244	LEU
1	C	245	LEU
1	C	250	ASN
1	C	263	LEU
1	C	314	LEU
1	D	73	GLU
1	D	81	GLU
1	D	99	GLU
1	D	218	LEU
1	D	233	ARG
1	D	252	LEU
1	D	255	ARG
1	D	259	ARG
1	D	262	LEU
1	D	270	GLU
1	D	273	LEU
1	D	287	GLU
1	D	293	LEU
1	D	304	LEU
1	D	314	LEU
1	E	15	TRP
1	E	21	PRO
1	E	22	GLN
1	E	31	GLU
1	E	37	LEU
1	E	80	LEU
1	E	88	ARG
1	E	90	ILE
1	E	94	ARG
1	E	142	ARG
1	E	176	LYS

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Mol	Chain	Res	Type
1	E	195	GLN
1	E	244	LEU
1	E	245	LEU
1	E	247	LEU
1	E	252	LEU
1	E	256	GLU
1	E	259	ARG
1	E	262	LEU
1	E	267	LEU
1	E	292	LEU
1	E	293	LEU
1	E	304	LEU
1	E	309	ASN
1	E	314	LEU
1	E	317	LEU
1	E	323	LEU
1	F	11	LEU
1	F	30	GLN
1	F	86	ASP
1	F	98	LYS
1	F	140	ASN
1	F	171	ASP
1	F	194	LEU
1	F	207	ARG
1	F	233	ARG
1	F	245	LEU
1	F	247	LEU
1	F	252	LEU
1	F	265	GLN
1	F	304	LEU
1	F	309	ASN
1	F	312	ILE
1	F	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	250	ASN
1	A	265	GLN
1	A	282	ASN
1	A	301	ASN

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Mol	Chain	Res	Type
1	A	309	ASN
1	B	78	ASN
1	B	83	ASN
1	B	91	ASN
1	B	195	GLN
1	B	210	ASN
1	B	213	GLN
1	B	250	ASN
1	B	265	GLN
1	B	282	ASN
1	C	91	ASN
1	C	124	GLN
1	C	128	GLN
1	C	184	ASN
1	C	210	ASN
1	C	226	ASN
1	C	250	ASN
1	C	265	GLN
1	C	275	GLN
1	C	277	HIS
1	C	282	ASN
1	C	320	GLN
1	D	22	GLN
1	D	74	ASN
1	D	140	ASN
1	D	195	GLN
1	D	226	ASN
1	D	250	ASN
1	D	265	GLN
1	D	282	ASN
1	E	30	GLN
1	E	77	HIS
1	E	78	ASN
1	E	124	GLN
1	E	128	GLN
1	E	158	GLN
1	E	265	GLN
1	E	282	ASN
1	E	309	ASN
1	F	30	GLN
1	F	77	HIS
1	F	127	GLN

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Mol	Chain	Res	Type
1	F	140	ASN
1	F	213	GLN
1	F	265	GLN
1	F	282	ASN
1	F	309	ASN
1	F	313	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	ADP	C	403	-	24,29,29	1.92	6 (25%)	29,45,45	0.87	0
2	ADP	B	402	-	24,29,29	1.99	9 (37%)	29,45,45	1.12	3 (10%)
2	ADP	A	401	-	24,29,29	2.18	7 (29%)	29,45,45	0.91	1 (3%)
2	ADP	E	404	-	24,29,29	2.02	8 (33%)	29,45,45	1.07	2 (6%)

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	ADP	C	403	-	-	4/12/32/32	0/3/3/3
2	ADP	B	402	-	-	3/12/32/32	0/3/3/3
2	ADP	A	401	-	-	4/12/32/32	0/3/3/3
2	ADP	E	404	-	-	4/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ADP	PA-O3A	7.34	1.67	1.59
2	E	404	ADP	PA-O3A	6.16	1.66	1.59
2	C	403	ADP	PA-O3A	5.93	1.65	1.59
2	B	402	ADP	PA-O3A	5.86	1.65	1.59
2	A	401	ADP	C8-N7	-3.85	1.27	1.34
2	B	402	ADP	C8-N7	-3.81	1.27	1.34
2	E	404	ADP	C8-N7	-3.56	1.28	1.34
2	C	403	ADP	C8-N7	-3.39	1.28	1.34
2	A	401	ADP	O4'-C1'	3.04	1.44	1.40
2	C	403	ADP	O4'-C1'	2.80	1.44	1.40
2	A	401	ADP	C2-N3	2.77	1.36	1.32
2	E	404	ADP	O4'-C1'	2.75	1.44	1.40
2	C	403	ADP	C2-N3	2.73	1.36	1.32
2	E	404	ADP	C1'-N9	2.70	1.56	1.49
2	B	402	ADP	O4'-C1'	2.67	1.44	1.40
2	C	403	ADP	C1'-N9	2.60	1.56	1.49
2	B	402	ADP	C2-N3	2.60	1.36	1.32
2	A	401	ADP	O4'-C4'	2.59	1.50	1.45
2	E	404	ADP	C2-N3	2.57	1.36	1.32
2	B	402	ADP	O4'-C4'	2.51	1.50	1.45
2	E	404	ADP	C2'-C3'	2.49	1.60	1.53
2	B	402	ADP	PA-O2A	-2.38	1.44	1.55
2	B	402	ADP	C2'-C3'	2.31	1.59	1.53
2	A	401	ADP	C2'-C3'	2.30	1.59	1.53
2	E	404	ADP	O4'-C4'	2.24	1.50	1.45
2	C	403	ADP	O4'-C4'	2.19	1.49	1.45
2	E	404	ADP	PA-O2A	-2.14	1.45	1.55
2	A	401	ADP	PA-O2A	-2.12	1.45	1.55
2	B	402	ADP	C1'-N9	2.06	1.55	1.49
2	B	402	ADP	O2'-C2'	2.01	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	404	ADP	C4'-O4'-C1'	3.30	112.95	109.92
2	B	402	ADP	C4'-O4'-C1'	3.21	112.86	109.92
2	B	402	ADP	C2'-C3'-C4'	2.52	107.47	102.61
2	B	402	ADP	O3A-PA-O1A	-2.36	103.61	110.70
2	E	404	ADP	O3A-PA-O1A	-2.05	104.55	110.70
2	A	401	ADP	O5'-C5'-C4'	2.02	115.87	108.99

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	403	ADP	PA-O3A-PB-O2B
2	A	401	ADP	C3'-C4'-C5'-O5'
2	B	402	ADP	O4'-C4'-C5'-O5'
2	B	402	ADP	C3'-C4'-C5'-O5'
2	C	403	ADP	O4'-C4'-C5'-O5'
2	C	403	ADP	C3'-C4'-C5'-O5'
2	E	404	ADP	O4'-C4'-C5'-O5'
2	E	404	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	O4'-C4'-C5'-O5'
2	A	401	ADP	PA-O3A-PB-O1B
2	A	401	ADP	C4'-C5'-O5'-PA
2	C	403	ADP	C4'-C5'-O5'-PA
2	B	402	ADP	C4'-C5'-O5'-PA
2	E	404	ADP	C4'-C5'-O5'-PA
2	E	404	ADP	PA-O3A-PB-O3B

There are no ring outliers.

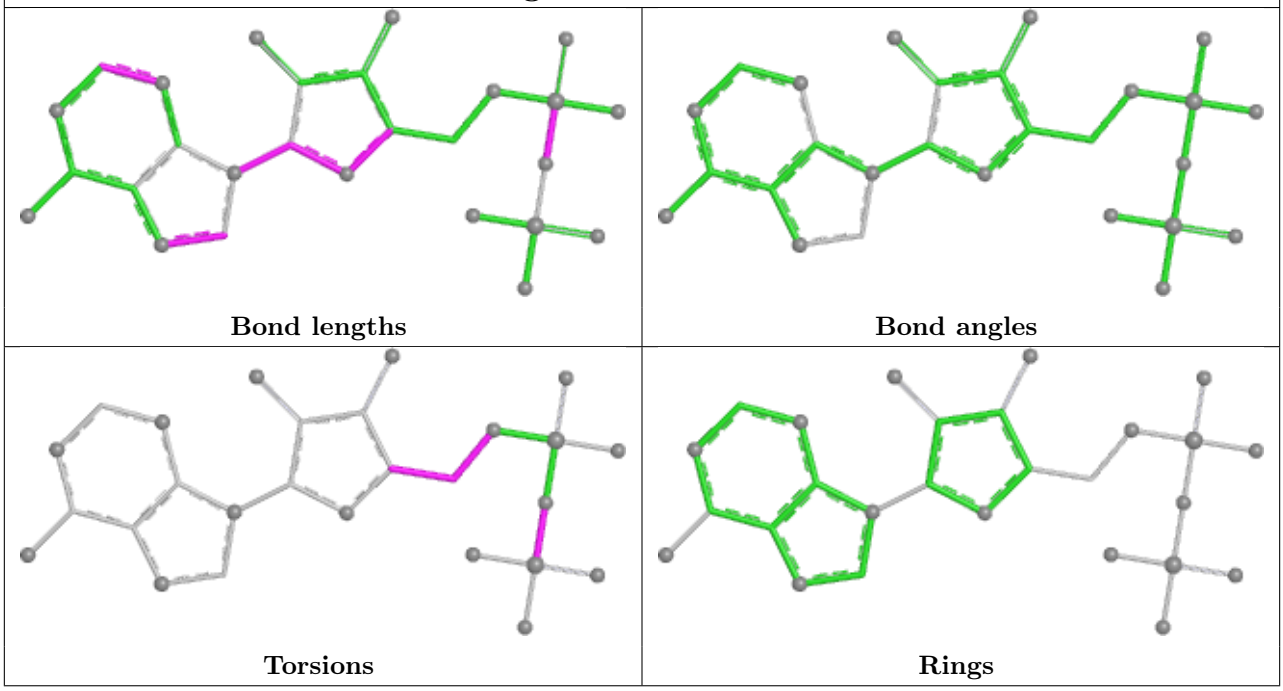
4 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	ADP	7	0
2	B	402	ADP	11	0
2	A	401	ADP	11	0
2	E	404	ADP	13	0

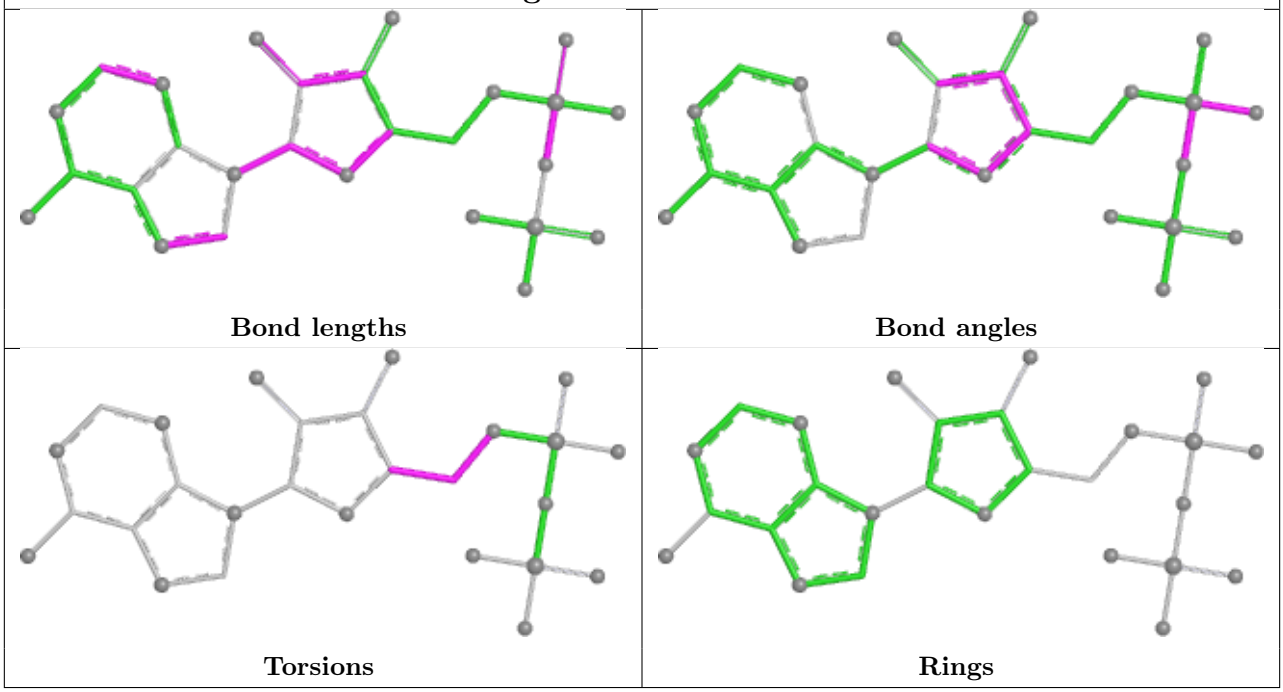
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

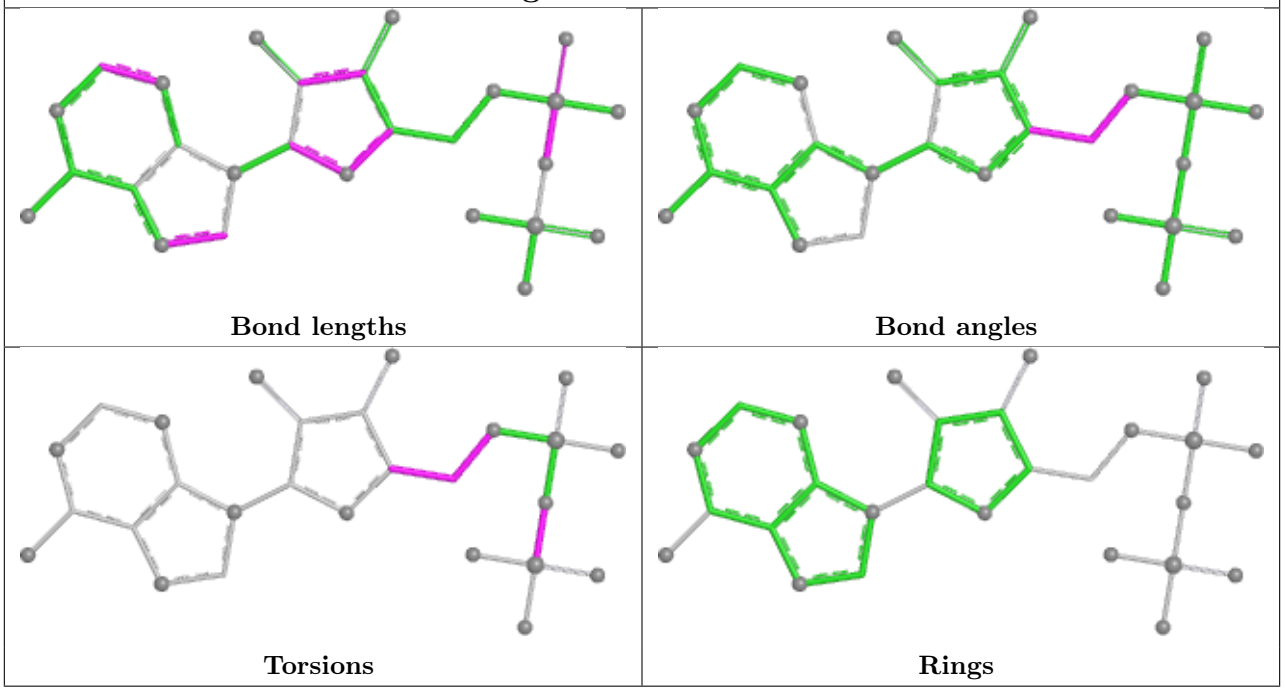
Ligand ADP C 403



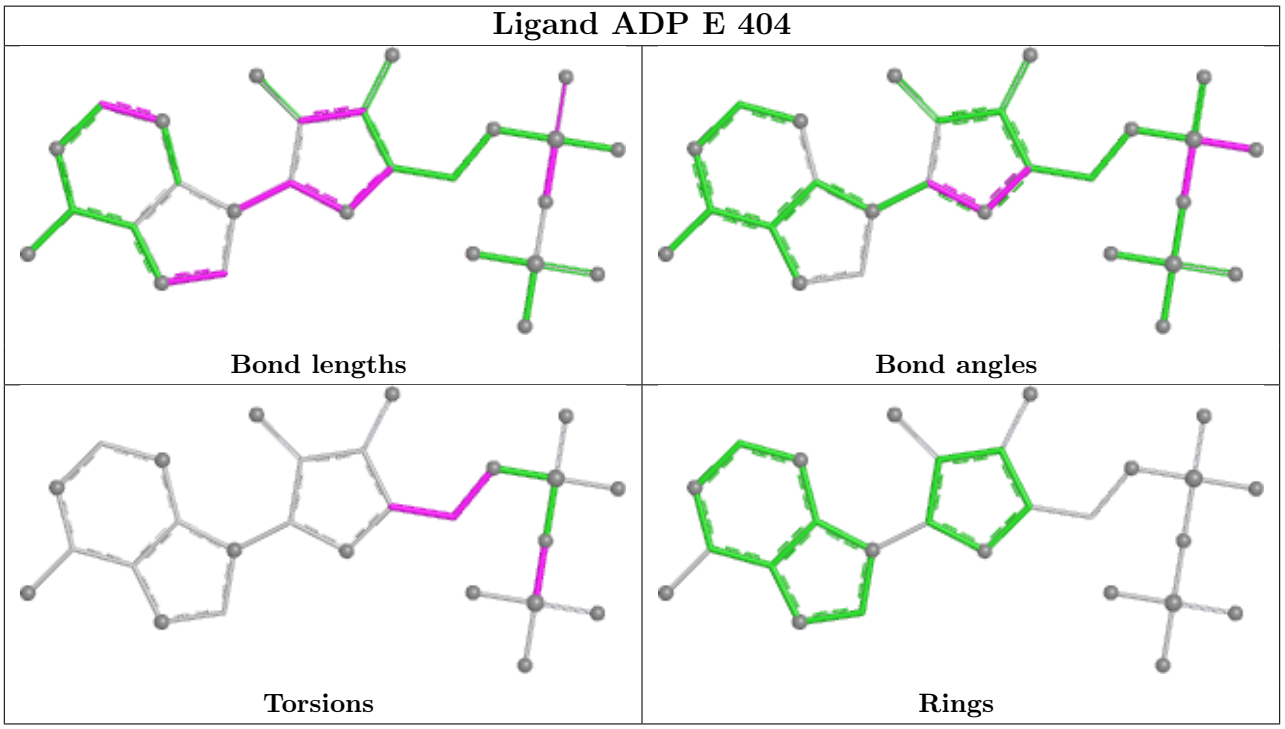
Ligand ADP B 402



Ligand ADP A 401



Ligand ADP E 404



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	326/327 (99%)	-0.19	3 (0%) 84 80	8, 39, 69, 98	0
1	B	326/327 (99%)	-0.25	0 100 100	12, 36, 67, 93	0
1	C	319/327 (97%)	0.55	35 (10%) 5 3	14, 75, 103, 107	0
1	D	326/327 (99%)	0.43	30 (9%) 9 5	17, 80, 101, 106	0
1	E	326/327 (99%)	-0.01	8 (2%) 57 47	21, 59, 91, 104	0
1	F	326/327 (99%)	-0.05	6 (1%) 68 61	17, 59, 93, 105	0
All	All	1949/1962 (99%)	0.08	82 (4%) 36 26	8, 53, 99, 107	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	93	ILE	9.2
1	C	97	VAL	8.2
1	C	90	ILE	7.8
1	F	2	SER	6.8
1	E	93	ILE	6.6
1	D	29	GLY	6.0
1	C	107	GLY	5.8
1	C	108	GLY	5.5
1	C	91	ASN	5.4
1	D	34	VAL	5.1
1	D	2	SER	4.5
1	E	90	ILE	4.0
1	A	90	ILE	4.0
1	C	187	LEU	4.0
1	E	92	VAL	4.0
1	D	45	SER	3.9
1	C	215	ALA	3.7
1	D	111	PHE	3.6
1	C	133	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	89	GLY	3.4
1	D	42	LYS	3.4
1	C	96	LYS	3.4
1	D	57	VAL	3.3
1	C	101	ALA	3.2
1	D	97	VAL	3.2
1	C	94	ARG	3.1
1	E	2	SER	3.1
1	D	110	SER	3.0
1	D	106	ILE	3.0
1	C	80	LEU	3.0
1	D	140	ASN	2.9
1	D	90	ILE	2.9
1	A	92	VAL	2.9
1	C	88	ARG	2.9
1	D	103	THR	2.9
1	D	32	HIS	2.9
1	C	95	GLU	2.8
1	D	107	GLY	2.8
1	C	11	LEU	2.7
1	C	189	LEU	2.7
1	C	211	ILE	2.7
1	C	99	GLU	2.6
1	C	212	LEU	2.6
1	D	105	PRO	2.6
1	F	11	LEU	2.6
1	D	100	PHE	2.6
1	A	93	ILE	2.5
1	C	86	ASP	2.5
1	C	13	LYS	2.5
1	C	222	ILE	2.5
1	E	89	GLY	2.5
1	D	139	SER	2.5
1	D	40	TYR	2.5
1	F	90	ILE	2.5
1	C	180	TYR	2.5
1	C	220	LYS	2.4
1	D	141	VAL	2.4
1	D	137	PHE	2.3
1	E	94	ARG	2.3
1	C	134	MET	2.3
1	D	43	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	208	ALA	2.3
1	D	28	VAL	2.3
1	D	30	GLN	2.3
1	D	101	ALA	2.2
1	D	128	GLN	2.2
1	C	10	VAL	2.2
1	C	106	ILE	2.2
1	C	78	ASN	2.2
1	D	113	ILE	2.2
1	E	88	ARG	2.2
1	C	140	ASN	2.2
1	D	159	SER	2.2
1	F	89	GLY	2.1
1	C	100	PHE	2.1
1	D	37	LEU	2.1
1	D	67	ALA	2.1
1	F	10	VAL	2.1
1	F	188	GLU	2.1
1	C	213	GLN	2.0
1	C	126	ALA	2.0
1	E	194	LEU	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, 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	ADP	C	403	27/27	0.74	0.39	105,110,124,124	0
2	ADP	A	401	27/27	0.79	0.45	105,106,111,112	0

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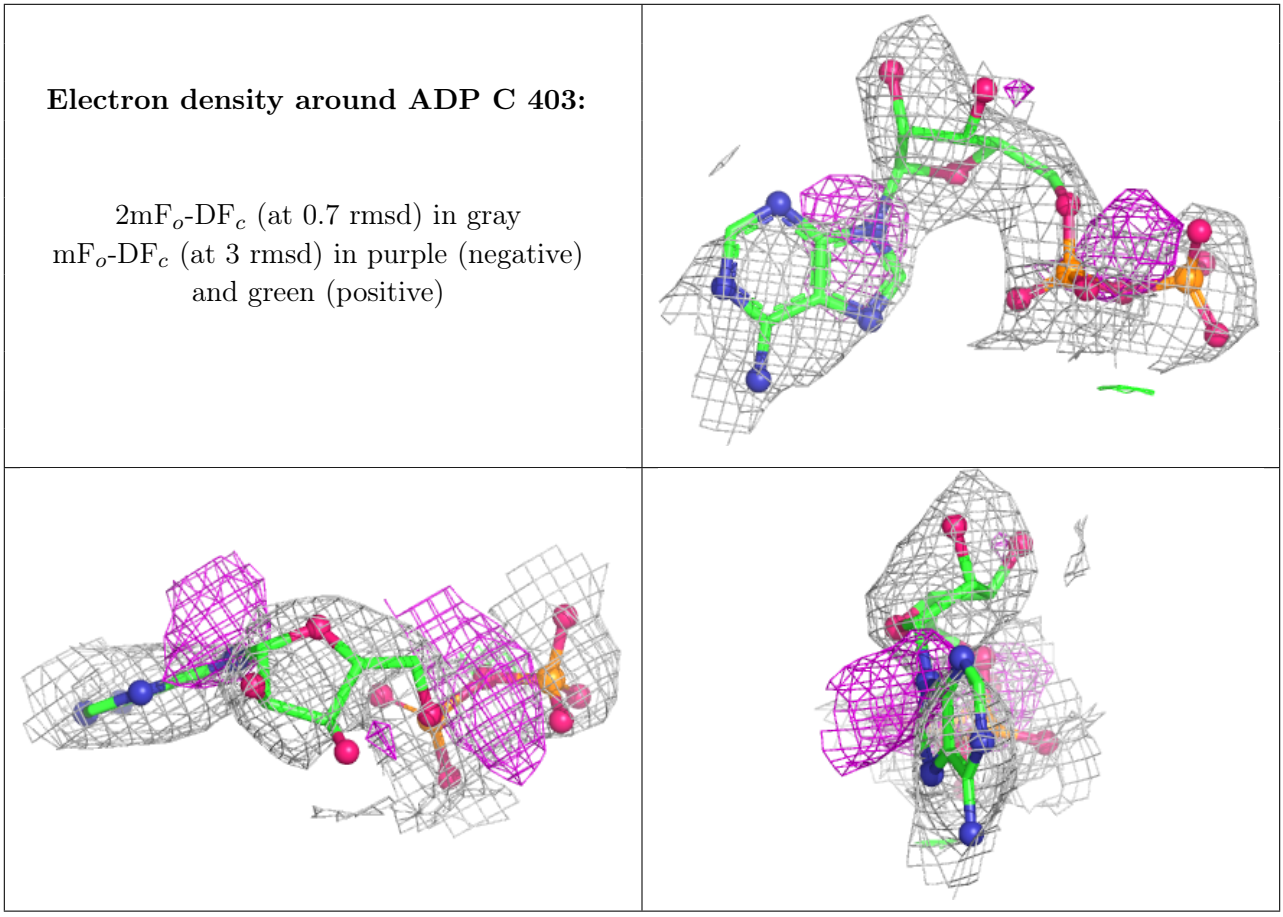
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	E	404	27/27	0.82	0.40	106,108,112,113	0
2	ADP	B	402	27/27	0.85	0.37	77,79,80,81	0

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.

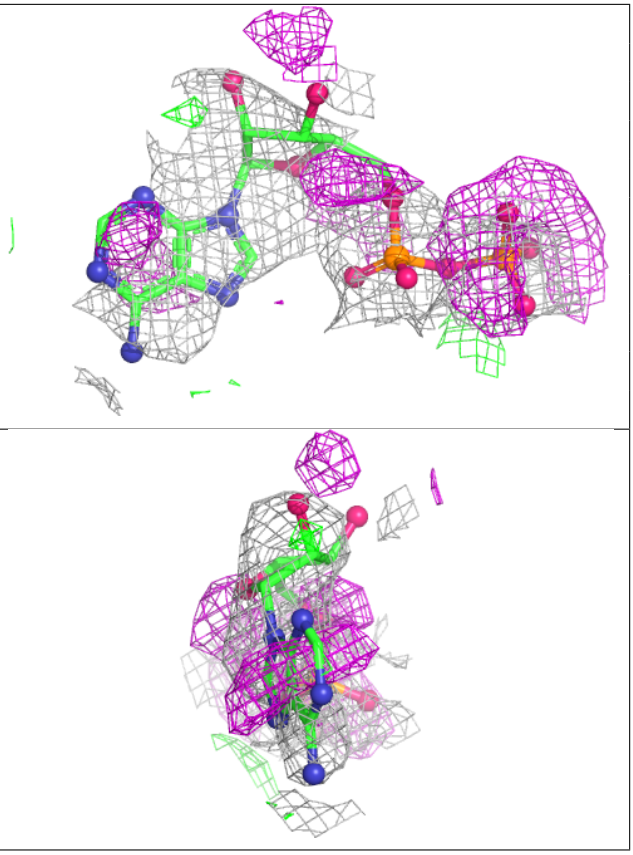
Electron density around ADP C 403:

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



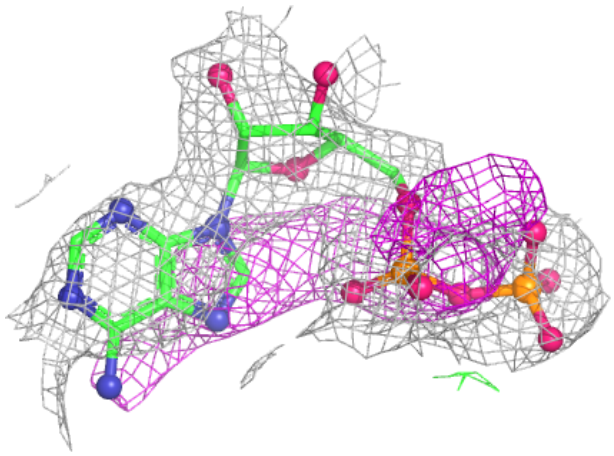
Electron density around ADP A 401:

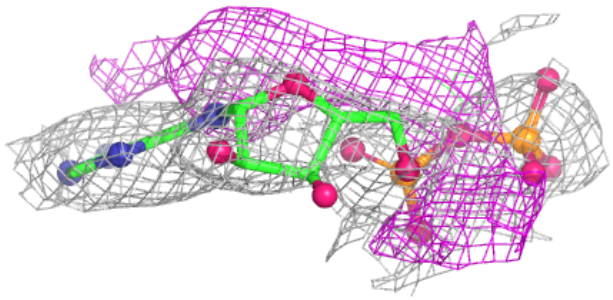
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

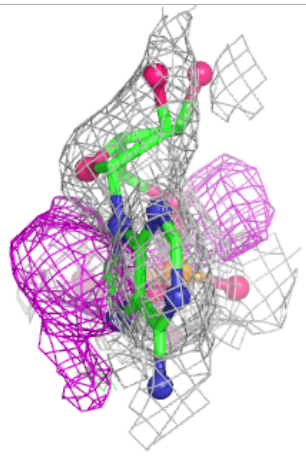


Electron density around ADP E 404:

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

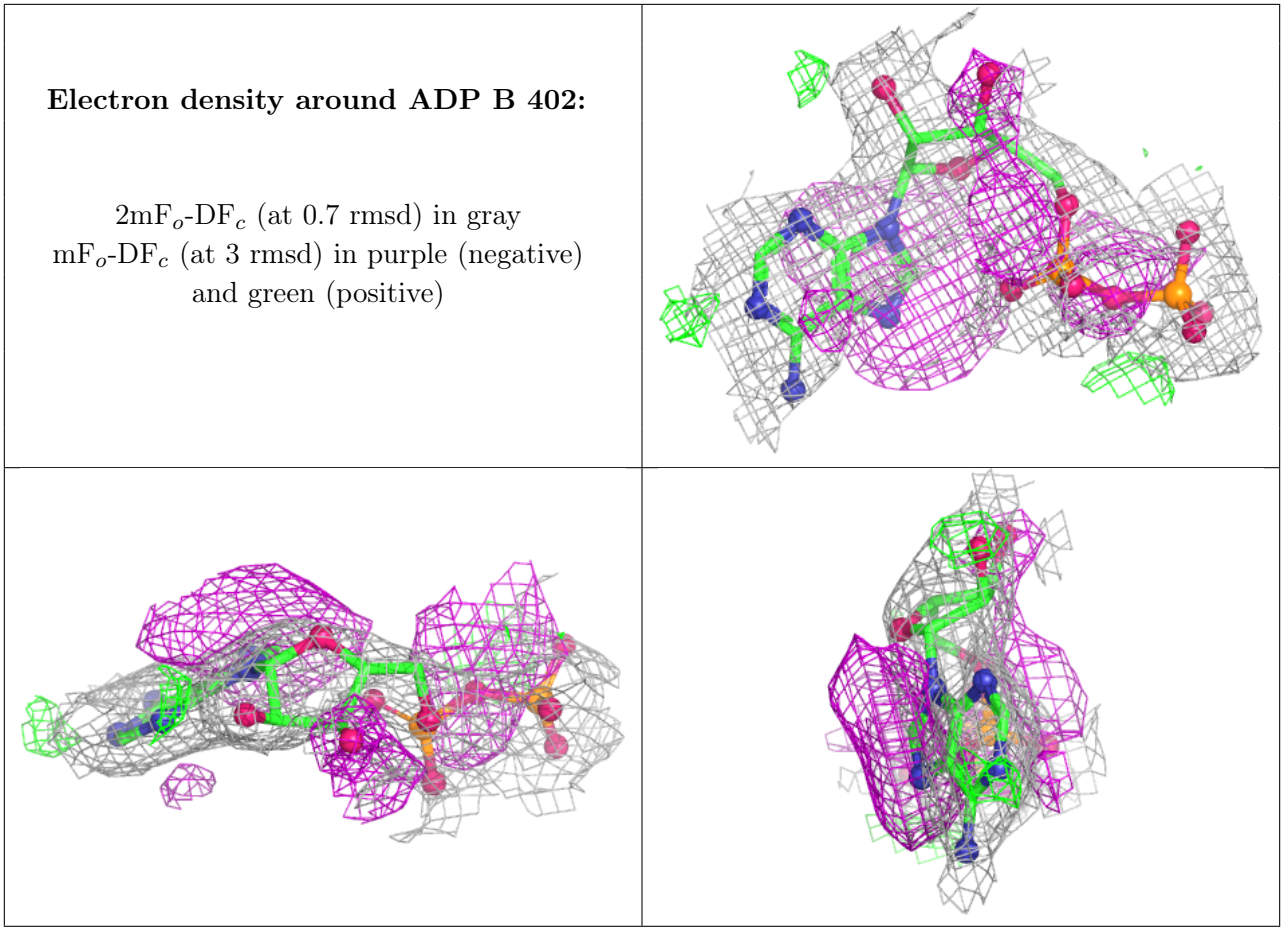






Electron density around ADP B 402:

$2mF_o$-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.