Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 10:58 AM EST

PDB ID	:	2P9S
Title	:	Structure of bovine Arp2/3 complex co-crystallized with ATP/Mg2+
Authors	:	Nolen, B.J.; Pollard, T.D.
Deposited on	:	2007-03-26
Resolution	:	2.68 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:

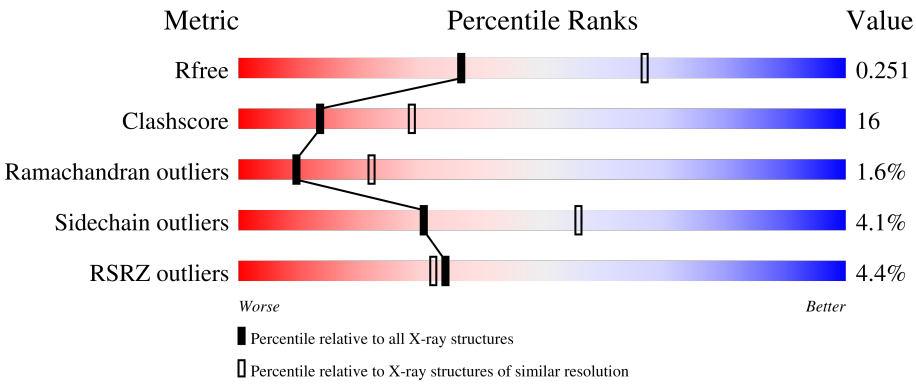
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	418	2%, 71%, 21%, • 5%
2	B	394	8%, 30%, 18%, •, 50%
3	C	372	.%, 61%, 28%, •• 8%
4	D	300	.%, 70%, 22%, • 7%
5	E	178	7%, 58%, 34%, • •

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Mol	Chain	Length	Quality of chain
6	F	168	% 76% 21%
7	G	151	9% 59% 27% 11%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13608 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 Actin-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3125	2006	517	587	15	0	0	0

- Molecule 2 is a protein called Actin-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	197	1487	951	251	281	4	0	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	341	2641	1676	463	483	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	58	VAL	ILE	conflict	UNP Q58CQ2

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	280	2249	1430	392	419	8	0	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	173	1411	906	235	261	9	0	0	0

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	167	1371	875	239	248	9	0	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	135	1028	643	177	205	3	0	0	0

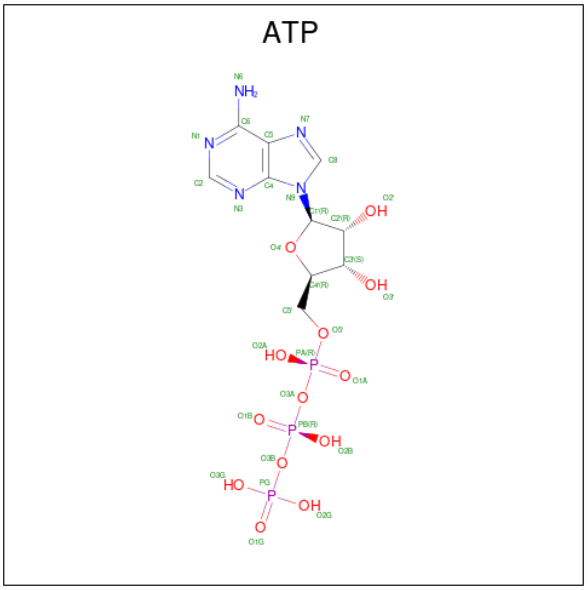
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	17	ASP	GLY	conflict	UNP Q3SYX9
G	28	ASP	GLU	conflict	UNP Q3SYX9

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	A	1	1	1	0	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
9	B	1	31	10	5	13	3	0	0

- Molecule 10 is water.

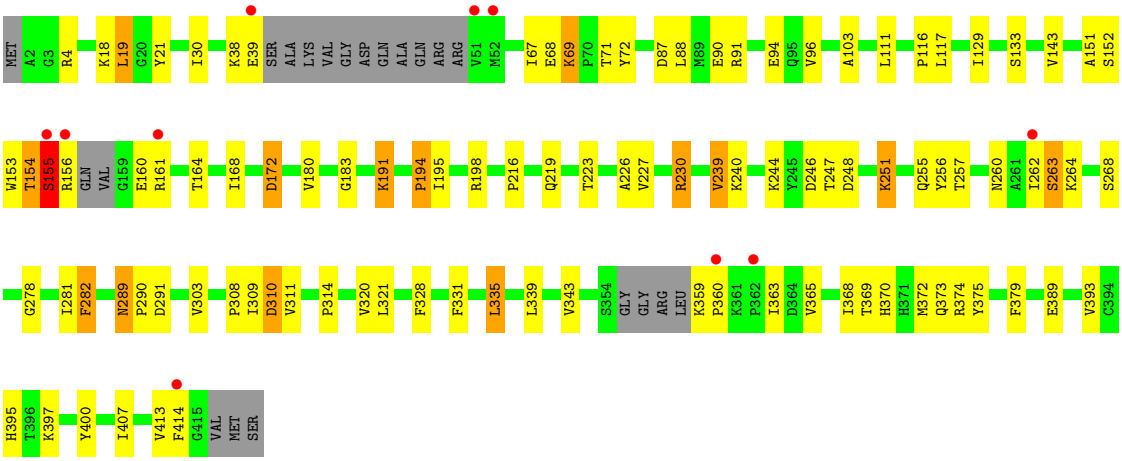
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	50	50	50	0	0
			Total	O		
10	B	15	15	15	0	0
			Total	O		
10	C	61	61	61	0	0
			Total	O		
10	D	47	47	47	0	0
			Total	O		
10	E	14	14	14	0	0
			Total	O		
10	F	39	39	39	0	0
			Total	O		
10	G	7	7	7	0	0

3 Residue-property plots (i)

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

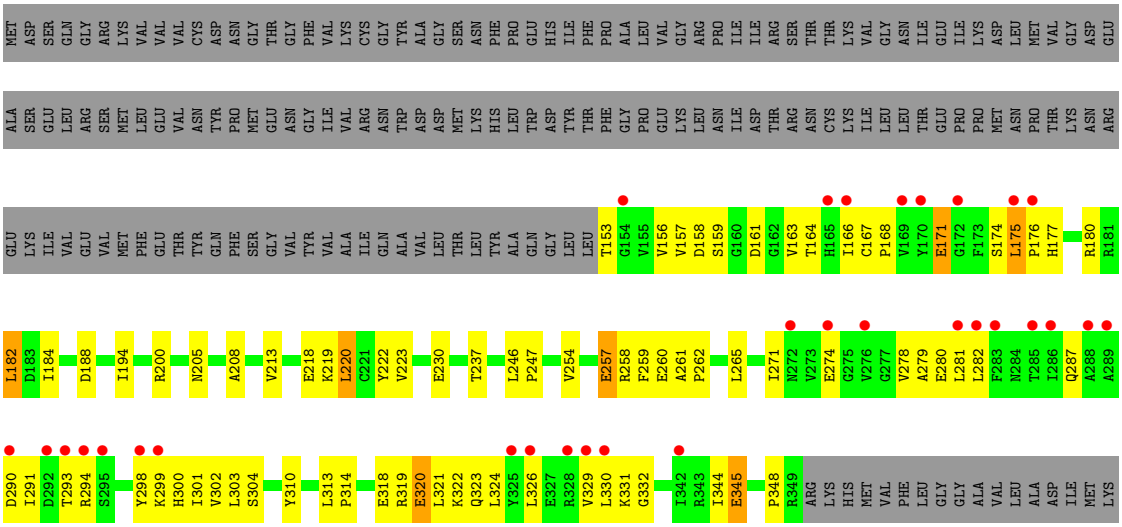
- Molecule 1: Actin-like protein 3

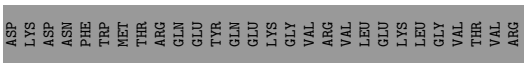
Chain A:



- Molecule 2: Actin-like protein 2

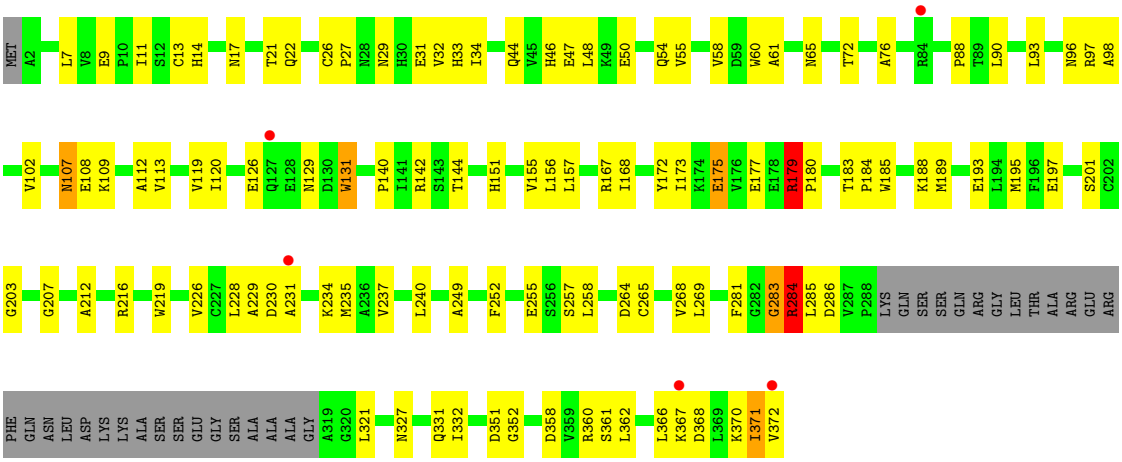
Chain B:





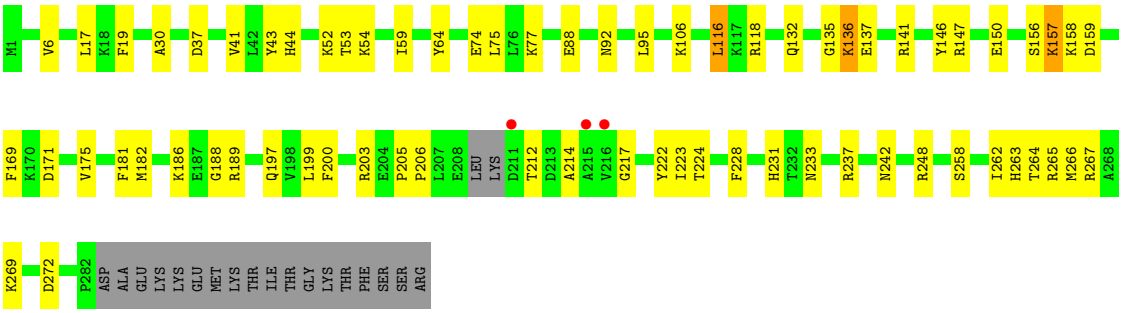
• Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:



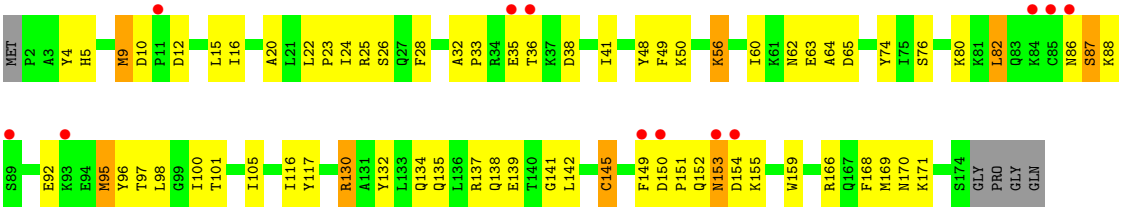
• Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



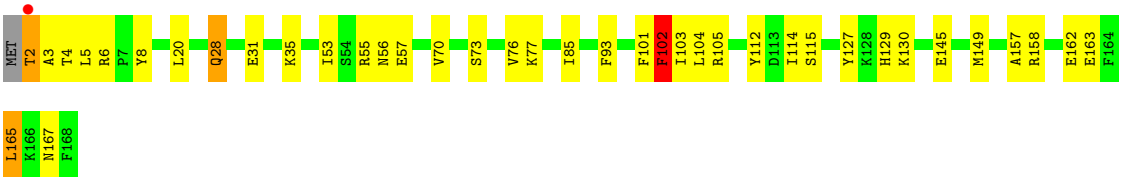
• Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



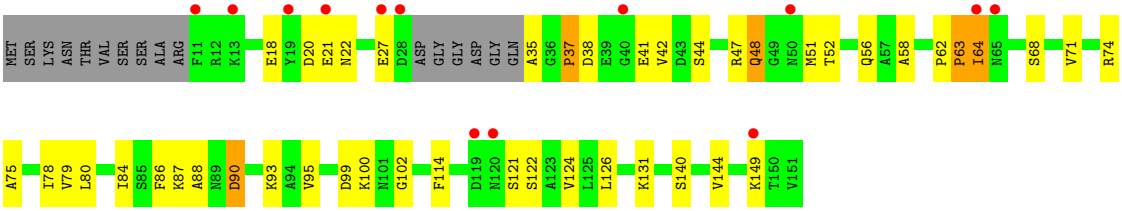
• Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.02Å 128.69Å 201.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.68 46.45 – 2.68	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.68) 95.3 (46.45-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	10.40	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.261 0.213 , 0.251	Depositor DCC
R_{free} test set	4068 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.0	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	0.93	EDS
Total number of atoms	13608	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 (i)

5.1 Standard geometry (i)

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

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	0.42	0/3205	0.63	1/4358 (0.0%)
2	B	0.34	0/1514	0.59	0/2059
3	C	0.40	0/2710	0.70	1/3680 (0.0%)
4	D	0.39	0/2297	0.59	0/3101
5	E	0.36	0/1445	0.62	0/1949
6	F	0.40	0/1393	0.61	0/1868
7	G	0.32	0/1040	0.55	0/1401
All	All	0.39	0/13604	0.62	2/18416 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	SER	N-CA-C	7.53	131.34	111.00
3	C	283	GLY	N-CA-C	6.30	128.86	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3125	0	3001	87	0
2	B	1487	0	1440	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2641	0	2589	100	0
4	D	2249	0	2206	62	0
5	E	1411	0	1413	71	0
6	F	1371	0	1410	34	0
7	G	1028	0	1029	31	0
8	A	1	0	0	0	0
9	A	31	0	12	2	0
9	B	31	0	12	3	0
10	A	50	0	0	2	0
10	B	15	0	0	0	0
10	C	61	0	0	1	0
10	D	47	0	0	1	0
10	E	14	0	0	0	0
10	F	39	0	0	0	0
10	G	7	0	0	0	0
All	All	13608	0	13112	425	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 16.

All (425) 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)
3:C:216:ARG:HG2	3:C:230:ASP:HB3	1.32	1.10
3:C:183:THR:HG22	3:C:185:TRP:H	1.24	1.01
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.45	0.99
3:C:14:HIS:H	3:C:331:GLN:HE22	1.07	0.91
3:C:201:SER:HB3	7:G:149:LYS:NZ	1.90	0.87
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.57	0.86
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.42	0.84
1:A:257:THR:HG22	1:A:268:SER:HB3	1.61	0.83
3:C:107:ASN:ND2	3:C:109:LYS:H	1.76	0.83
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.63	0.80
3:C:201:SER:HB3	7:G:149:LYS:HZ3	1.47	0.80
3:C:29:ASN:HB3	3:C:31:GLU:H	1.47	0.80
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.82	0.79
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.64	0.79
5:E:86:ASN:HB3	5:E:154:ASP:OD1	1.84	0.78
1:A:154:THR:O	1:A:155:SER:HB2	1.84	0.77
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.64	0.77
3:C:183:THR:HG23	3:C:184:PRO:HD2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD21	2:B:301:ILE:HD13	1.69	0.75
6:F:20:LEU:HD23	6:F:70:VAL:HG21	1.68	0.75
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.67	0.75
3:C:14:HIS:N	3:C:331:GLN:HE22	1.84	0.74
1:A:262:ILE:C	1:A:264:LYS:H	1.90	0.74
3:C:14:HIS:H	3:C:331:GLN:NE2	1.86	0.73
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.67	0.73
3:C:107:ASN:C	3:C:107:ASN:HD22	1.91	0.73
5:E:88:LYS:H	5:E:153:ASN:ND2	1.87	0.73
7:G:51:MET:HG3	7:G:87:LYS:NZ	2.04	0.72
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.70	0.72
4:D:137:GLU:OE2	4:D:158:LYS:HE2	1.89	0.72
3:C:17:ASN:ND2	3:C:22:GLN:HG3	2.05	0.72
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.54	0.72
7:G:51:MET:HG3	7:G:87:LYS:HZ3	1.55	0.71
6:F:2:THR:HG23	6:F:3:ALA:H	1.56	0.71
2:B:166:ILE:HD12	2:B:281:LEU:CD2	2.21	0.70
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.54	0.70
4:D:197:GLN:NE2	4:D:199:LEU:HD11	2.07	0.70
4:D:266:MET:HE3	6:F:93:PHE:CD1	2.27	0.69
5:E:150:ASP:C	5:E:152:GLN:H	1.96	0.69
1:A:321:LEU:HD12	1:A:369:THR:HG22	1.75	0.69
3:C:216:ARG:HG2	3:C:230:ASP:CB	2.18	0.68
3:C:34:ILE:HB	3:C:46:HIS:HB2	1.74	0.68
3:C:284:ARG:NH1	3:C:286:ASP:O	2.25	0.68
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.74	0.68
3:C:183:THR:HG22	3:C:185:TRP:N	2.05	0.67
2:B:318:GLU:HG3	2:B:344:ILE:HD12	1.75	0.67
7:G:38:ASP:O	7:G:42:VAL:HG23	1.95	0.66
1:A:262:ILE:O	1:A:264:LYS:N	2.28	0.66
3:C:107:ASN:HD22	3:C:108:GLU:N	1.93	0.66
3:C:269:LEU:H	3:C:283:GLY:HA2	1.61	0.66
2:B:218:GLU:HG2	9:B:502:ATP:C5	2.30	0.66
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.11	0.66
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.25	0.66
1:A:311:VAL:C	1:A:314:PRO:HD2	2.17	0.66
6:F:4:THR:HG23	6:F:55:ARG:HE	1.60	0.65
1:A:239:VAL:HG22	5:E:4:TYR:CZ	2.31	0.65
1:A:87:ASP:OD2	4:D:264:THR:HG22	1.97	0.65
2:B:230:GLU:OE2	6:F:35:LYS:HE3	1.97	0.65
5:E:22:LEU:HD23	5:E:41:ILE:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.31	0.64
5:E:76:SER:O	5:E:80:LYS:HG3	1.98	0.64
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.30	0.64
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.80	0.64
5:E:20:ALA:HB1	5:E:22:LEU:HD13	1.80	0.63
3:C:183:THR:HG23	3:C:184:PRO:CD	2.29	0.63
2:B:153:THR:CB	2:B:171:GLU:H	2.12	0.63
4:D:206:PRO:HD3	4:D:222:TYR:CG	2.33	0.63
7:G:121:SER:O	7:G:124:VAL:HG12	2.00	0.62
5:E:16:ILE:HG23	5:E:16:ILE:O	2.00	0.62
5:E:24:ILE:HD11	5:E:135:GLN:HG2	1.81	0.62
4:D:228:PHE:H	4:D:231:HIS:HD2	1.48	0.62
1:A:343:VAL:HG13	1:A:363:ILE:HD12	1.82	0.61
5:E:150:ASP:O	5:E:152:GLN:N	2.34	0.61
1:A:152:SER:C	1:A:154:THR:N	2.52	0.61
4:D:205:PRO:HB3	4:D:222:TYR:CZ	2.36	0.61
5:E:95:MET:HG2	5:E:141:GLY:O	2.01	0.61
2:B:205:ASN:HD22	2:B:208:ALA:H	1.48	0.60
1:A:87:ASP:CG	4:D:264:THR:HG22	2.22	0.60
3:C:229:ALA:HB2	3:C:237:VAL:HG22	1.83	0.60
6:F:101:PHE:O	6:F:103:ILE:N	2.35	0.60
3:C:142:ARG:HG3	3:C:142:ARG:HH11	1.66	0.60
3:C:281:PHE:CE1	3:C:283:GLY:HA3	2.36	0.60
5:E:150:ASP:C	5:E:152:GLN:N	2.55	0.60
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.84	0.60
1:A:164:THR:HA	1:A:180:VAL:O	2.03	0.59
4:D:233:ASN:O	4:D:237:ARG:HB2	2.01	0.59
3:C:370:LYS:O	3:C:371:ILE:HB	2.02	0.59
5:E:25:ARG:HH11	5:E:25:ARG:HG2	1.67	0.59
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.28	0.59
1:A:154:THR:CG2	1:A:370:HIS:HB2	2.33	0.59
3:C:21:THR:HG22	3:C:22:GLN:HG2	1.83	0.59
6:F:101:PHE:O	6:F:102:PHE:CD1	2.56	0.59
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.84	0.58
1:A:152:SER:C	1:A:154:THR:H	2.06	0.58
2:B:157:VAL:HB	2:B:303:LEU:HD13	1.84	0.58
5:E:86:ASN:O	5:E:87:SER:CB	2.52	0.58
3:C:27:PRO:HG3	3:C:33:HIS:CD2	2.38	0.58
4:D:17:LEU:HG	10:D:323:HOH:O	2.03	0.58
5:E:74:TYR:OH	5:E:98:LEU:HD12	2.04	0.58
1:A:311:VAL:O	1:A:314:PRO:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ILE:HG13	3:C:352:GLY:HA2	1.86	0.57
3:C:107:ASN:HD22	3:C:109:LYS:H	1.53	0.57
6:F:4:THR:HG23	6:F:55:ARG:NE	2.19	0.57
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.86	0.57
7:G:95:VAL:HG21	7:G:131:LYS:HB3	1.86	0.57
3:C:264:ASP:O	3:C:265:CYS:HB2	2.05	0.56
4:D:189:ARG:NH1	4:D:197:GLN:HB2	2.20	0.56
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.19	0.56
1:A:370:HIS:O	1:A:373:GLN:HG3	2.05	0.56
3:C:29:ASN:O	3:C:54:GLN:HA	2.05	0.56
3:C:252:PHE:HA	3:C:258:LEU:HD23	1.88	0.56
7:G:87:LYS:HD3	7:G:87:LYS:N	2.20	0.56
2:B:184:ILE:HD13	2:B:271:ILE:HD13	1.88	0.56
4:D:197:GLN:HE21	4:D:199:LEU:HD11	1.70	0.56
4:D:19:PHE:HB3	4:D:106:LYS:HD3	1.87	0.56
2:B:174:SER:O	2:B:176:PRO:HD3	2.06	0.56
1:A:19:LEU:HD23	1:A:19:LEU:N	2.21	0.56
1:A:289:ASN:HD22	1:A:290:PRO:CD	2.18	0.56
3:C:50:GLU:OE1	3:C:88:PRO:HG3	2.06	0.56
6:F:2:THR:C	6:F:4:THR:H	2.09	0.56
5:E:86:ASN:O	5:E:87:SER:HB3	2.06	0.56
1:A:257:THR:HG22	1:A:268:SER:CB	2.34	0.55
2:B:302:VAL:HA	2:B:345:GLU:CB	2.37	0.55
2:B:282:LEU:HD23	2:B:321:LEU:HD11	1.89	0.55
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.37	0.55
7:G:20:ASP:OD1	7:G:22:ASN:HB2	2.05	0.55
5:E:169:MET:O	5:E:171:LYS:HG2	2.07	0.55
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.88	0.55
4:D:132:GLN:HE21	4:D:159:ASP:HA	1.72	0.55
3:C:184:PRO:HB2	3:C:231:ALA:CB	2.37	0.55
5:E:95:MET:HG2	5:E:141:GLY:CA	2.36	0.55
4:D:182:MET:HG3	4:D:200:PHE:CD1	2.42	0.54
1:A:309:ILE:HG23	1:A:310:ASP:H	1.72	0.54
3:C:96:ASN:O	3:C:97:ARG:HD3	2.07	0.54
2:B:158:ASP:HA	2:B:304:SER:O	2.08	0.54
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.38	0.54
2:B:287:GLN:NE2	2:B:298:TYR:OH	2.41	0.54
2:B:163:VAL:HG22	2:B:164:THR:N	2.23	0.54
5:E:50:LYS:NZ	5:E:159:TRP:O	2.41	0.54
5:E:152:GLN:HB3	5:E:155:LYS:CE	2.38	0.54
2:B:180:ARG:HB2	2:B:281:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ILE:HD13	2:B:271:ILE:CD1	2.38	0.53
3:C:155:VAL:HG11	3:C:180:PRO:HG2	1.90	0.53
6:F:53:ILE:N	6:F:53:ILE:HD12	2.22	0.53
1:A:19:LEU:HD13	1:A:96:VAL:HG13	1.89	0.53
3:C:107:ASN:ND2	3:C:107:ASN:C	2.61	0.53
3:C:257:SER:OG	3:C:372:VAL:N	2.37	0.53
5:E:105:ILE:HD13	5:E:130:ARG:NH1	2.23	0.53
3:C:358:ASP:OD1	3:C:360:ARG:HG2	2.09	0.53
1:A:395:HIS:HA	10:A:542:HOH:O	2.08	0.53
2:B:219:LYS:HG2	2:B:220:LEU:HD13	1.91	0.53
5:E:97:THR:O	5:E:101:THR:HG23	2.08	0.53
3:C:201:SER:HB3	7:G:149:LYS:HZ2	1.69	0.53
5:E:153:ASN:OD1	5:E:154:ASP:N	2.42	0.53
2:B:175:LEU:O	2:B:177:HIS:O	2.27	0.53
5:E:152:GLN:HB3	5:E:155:LYS:HZ3	1.72	0.52
7:G:122:SER:O	7:G:126:LEU:HG	2.08	0.52
4:D:37:ASP:HB3	4:D:41:VAL:HB	1.91	0.52
4:D:263:HIS:HB3	4:D:267:ARG:NH1	2.24	0.52
7:G:51:MET:HB3	7:G:86:PHE:CE1	2.44	0.52
3:C:173:ILE:O	3:C:177:GLU:HG2	2.09	0.52
1:A:183:GLY:HA3	1:A:413:VAL:HG21	1.91	0.52
1:A:223:THR:O	1:A:227:VAL:HG23	2.09	0.52
3:C:129:ASN:HB2	3:C:131:TRP:CZ3	2.44	0.52
2:B:290:ASP:O	2:B:294:ARG:HG3	2.10	0.52
2:B:303:LEU:HD21	2:B:344:ILE:CG2	2.40	0.52
1:A:240:LYS:O	1:A:244:LYS:HG3	2.09	0.52
1:A:393:VAL:HG21	1:A:414:PHE:CE2	2.45	0.52
6:F:101:PHE:C	6:F:103:ILE:H	2.13	0.52
1:A:111:LEU:HD23	1:A:111:LEU:C	2.30	0.52
6:F:145:GLU:O	6:F:149:MET:HG3	2.10	0.52
7:G:47:ARG:O	7:G:48:GLN:HG3	2.09	0.52
1:A:153:TRP:CE3	1:A:161:ARG:HD2	2.45	0.51
1:A:289:ASN:HD22	1:A:290:PRO:N	2.08	0.51
1:A:67:ILE:HG22	1:A:68:GLU:HG2	1.93	0.51
1:A:194:PRO:C	1:A:195:ILE:HD12	2.31	0.51
1:A:389:GLU:CD	1:A:414:PHE:HB2	2.31	0.51
4:D:205:PRO:HA	4:D:222:TYR:CD1	2.45	0.51
1:A:359:LYS:N	1:A:360:PRO:HD3	2.26	0.51
2:B:246:LEU:HB3	2:B:247:PRO:HD2	1.92	0.51
7:G:35:ALA:HB1	7:G:63:PRO:HA	1.91	0.51
7:G:140:SER:O	7:G:144:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.41	0.51
5:E:95:MET:HG2	5:E:141:GLY:C	2.30	0.51
1:A:343:VAL:CG1	1:A:363:ILE:HD12	2.41	0.51
5:E:9:MET:SD	5:E:63:GLU:HG2	2.51	0.51
4:D:135:GLY:O	4:D:137:GLU:HG3	2.11	0.51
5:E:95:MET:HG2	5:E:141:GLY:HA3	1.92	0.51
1:A:172:ASP:OD2	1:A:198:ARG:NE	2.44	0.51
5:E:88:LYS:O	5:E:92:GLU:HG3	2.11	0.51
1:A:21:TYR:OH	1:A:103:ALA:HB2	2.11	0.50
5:E:5:HIS:HD2	5:E:65:ASP:OD2	1.93	0.50
1:A:18:LYS:HD2	1:A:18:LYS:N	2.26	0.50
2:B:290:ASP:HB2	2:B:293:THR:OG1	2.11	0.50
3:C:234:LYS:O	3:C:235:MET:HB2	2.12	0.50
5:E:60:ILE:HD11	5:E:116:ILE:HG21	1.93	0.50
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.46	0.50
3:C:285:LEU:HB3	3:C:362:LEU:HD13	1.94	0.50
4:D:169:PHE:HB2	4:D:175:VAL:HG22	1.94	0.50
5:E:166:ARG:HG2	5:E:166:ARG:HH11	1.76	0.50
1:A:308:PRO:O	1:A:311:VAL:HG12	2.12	0.50
4:D:263:HIS:HB3	4:D:267:ARG:HH12	1.76	0.50
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.94	0.49
1:A:38:LYS:HD3	1:A:72:TYR:CE2	2.48	0.49
1:A:397:LYS:O	1:A:400:TYR:HB3	2.13	0.49
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.48	0.49
3:C:26:CYS:SG	3:C:55:VAL:HB	2.52	0.49
1:A:310:ASP:OD2	1:A:310:ASP:N	2.45	0.49
5:E:22:LEU:HD23	5:E:41:ILE:HD13	1.93	0.49
1:A:278:GLY:O	1:A:281:ILE:HG12	2.11	0.49
5:E:26:SER:HB2	5:E:139:GLU:HG2	1.95	0.49
4:D:199:LEU:HB2	4:D:224:THR:HB	1.94	0.49
1:A:309:ILE:HG23	1:A:310:ASP:N	2.28	0.48
1:A:191:LYS:HB2	1:A:303:VAL:CG2	2.43	0.48
2:B:330:LEU:C	2:B:332:GLY:H	2.16	0.48
3:C:29:ASN:CB	3:C:31:GLU:H	2.23	0.48
4:D:64:TYR:CD2	4:D:92:ASN:HB3	2.48	0.48
1:A:154:THR:HG22	1:A:370:HIS:HB2	1.94	0.48
6:F:158:ARG:O	6:F:162:GLU:HG3	2.14	0.48
1:A:4:ARG:HG3	1:A:4:ARG:HH11	1.79	0.48
4:D:206:PRO:HD3	4:D:222:TYR:CB	2.44	0.48
5:E:22:LEU:CD2	5:E:41:ILE:HD13	2.44	0.48
7:G:80:LEU:O	7:G:84:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:HA	1:A:373:GLN:OE1	2.14	0.48
4:D:181:PHE:CE2	6:F:157:ALA:HA	2.49	0.48
7:G:99:ASP:O	7:G:102:GLY:N	2.41	0.48
3:C:7:LEU:HD12	3:C:9:GLU:HB2	1.96	0.48
3:C:157:LEU:O	3:C:168:ILE:HA	2.14	0.47
5:E:95:MET:CG	5:E:141:GLY:HA3	2.44	0.47
1:A:339:LEU:HD23	1:A:365:VAL:CG1	2.44	0.47
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.25	0.47
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.26	0.47
5:E:95:MET:HA	5:E:95:MET:CE	2.44	0.47
5:E:56:LYS:HG3	5:E:170:ASN:HD21	1.80	0.47
6:F:163:GLU:O	6:F:167:ASN:ND2	2.47	0.47
1:A:262:ILE:C	1:A:264:LYS:N	2.58	0.47
7:G:52:THR:O	7:G:56:GLN:HG3	2.15	0.47
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.74	0.47
1:A:30:ILE:HD13	1:A:375:TYR:OH	2.14	0.47
6:F:5:LEU:HD13	6:F:55:ARG:NH1	2.29	0.47
7:G:87:LYS:HD3	7:G:87:LYS:H	1.80	0.47
3:C:13:CYS:SG	3:C:58:VAL:HG23	2.55	0.46
3:C:72:THR:HA	3:C:98:ALA:HB1	1.97	0.46
4:D:59:ILE:HB	4:D:116:LEU:HD13	1.97	0.46
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.96	0.46
3:C:184:PRO:HB2	3:C:231:ALA:HB1	1.97	0.46
7:G:62:PRO:C	7:G:64:ILE:H	2.19	0.46
5:E:35:GLU:OE1	5:E:36:THR:N	2.48	0.46
2:B:254:VAL:HG12	2:B:258:ARG:HG3	1.98	0.46
3:C:212:ALA:HB3	3:C:255:GLU:OE2	2.16	0.46
3:C:370:LYS:O	3:C:371:ILE:CB	2.63	0.46
2:B:291:ILE:O	2:B:291:ILE:HG22	2.16	0.46
3:C:175:GLU:H	3:C:175:GLU:HG2	1.40	0.46
1:A:395:HIS:HB3	1:A:407:ILE:HD12	1.96	0.46
3:C:44:GLN:HE21	3:C:47:GLU:HG3	1.81	0.46
1:A:90:GLU:HG3	1:A:129:ILE:HG23	1.97	0.46
2:B:161:ASP:HB2	9:B:502:ATP:H5'1	1.97	0.46
4:D:44:HIS:ND1	4:D:88:GLU:OE2	2.49	0.45
4:D:169:PHE:HB2	4:D:175:VAL:CG2	2.46	0.45
1:A:153:TRP:CD2	1:A:161:ARG:HD2	2.52	0.45
4:D:228:PHE:H	4:D:231:HIS:CD2	2.31	0.45
3:C:7:LEU:HD13	3:C:27:PRO:HB2	1.99	0.45
4:D:156:SER:O	4:D:157:LYS:HD2	2.17	0.45
4:D:182:MET:HG3	4:D:200:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:ALA:CB	5:E:22:LEU:HD13	2.45	0.45
7:G:87:LYS:HE2	7:G:90:ASP:CG	2.37	0.45
1:A:68:GLU:O	1:A:69:LYS:C	2.55	0.45
1:A:152:SER:HB3	1:A:320:VAL:HG11	1.98	0.45
3:C:184:PRO:HB2	3:C:231:ALA:HB3	1.98	0.45
3:C:226:VAL:HG12	3:C:240:LEU:HB3	1.98	0.45
3:C:264:ASP:O	3:C:265:CYS:CB	2.64	0.45
5:E:24:ILE:CD1	5:E:135:GLN:HG2	2.47	0.45
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.99	0.45
4:D:203:ARG:HA	4:D:217:GLY:O	2.17	0.45
5:E:150:ASP:OD2	5:E:152:GLN:HB2	2.17	0.45
1:A:168:ILE:CD1	1:A:335:LEU:HD11	2.47	0.45
2:B:330:LEU:O	2:B:332:GLY:N	2.50	0.45
3:C:144:THR:CB	6:F:28:GLN:HE21	2.30	0.45
3:C:327:ASN:HB2	3:C:351:ASP:HB3	1.99	0.45
6:F:2:THR:OG1	6:F:3:ALA:N	2.50	0.45
3:C:172:TYR:C	3:C:172:TYR:CD2	2.90	0.44
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.52	0.44
1:A:38:LYS:O	1:A:39:GLU:HB3	2.17	0.44
1:A:393:VAL:HG21	1:A:414:PHE:CD2	2.52	0.44
3:C:189:MET:HA	3:C:195:MET:HE3	1.98	0.44
4:D:263:HIS:HD2	4:D:266:MET:HE2	1.82	0.44
1:A:116:PRO:O	1:A:117:LEU:CB	2.64	0.44
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.98	0.44
3:C:102:VAL:HG23	3:C:113:VAL:HG22	1.98	0.44
3:C:183:THR:CG2	3:C:184:PRO:N	2.81	0.44
3:C:228:LEU:C	3:C:228:LEU:HD23	2.38	0.44
7:G:114:PHE:CZ	7:G:126:LEU:HD23	2.52	0.44
3:C:207:GLY:O	3:C:219:TRP:HA	2.18	0.44
4:D:136:LYS:HE3	4:D:136:LYS:HB2	1.83	0.44
3:C:61:ALA:HB1	3:C:108:GLU:OE1	2.17	0.44
6:F:105:ARG:HG2	6:F:105:ARG:HH11	1.83	0.44
4:D:159:ASP:OD2	4:D:159:ASP:N	2.48	0.44
4:D:197:GLN:HE21	4:D:199:LEU:CD1	2.31	0.44
6:F:2:THR:HG23	6:F:3:ALA:N	2.29	0.44
1:A:129:ILE:O	1:A:133:SER:HB2	2.18	0.44
3:C:119:VAL:HG22	3:C:120:ILE:N	2.33	0.44
4:D:199:LEU:N	4:D:199:LEU:HD12	2.33	0.44
5:E:28:PHE:HE1	5:E:142:LEU:HD22	1.82	0.44
2:B:318:GLU:CG	2:B:344:ILE:HD12	2.46	0.44
4:D:223:ILE:HD12	4:D:223:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:85:ILE:HD12	6:F:85:ILE:C	2.38	0.43
2:B:299:LYS:O	2:B:300:HIS:ND1	2.51	0.43
3:C:60:TRP:HE1	3:C:65:ASN:ND2	2.16	0.43
4:D:212:THR:C	4:D:214:ALA:H	2.20	0.43
5:E:142:LEU:O	5:E:145:CYS:HB2	2.18	0.43
1:A:369:THR:HG23	10:A:527:HOH:O	2.18	0.43
1:A:372:MET:HE2	1:A:379:PHE:CD1	2.54	0.43
2:B:280:GLU:HA	2:B:324:LEU:HD11	2.00	0.43
4:D:37:ASP:HB2	4:D:43:TYR:CE1	2.53	0.43
3:C:13:CYS:HA	3:C:331:GLN:NE2	2.33	0.43
1:A:151:ALA:O	1:A:154:THR:HB	2.18	0.43
3:C:189:MET:HA	3:C:195:MET:CE	2.49	0.43
5:E:16:ILE:O	5:E:16:ILE:CG2	2.66	0.43
6:F:53:ILE:HA	7:G:114:PHE:CD1	2.53	0.43
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.54	0.43
5:E:32:ALA:HA	5:E:33:PRO:HD3	1.89	0.43
3:C:21:THR:HG22	3:C:22:GLN:CG	2.48	0.43
4:D:74:GLU:H	4:D:74:GLU:CD	2.22	0.43
5:E:74:TYR:CE2	5:E:137:ARG:HA	2.54	0.43
5:E:132:TYR:O	5:E:135:GLN:HB3	2.19	0.43
6:F:8:TYR:CG	6:F:55:ARG:HB2	2.54	0.43
7:G:37:PRO:HG3	7:G:58:ALA:O	2.18	0.43
3:C:33:HIS:HD2	10:C:395:HOH:O	2.02	0.43
3:C:183:THR:CG2	3:C:185:TRP:H	2.12	0.43
3:C:193:GLU:HB3	3:C:195:MET:HE2	2.00	0.43
4:D:189:ARG:NH2	4:D:197:GLN:HG3	2.33	0.43
4:D:64:TYR:HB3	4:D:92:ASN:ND2	2.33	0.43
4:D:77:LYS:HD2	4:D:77:LYS:HA	1.76	0.43
4:D:182:MET:HE3	4:D:182:MET:HA	2.01	0.43
6:F:2:THR:O	6:F:3:ALA:HB3	2.19	0.43
1:A:156:ARG:CB	1:A:368:ILE:HG23	2.48	0.42
1:A:226:ALA:O	1:A:230:ARG:HD3	2.19	0.42
2:B:223:VAL:HG23	2:B:310:TYR:CB	2.49	0.42
4:D:258:SER:O	4:D:262:ILE:HG12	2.19	0.42
6:F:76:VAL:HG12	6:F:77:LYS:N	2.34	0.42
2:B:159:SER:HB2	2:B:164:THR:HG23	2.02	0.42
2:B:281:LEU:O	2:B:281:LEU:HD23	2.19	0.42
2:B:222:TYR:O	2:B:259:PHE:HA	2.19	0.42
3:C:44:GLN:NE2	3:C:47:GLU:HG3	2.34	0.42
3:C:283:GLY:O	3:C:284:ARG:HB2	2.19	0.42
4:D:118:ARG:HD3	4:D:118:ARG:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.20	0.42
5:E:24:ILE:O	5:E:24:ILE:HG13	2.19	0.42
1:A:152:SER:O	1:A:154:THR:N	2.51	0.42
1:A:343:VAL:HG11	1:A:363:ILE:HB	2.00	0.42
3:C:142:ARG:HG3	3:C:142:ARG:NH1	2.33	0.42
4:D:248:ARG:HD3	4:D:248:ARG:C	2.40	0.42
1:A:19:LEU:HD23	1:A:19:LEU:H	1.84	0.42
1:A:91:ARG:O	1:A:94:GLU:HB2	2.20	0.42
2:B:318:GLU:O	2:B:322:LYS:HG3	2.20	0.42
3:C:228:LEU:HD23	3:C:229:ALA:N	2.34	0.42
3:C:268:VAL:HA	3:C:284:ARG:H	1.85	0.42
4:D:141:ARG:NH2	4:D:212:THR:CG2	2.82	0.42
4:D:269:LYS:HD2	4:D:269:LYS:HA	1.85	0.42
5:E:87:SER:N	5:E:154:ASP:HA	2.33	0.42
7:G:74:ARG:O	7:G:78:ILE:HG13	2.20	0.42
1:A:328:PHE:CE1	9:A:501:ATP:H2	2.37	0.42
3:C:226:VAL:CG1	3:C:240:LEU:HB3	2.49	0.42
4:D:75:LEU:HD23	4:D:75:LEU:C	2.39	0.42
4:D:132:GLN:HB2	4:D:156:SER:OG	2.19	0.42
1:A:282:PHE:CD2	1:A:331:PHE:HE1	2.38	0.42
5:E:62:ASN:C	5:E:64:ALA:N	2.73	0.42
6:F:2:THR:CG2	6:F:3:ALA:H	2.22	0.42
6:F:130:LYS:HA	6:F:130:LYS:CE	2.42	0.42
1:A:247:THR:HG22	1:A:248:ASP:N	2.35	0.42
1:A:248:ASP:OD2	1:A:251:LYS:HD3	2.20	0.42
2:B:167:CYS:HA	2:B:168:PRO:HD3	1.88	0.42
3:C:183:THR:HB	3:C:189:MET:CE	2.50	0.42
6:F:73:SER:HB3	6:F:112:TYR:CG	2.55	0.42
2:B:184:ILE:HG13	2:B:265:LEU:HD23	2.01	0.41
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.50	0.41
1:A:160:GLU:OE1	1:A:160:GLU:HA	2.20	0.41
4:D:6:VAL:HG21	4:D:242:ASN:HB3	2.02	0.41
5:E:134:GLN:O	5:E:138:GLN:HG2	2.20	0.41
3:C:102:VAL:HA	3:C:112:ALA:O	2.20	0.41
4:D:146:TYR:OH	4:D:248:ARG:HG3	2.19	0.41
4:D:269:LYS:O	4:D:272:ASP:HB2	2.21	0.41
5:E:152:GLN:O	5:E:153:ASN:O	2.39	0.41
5:E:60:ILE:CD1	5:E:116:ILE:HG23	2.51	0.41
5:E:82:LEU:HD12	5:E:82:LEU:HA	1.88	0.41
5:E:145:CYS:O	5:E:149:PHE:HD1	2.03	0.41
4:D:188:GLY:HA3	6:F:165:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:93:LYS:NZ	7:G:93:LYS:HB3	2.36	0.41
1:A:168:ILE:HD13	1:A:335:LEU:HD11	2.02	0.41
2:B:254:VAL:HG13	2:B:257:GLU:HG2	2.03	0.41
3:C:366:LEU:HD12	3:C:366:LEU:N	2.35	0.41
4:D:186:LYS:NZ	4:D:200:PHE:H	2.19	0.41
5:E:166:ARG:HG2	5:E:166:ARG:NH1	2.36	0.41
6:F:20:LEU:HD23	6:F:20:LEU:HA	1.92	0.41
1:A:87:ASP:OD2	4:D:267:ARG:HD2	2.21	0.41
1:A:289:ASN:HA	1:A:290:PRO:HD3	1.92	0.41
1:A:289:ASN:ND2	1:A:291:ASP:H	2.18	0.41
2:B:319:ARG:O	2:B:323:GLN:HG3	2.21	0.41
5:E:168:PHE:CE2	5:E:169:MET:HE2	2.56	0.41
1:A:328:PHE:CZ	9:A:501:ATP:H2	2.38	0.41
2:B:166:ILE:HD12	2:B:281:LEU:HD23	2.02	0.41
3:C:167:ARG:HG2	3:C:197:GLU:HG3	2.03	0.41
3:C:193:GLU:HG2	3:C:195:MET:HE1	2.02	0.41
3:C:252:PHE:CE1	3:C:258:LEU:HD21	2.56	0.41
3:C:358:ASP:HB3	3:C:361:SER:HB2	2.01	0.41
4:D:30:ALA:HA	4:D:52:LYS:HG2	2.03	0.41
6:F:114:ILE:HG13	6:F:115:SER:N	2.36	0.41
4:D:53:THR:C	4:D:54:LYS:HD2	2.42	0.41
5:E:152:GLN:CB	5:E:155:LYS:HD2	2.51	0.41
7:G:41:GLU:O	7:G:44:SER:HB3	2.20	0.41
1:A:260:ASN:HB3	1:A:262:ILE:O	2.20	0.40
5:E:22:LEU:HA	5:E:23:PRO:HD3	1.80	0.40
6:F:20:LEU:HD23	6:F:70:VAL:CG2	2.45	0.40
7:G:75:ALA:O	7:G:79:VAL:HG23	2.21	0.40
2:B:163:VAL:CG2	2:B:164:THR:N	2.84	0.40
2:B:223:VAL:HG23	2:B:310:TYR:HB3	2.04	0.40
2:B:326:LEU:O	2:B:326:LEU:HG	2.20	0.40
5:E:130:ARG:HH11	5:E:130:ARG:HB2	1.86	0.40
1:A:374:ARG:HG2	1:A:375:TYR:CE2	2.56	0.40
2:B:161:ASP:OD2	9:B:502:ATP:H3'	2.21	0.40
3:C:32:VAL:HB	3:C:48:LEU:HB2	2.03	0.40
5:E:96:TYR:O	5:E:100:ILE:HG12	2.21	0.40
1:A:262:ILE:HG22	1:A:263:SER:N	2.36	0.40
3:C:183:THR:HG21	3:C:185:TRP:HD1	1.87	0.40
5:E:87:SER:HA	5:E:153:ASN:OD1	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	389/418 (93%)	356 (92%)	29 (8%)	4 (1%)	15 34
2	B	195/394 (50%)	175 (90%)	14 (7%)	6 (3%)	4 8
3	C	337/372 (91%)	315 (94%)	18 (5%)	4 (1%)	13 29
4	D	276/300 (92%)	260 (94%)	15 (5%)	1 (0%)	34 58
5	E	171/178 (96%)	158 (92%)	9 (5%)	4 (2%)	6 14
6	F	165/168 (98%)	155 (94%)	8 (5%)	2 (1%)	13 29
7	G	131/151 (87%)	113 (86%)	13 (10%)	5 (4%)	3 6
All	All	1664/1981 (84%)	1532 (92%)	106 (6%)	26 (2%)	9 22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	SER
2	B	171	GLU
2	B	345	GLU
3	C	371	ILE
5	E	87	SER
5	E	153	ASN
6	F	102	PHE
3	C	203	GLY
7	G	37	PRO
1	A	69	LYS
1	A	263	SER
2	B	331	LYS
3	C	179	ARG
7	G	48	GLN
2	B	278	VAL
2	B	348	PRO
3	C	284	ARG
4	D	136	LYS

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Mol	Chain	Res	Type
7	G	88	ALA
7	G	100	LYS
5	E	49	PHE
5	E	151	PRO
6	F	56	ASN
1	A	194	PRO
2	B	329	VAL
7	G	63	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	333/363 (92%)	317 (95%)	16 (5%)	25	49
2	B	151/345 (44%)	143 (95%)	8 (5%)	22	45
3	C	288/313 (92%)	277 (96%)	11 (4%)	33	59
4	D	242/264 (92%)	238 (98%)	4 (2%)	60	82
5	E	156/159 (98%)	149 (96%)	7 (4%)	27	52
6	F	154/155 (99%)	146 (95%)	8 (5%)	23	46
7	G	111/124 (90%)	106 (96%)	5 (4%)	27	52
All	All	1435/1723 (83%)	1376 (96%)	59 (4%)	30	56

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	71	THR
1	A	88	LEU
1	A	143	VAL
1	A	154	THR
1	A	155	SER
1	A	172	ASP
1	A	191	LYS
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	251	LYS
1	A	255	GLN
1	A	282	PHE
1	A	289	ASN
1	A	310	ASP
1	A	335	LEU
2	B	175	LEU
2	B	182	LEU
2	B	200	ARG
2	B	220	LEU
2	B	237	THR
2	B	257	GLU
2	B	274	GLU
2	B	320	GLU
3	C	90	LEU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	175	GLU
3	C	179	ARG
3	C	188	LYS
3	C	284	ARG
3	C	321	LEU
3	C	367	LYS
3	C	368	ASP
4	D	116	LEU
4	D	157	LYS
4	D	171	ASP
4	D	265	ARG
5	E	9	MET
5	E	38	ASP
5	E	56	LYS
5	E	82	LEU
5	E	95	MET
5	E	130	ARG
5	E	145	CYS
6	F	2	THR
6	F	6	ARG
6	F	28	GLN
6	F	31	GLU
6	F	57	GLU

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Mol	Chain	Res	Type
6	F	102	PHE
6	F	104	LEU
6	F	165	LEU
7	G	18	GLU
7	G	21	GLU
7	G	27	GLU
7	G	64	ILE
7	G	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	144	GLN
1	A	205	GLN
1	A	206	GLN
1	A	243	ASN
1	A	289	ASN
1	A	318	ASN
1	A	395	HIS
1	A	411	ASN
2	B	205	ASN
2	B	284	ASN
2	B	287	GLN
2	B	323	GLN
3	C	44	GLN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN
4	D	132	GLN
4	D	140	ASN
4	D	145	HIS
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
6	F	28	GLN
6	F	78	GLN
6	F	125	GLN
6	F	167	ASN
7	G	48	GLN

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Mol	Chain	Res	Type
7	G	61	ASN
7	G	96	GLN

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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
9	ATP	A	501	8	26,33,33	1.34	3 (11%)	31,52,52	1.68	5 (16%)
9	ATP	B	502	-	26,33,33	1.37	3 (11%)	31,52,52	1.64	4 (12%)

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
9	ATP	A	501	8	-	2/18/38/38	0/3/3/3
9	ATP	B	502	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	ATP	C2-N1	3.73	1.40	1.33
9	A	501	ATP	C2-N1	3.61	1.40	1.33
9	B	502	ATP	PG-O1G	3.49	1.61	1.50
9	A	501	ATP	PG-O1G	3.40	1.61	1.50
9	B	502	ATP	O4'-C1'	2.23	1.44	1.41
9	A	501	ATP	O4'-C1'	2.05	1.43	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	502	ATP	N3-C2-N1	-5.43	120.19	128.68
9	A	501	ATP	N3-C2-N1	-5.42	120.21	128.68
9	B	502	ATP	PB-O3B-PG	-3.83	119.67	132.83
9	B	502	ATP	PA-O3A-PB	-3.40	121.16	132.83
9	A	501	ATP	O4'-C1'-C2'	-3.28	102.13	106.93
9	A	501	ATP	PA-O3A-PB	-3.28	121.57	132.83
9	A	501	ATP	PB-O3B-PG	-3.04	122.39	132.83
9	A	501	ATP	O3G-PG-O3B	2.63	113.47	104.64
9	B	502	ATP	O3G-PG-O3B	2.50	113.02	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	501	ATP	PG-O3B-PB-O1B
9	A	501	ATP	PG-O3B-PB-O2B

There are no ring outliers.

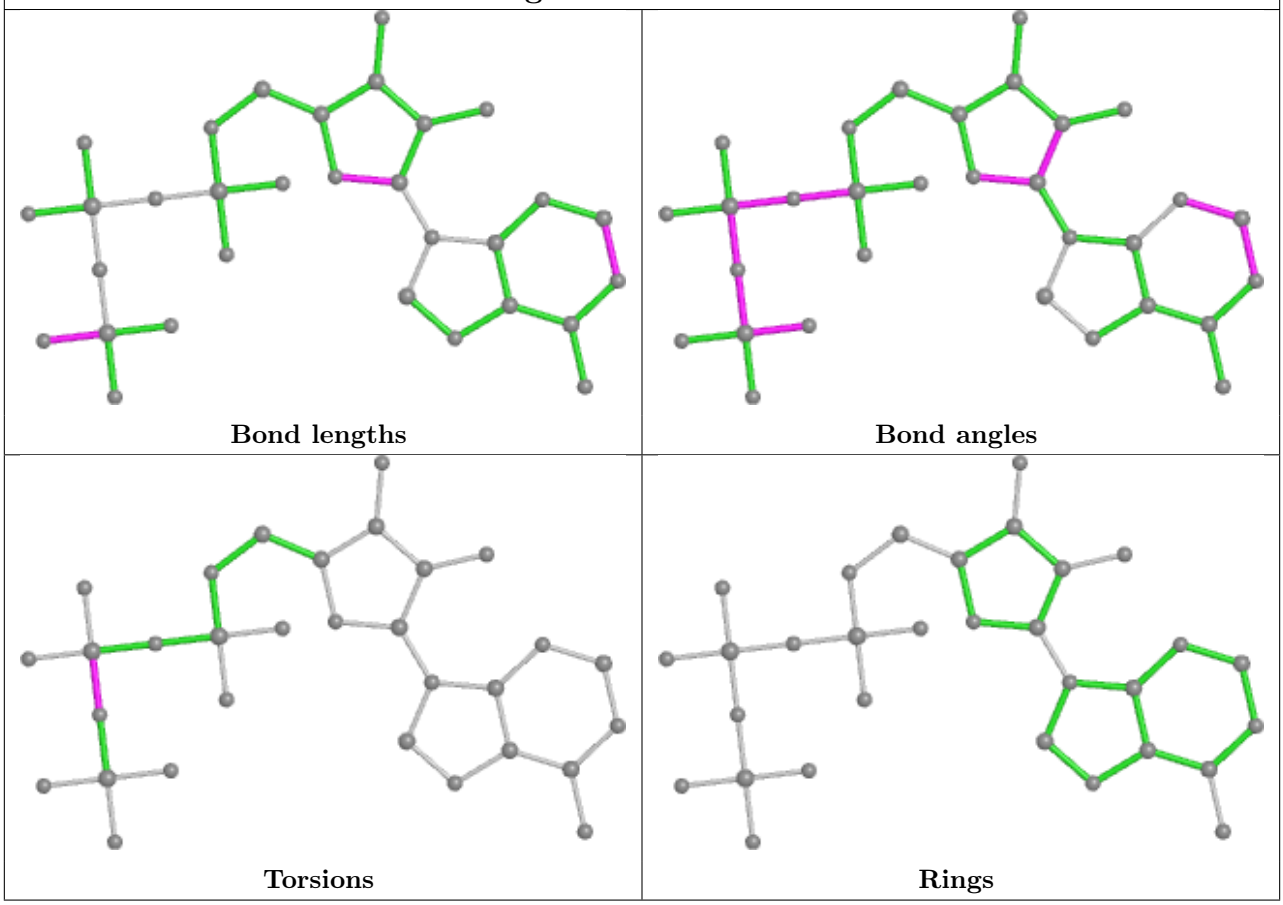
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	501	ATP	2	0
9	B	502	ATP	3	0

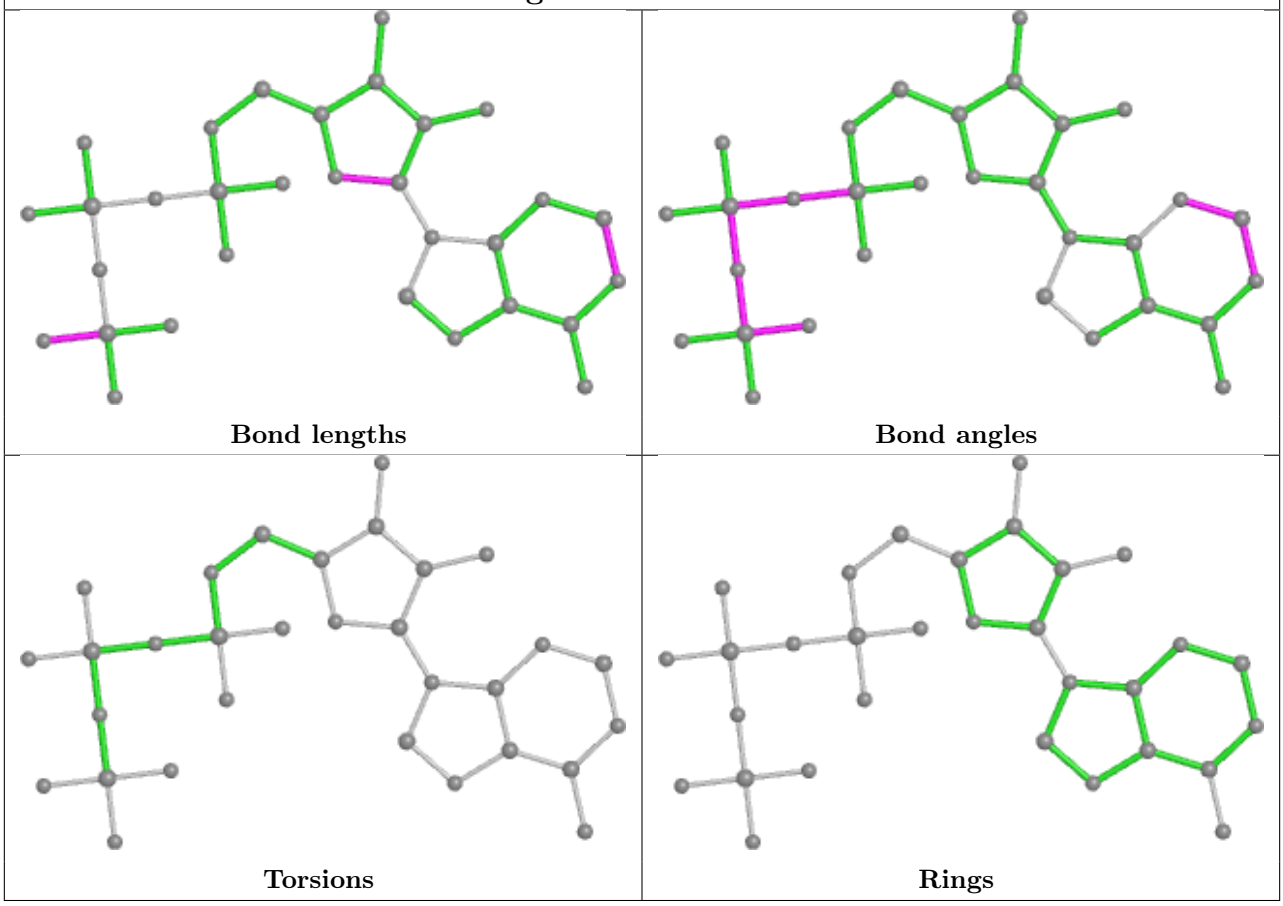
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 501



Ligand ATP B 502



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	397/418 (94%)	-0.02	10 (2%)	57	57	25, 48, 81, 96	0
2	B	197/394 (50%)	0.49	31 (15%)	2	1	34, 62, 96, 111	0
3	C	341/372 (91%)	-0.02	5 (1%)	73	74	27, 41, 69, 92	0
4	D	280/300 (93%)	-0.07	3 (1%)	80	81	27, 44, 78, 87	0
5	E	173/178 (97%)	0.25	12 (6%)	16	14	37, 58, 85, 100	0
6	F	167/168 (99%)	-0.14	1 (0%)	89	90	30, 43, 59, 89	0
7	G	135/151 (89%)	0.54	13 (9%)	8	6	35, 72, 96, 103	0
All	All	1690/1981 (85%)	0.09	75 (4%)	34	32	25, 49, 88, 111	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	10.4
1	A	52	MET	5.5
5	E	154	ASP	5.3
2	B	290	ASP	4.4
7	G	120	ASN	4.4
3	C	127	GLN	4.1
2	B	154	GLY	3.9
4	D	215	ALA	3.9
7	G	50	ASN	3.6
5	E	84	LYS	3.6
2	B	298	TYR	3.5
5	E	85	CYS	3.5
7	G	13	LYS	3.5
2	B	170	TYR	3.4
2	B	330	LEU	3.3
2	B	293	THR	3.2
2	B	294	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	286	ILE	3.2
7	G	40	GLY	3.1
7	G	28	ASP	3.1
1	A	262	ILE	3.1
7	G	149	LYS	3.1
2	B	165	HIS	3.0
2	B	176	PRO	3.0
1	A	39	GLU	2.9
4	D	216	VAL	2.9
2	B	342	ILE	2.9
5	E	35	GLU	2.9
2	B	299	LYS	2.9
3	C	367	LYS	2.9
2	B	169	VAL	2.8
5	E	89	SER	2.8
2	B	329	VAL	2.8
5	E	93	LYS	2.8
7	G	19	TYR	2.8
2	B	175	LEU	2.7
2	B	274	GLU	2.7
1	A	155	SER	2.7
2	B	325	TYR	2.7
1	A	360	PRO	2.6
1	A	362	PRO	2.6
2	B	285	THR	2.6
2	B	281	LEU	2.6
7	G	27	GLU	2.5
2	B	292	ASP	2.5
1	A	156	ARG	2.4
2	B	328	ARG	2.4
5	E	36	THR	2.4
2	B	289	ALA	2.4
1	A	161	ARG	2.4
5	E	153	ASN	2.3
4	D	211	ASP	2.3
5	E	149	PHE	2.3
7	G	119	ASP	2.3
2	B	276	VAL	2.2
7	G	11	PHE	2.2
2	B	326	LEU	2.2
1	A	414	PHE	2.2
2	B	272	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	84	ARG	2.2
7	G	21	GLU	2.1
5	E	86	ASN	2.1
6	F	2	THR	2.1
2	B	166	ILE	2.1
2	B	283	PHE	2.1
5	E	150	ASP	2.1
3	C	372	VAL	2.1
2	B	172	GLY	2.1
7	G	64	ILE	2.1
5	E	11	PRO	2.1
7	G	65	ASN	2.1
2	B	288	ALA	2.0
2	B	282	LEU	2.0
3	C	231	ALA	2.0
2	B	295	SER	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)

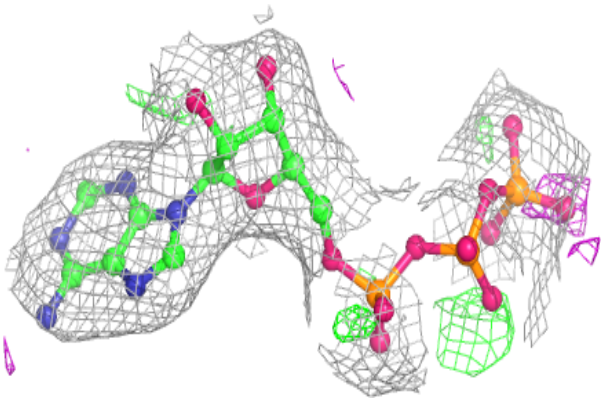
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

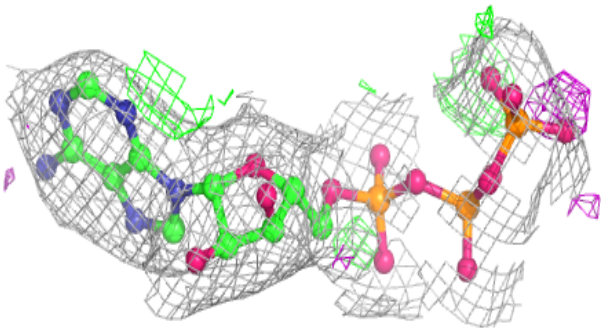
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	A	500	1/1	0.94	0.44	43,43,43,43	0
9	ATP	B	502	31/31	0.94	0.13	51,58,88,89	0
9	ATP	A	501	31/31	0.97	0.15	41,45,48,51	0

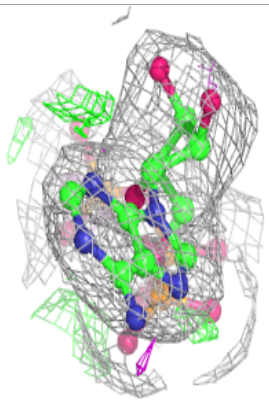
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 502:

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

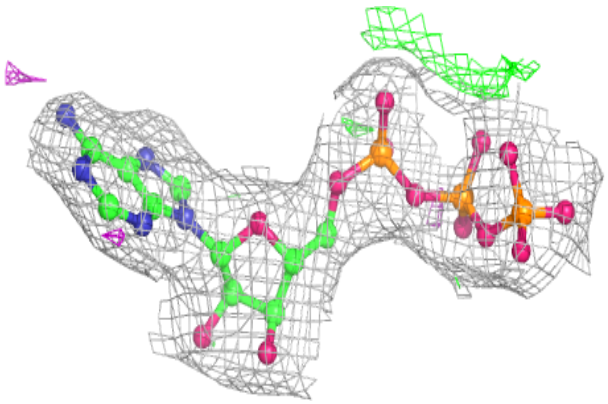


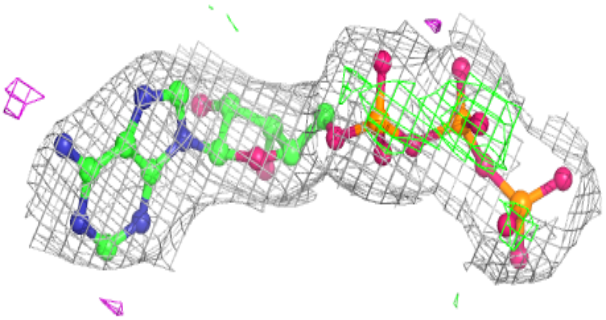


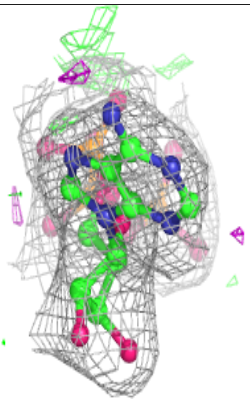


Electron density around ATP A 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.