Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:17 PM EST

PDB ID	:	3ULE
Title	:	Structure of Bos taurus Arp2/3 complex with bound inhibitor CK-869 and ATP
Authors	:	Nolen, B.J.; Han, M.
Deposited on	:	2011-11-10
Resolution	:	2.50 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:

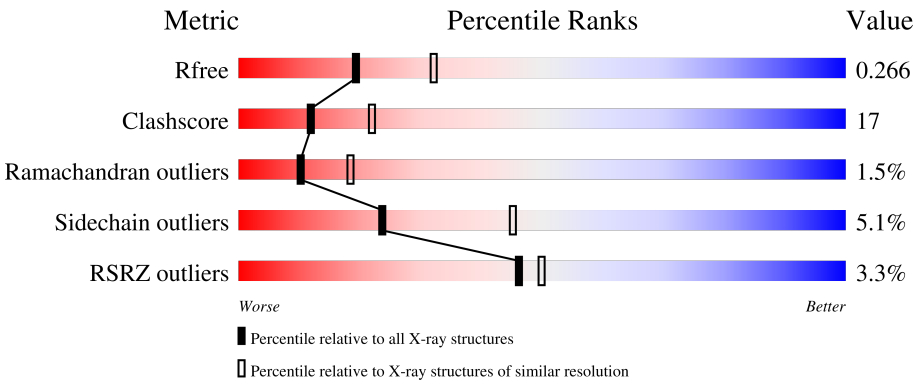
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 67% 25% • •
2	B	394	8% 34% 22% • 40%
3	C	372	.% 67% 23% • 8%
4	D	300	.% 69% 23% • 6%
5	E	178	.% 59% 34% 5% •

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Mol	Chain	Length	Quality of chain
6	F	168	% 77% 22% ••
7	G	151	5% 67% 19% 5% 9%

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
9	C69	A	1002	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14186 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-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	3198	2055	532	596	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1835	1181	308	340	6	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	2649	1681	464	485	19	0	0	0

- 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	281	2264	1441	393	422	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	174	1412	907	236	260	9	0	0	0

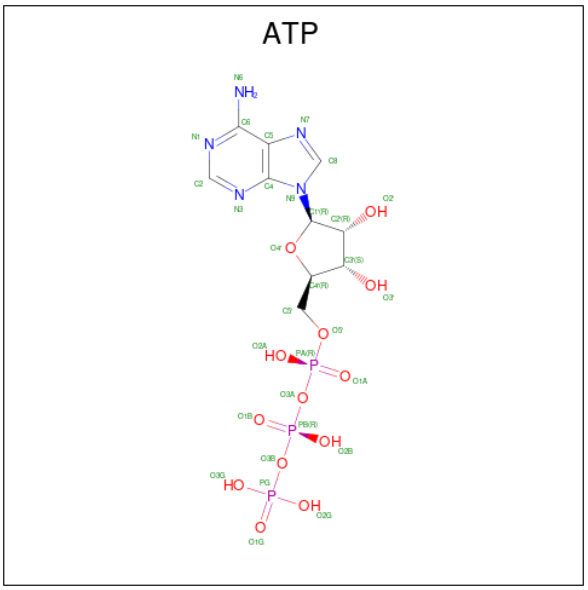
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

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.

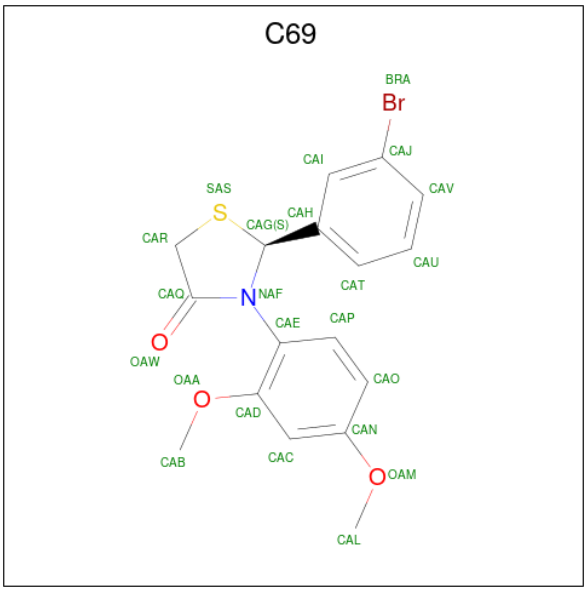
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	137	1045	654	183	205	3	0	0	0

- Molecule 8 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		
8	A	1	31	10	5	13	3	0	0
8	B	1	31	10	5	13	3	0	0

- Molecule 9 is (2S)-2-(3-bromophenyl)-3-(2,4-dimethoxyphenyl)-1,3-thiazolidin-4-one (three-letter code: C69) (formula: $C_{17}H_{16}BrNO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
9	A	1	23	1	17	1	3	1	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
10	A	1	1	1	0	0
10	B	1	1	1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	57	57	57	0	0
11	B	27	27	27	0	0
11	C	77	77	77	0	0
11	D	72	72	72	0	0
11	E	23	23	23	0	0
11	F	51	51	51	0	0

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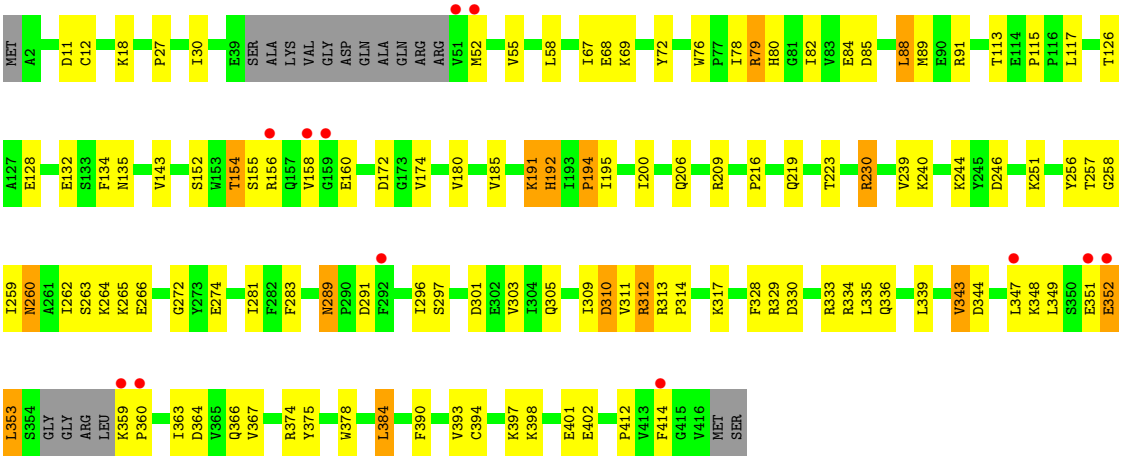
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	G	18	18	18	0	0

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.

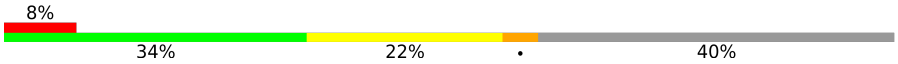
- Molecule 1: Actin-related protein 3

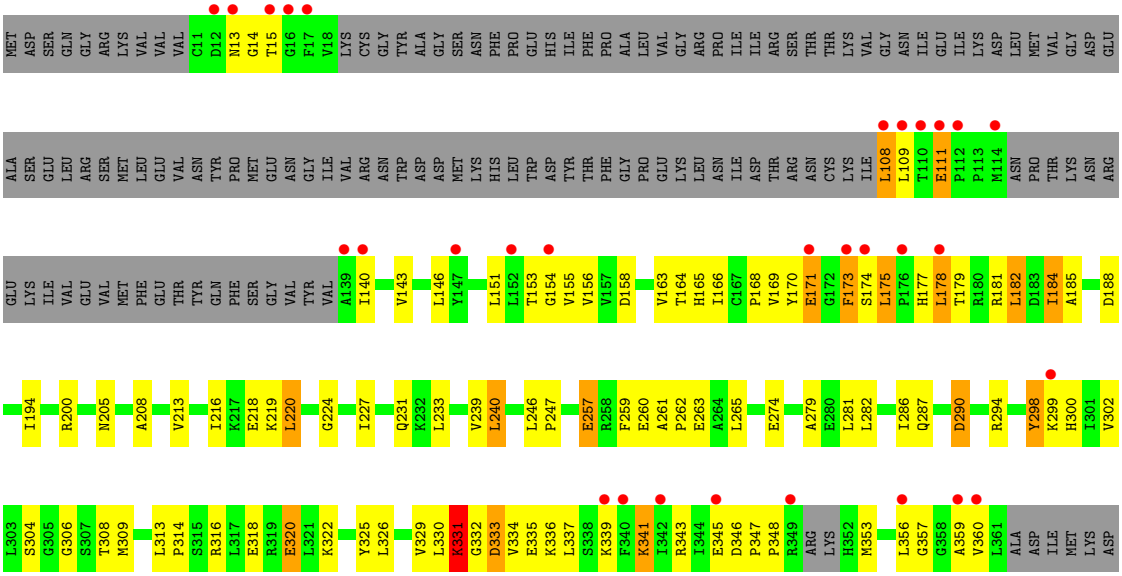
Chain A:

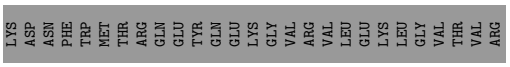


- Molecule 2: Actin-related protein 2

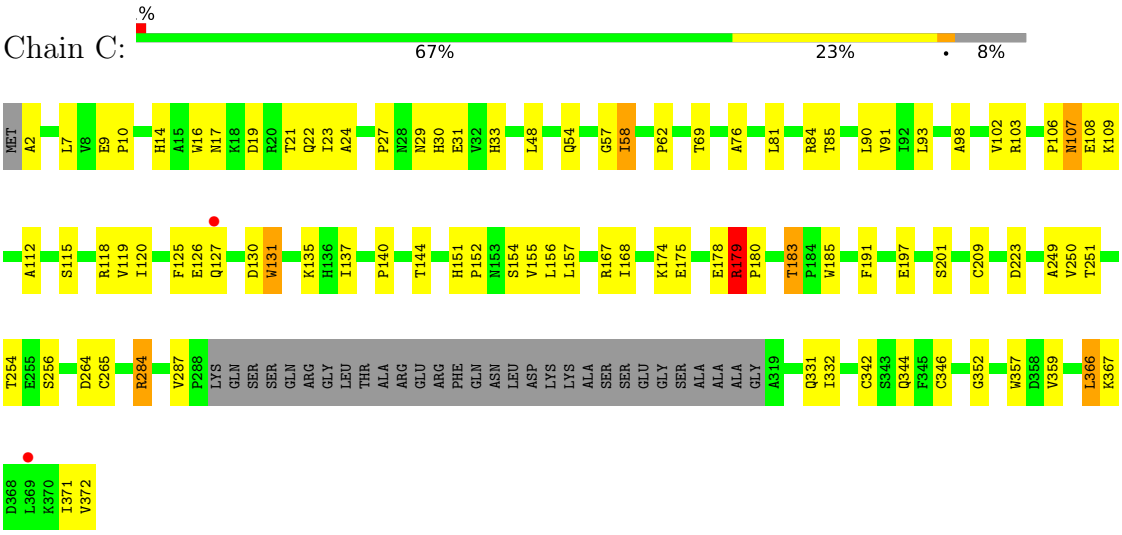
Chain B:



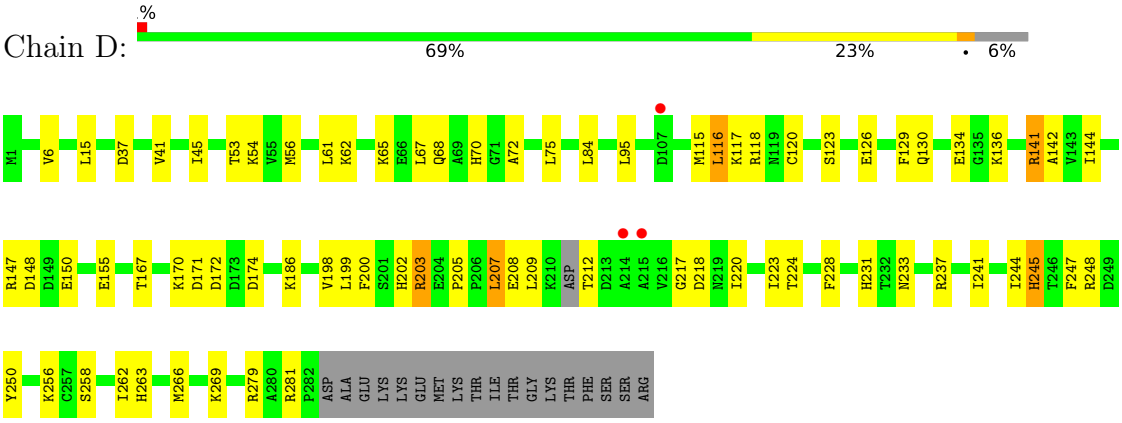




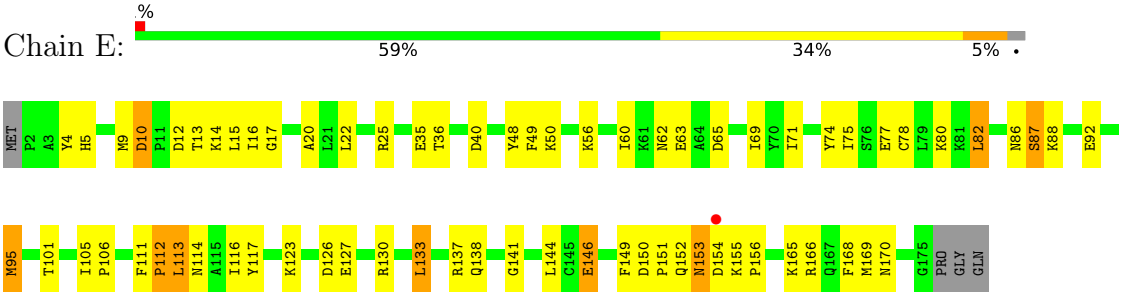
• Molecule 3: Actin-related protein 2/3 complex subunit 1B



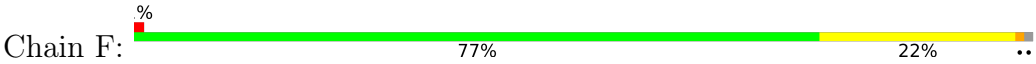
• Molecule 4: Actin-related protein 2/3 complex subunit 2

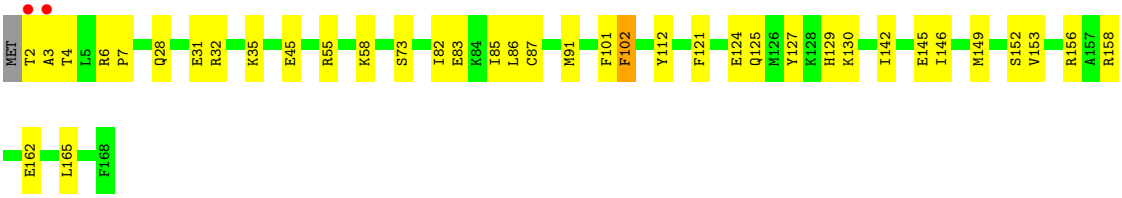


• Molecule 5: Actin-related protein 2/3 complex subunit 3



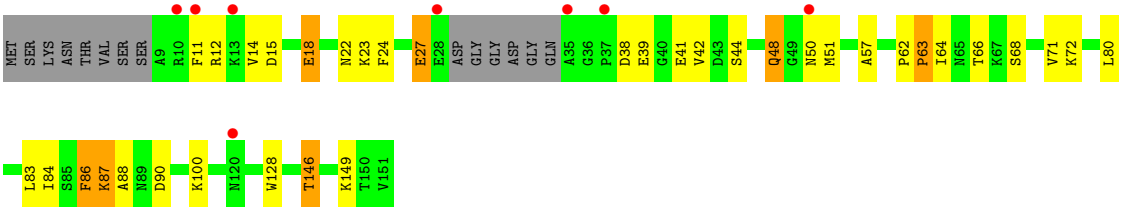
• Molecule 6: Actin-related protein 2/3 complex subunit 4





• 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	111.17Å 128.31Å 198.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 49.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 84.6 (49.62-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.274 0.217 , 0.266	Depositor DCC
R_{free} test set	4711 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14186	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: C69, CA, 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	0.37	0/3279	0.61	0/4450
2	B	0.33	0/1866	0.59	0/2525
3	C	0.37	0/2718	0.65	0/3689
4	D	0.38	0/2312	0.59	0/3121
5	E	0.35	0/1446	0.60	1/1950 (0.1%)
6	F	0.40	0/1393	0.63	0/1868
7	G	0.35	0/1057	0.61	0/1421
All	All	0.37	0/14071	0.61	1/19024 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	17	GLY	N-CA-C	-5.42	99.56	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	3198	0	3143	120	0
2	B	1835	0	1859	102	0
3	C	2649	0	2604	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2264	0	2230	64	0
5	E	1412	0	1414	64	0
6	F	1371	0	1410	26	0
7	G	1045	0	1059	29	0
8	A	31	0	12	3	0
8	B	31	0	12	2	0
9	A	23	0	16	9	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	57	0	0	2	0
11	B	27	0	0	1	0
11	C	77	0	0	6	0
11	D	72	0	0	2	0
11	E	23	0	0	3	0
11	F	51	0	0	1	0
11	G	18	0	0	1	0
All	All	14186	0	13759	478	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 17.

All (478) 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:17:ASN:HD21	3:C:21:THR:HG22	1.13	1.10
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.44	1.00
6:F:4:THR:HG23	6:F:55:ARG:HE	1.22	1.00
1:A:115:PRO:HD3	9:A:1002:C69:H2	1.45	0.97
3:C:223:ASP:CB	7:G:146:THR:HG21	1.97	0.94
2:B:205:ASN:HD22	2:B:208:ALA:H	0.96	0.93
1:A:384:LEU:HD21	1:A:414:PHE:CE1	2.03	0.92
1:A:309:ILE:HA	1:A:312:ARG:HH11	1.36	0.91
2:B:205:ASN:ND2	2:B:208:ALA:H	1.69	0.90
3:C:57:GLY:O	3:C:58:ILE:HG13	1.72	0.89
3:C:371:ILE:HG22	3:C:372:VAL:HG23	1.55	0.89
4:D:202:HIS:O	4:D:203:ARG:HB2	1.70	0.88
1:A:206:GLN:HE22	1:A:209:ARG:NH1	1.71	0.88
2:B:326:LEU:HD12	2:B:337:LEU:HD12	1.56	0.87
2:B:166:ILE:HD12	2:B:281:LEU:HD22	1.56	0.85
4:D:186:LYS:HZ3	4:D:200:PHE:H	1.21	0.85
5:E:126:ASP:O	5:E:130:ARG:HG3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD21	1:A:414:PHE:HE1	1.41	0.81
1:A:191:LYS:HE2	1:A:303:VAL:HG22	1.62	0.81
2:B:194:ILE:HG12	2:B:213:VAL:HG21	1.60	0.81
1:A:260:ASN:HD21	1:A:263:SER:HB3	1.44	0.81
3:C:107:ASN:C	3:C:107:ASN:HD22	1.84	0.80
1:A:79:ARG:HG2	1:A:82:ILE:HD11	1.64	0.80
3:C:57:GLY:O	3:C:58:ILE:CG1	2.30	0.79
3:C:90:LEU:HD23	3:C:91:VAL:N	1.98	0.77
1:A:260:ASN:ND2	1:A:263:SER:HB3	2.00	0.76
2:B:331:LYS:O	2:B:331:LYS:HD3	1.85	0.76
3:C:17:ASN:ND2	3:C:21:THR:HG22	1.95	0.76
7:G:38:ASP:OD2	7:G:41:GLU:HB2	1.85	0.76
2:B:205:ASN:HD22	2:B:208:ALA:N	1.80	0.75
2:B:261:ALA:HB3	2:B:262:PRO:HD3	1.68	0.74
2:B:163:VAL:HG21	2:B:181:ARG:HH21	1.49	0.74
1:A:393:VAL:HG21	1:A:414:PHE:CE2	2.21	0.74
1:A:246:ASP:OD1	5:E:50:LYS:HE3	1.87	0.74
6:F:4:THR:HG23	6:F:55:ARG:NE	2.02	0.74
3:C:107:ASN:ND2	3:C:109:LYS:H	1.87	0.73
3:C:2:ALA:N	11:C:450:HOH:O	2.21	0.73
2:B:299:LYS:HE2	2:B:341:LYS:HD3	1.71	0.72
3:C:144:THR:H	6:F:28:GLN:NE2	1.88	0.72
3:C:126:GLU:HB2	3:C:131:TRP:HZ3	1.52	0.72
3:C:21:THR:HG23	3:C:22:GLN:HG3	1.70	0.72
4:D:203:ARG:HD3	4:D:218:ASP:OD1	1.88	0.72
3:C:14:HIS:H	3:C:331:GLN:HE22	1.37	0.71
2:B:257:GLU:HA	2:B:260:GLU:HB2	1.72	0.71
1:A:84:GLU:HB3	9:A:1002:C69:H7	1.72	0.71
2:B:182:LEU:HD22	2:B:184:ILE:HG22	1.73	0.70
4:D:228:PHE:H	4:D:231:HIS:HD2	1.37	0.70
4:D:209:LEU:O	4:D:212:THR:N	2.24	0.70
2:B:239:VAL:HG23	2:B:240:LEU:HD13	1.73	0.70
1:A:67:ILE:HG22	1:A:68:GLU:HG3	1.73	0.70
6:F:158:ARG:O	6:F:162:GLU:HG3	1.92	0.70
1:A:194:PRO:C	1:A:195:ILE:HD12	2.13	0.69
5:E:75:ILE:HG23	5:E:144:LEU:HD11	1.74	0.69
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.56	0.69
3:C:155:VAL:HG21	3:C:180:PRO:HG3	1.74	0.69
1:A:335:LEU:HD23	1:A:367:VAL:HG21	1.74	0.68
2:B:290:ASP:O	2:B:294:ARG:HG3	1.94	0.68
1:A:393:VAL:HG21	1:A:414:PHE:CZ	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:ARG:HG2	4:D:141:ARG:HH11	1.59	0.67
2:B:279:ALA:CB	2:B:320:GLU:HG2	2.25	0.67
1:A:259:ILE:HA	1:A:265:LYS:O	1.96	0.66
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.10	0.66
1:A:309:ILE:HA	1:A:312:ARG:NH1	2.11	0.66
6:F:127:TYR:HB3	6:F:129:HIS:CE1	2.30	0.66
4:D:217:GLY:HA3	4:D:220:ILE:HD13	1.77	0.65
3:C:17:ASN:HD21	3:C:21:THR:CG2	2.01	0.65
1:A:384:LEU:HD21	1:A:414:PHE:CD1	2.32	0.65
9:A:1002:C69:H9	9:A:1002:C69:OAW	1.95	0.65
3:C:183:THR:CG2	3:C:185:TRP:H	2.08	0.65
1:A:84:GLU:HB3	9:A:1002:C69:CAL	2.26	0.65
1:A:206:GLN:HE22	1:A:209:ARG:HH11	1.43	0.64
7:G:68:SER:HB3	7:G:71:VAL:HG12	1.78	0.64
3:C:126:GLU:HB2	3:C:131:TRP:CZ3	2.33	0.64
4:D:141:ARG:HB3	4:D:155:GLU:HG3	1.80	0.64
9:A:1002:C69:H12	9:A:1002:C69:OAA	1.96	0.64
3:C:107:ASN:HD22	3:C:108:GLU:N	1.95	0.64
1:A:260:ASN:HD21	1:A:263:SER:CB	2.10	0.64
3:C:107:ASN:C	3:C:107:ASN:ND2	2.51	0.64
2:B:182:LEU:HD22	2:B:184:ILE:CG2	2.28	0.63
2:B:146:LEU:CD1	2:B:169:VAL:HB	2.27	0.63
5:E:152:GLN:HB3	5:E:155:LYS:NZ	2.13	0.63
6:F:58:LYS:HE2	6:F:58:LYS:HA	1.80	0.63
7:G:51:MET:HB3	7:G:86:PHE:CE1	2.33	0.63
4:D:237:ARG:HD3	11:D:413:HOH:O	1.99	0.63
5:E:150:ASP:O	5:E:152:GLN:N	2.32	0.63
11:A:1131:HOH:O	4:D:170:LYS:HE3	1.98	0.62
4:D:150:GLU:HG2	4:D:167:THR:HA	1.81	0.62
1:A:343:VAL:HG11	1:A:363:ILE:HG13	1.81	0.61
3:C:287:VAL:HG21	3:C:366:LEU:HD11	1.82	0.61
4:D:263:HIS:HD2	4:D:266:MET:CE	2.13	0.61
2:B:168:PRO:HG2	2:B:178:LEU:HD13	1.82	0.61
2:B:108:LEU:HD22	2:B:109:LEU:N	2.15	0.61
4:D:129:PHE:HD2	4:D:237:ARG:HG3	1.64	0.61
3:C:125:PHE:HE1	3:C:127:GLN:HA	1.67	0.60
1:A:216:PRO:CG	1:A:260:ASN:HB2	2.31	0.60
5:E:95:MET:HG3	5:E:141:GLY:HA3	1.82	0.60
1:A:200:ILE:HG12	1:A:281:ILE:HD11	1.84	0.60
1:A:313:ARG:NH1	1:A:363:ILE:HG22	2.16	0.60
3:C:21:THR:CG2	3:C:22:GLN:HG3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:ASP:HB2	7:G:146:THR:HG21	1.82	0.59
1:A:343:VAL:HG13	1:A:363:ILE:HD11	1.83	0.59
1:A:317:LYS:HE3	1:A:364:ASP:OD1	2.02	0.59
3:C:179:ARG:HG3	3:C:179:ARG:HH11	1.68	0.59
1:A:152:SER:C	1:A:154:THR:H	2.06	0.59
2:B:109:LEU:O	2:B:109:LEU:HD12	2.03	0.59
2:B:227:ILE:O	2:B:231:GLN:HG3	2.02	0.59
1:A:79:ARG:CG	1:A:82:ILE:HD11	2.32	0.59
2:B:175:LEU:HD12	2:B:178:LEU:HD21	1.84	0.59
2:B:337:LEU:HD23	2:B:337:LEU:O	2.02	0.59
2:B:333:ASP:OD2	2:B:336:LYS:HB2	2.03	0.58
2:B:163:VAL:HG22	2:B:164:THR:N	2.19	0.58
2:B:345:GLU:HG2	2:B:347:PRO:HD3	1.85	0.58
3:C:254:THR:OG1	3:C:372:VAL:HG22	2.04	0.58
2:B:336:LYS:HG2	2:B:339:LYS:HE3	1.84	0.58
2:B:184:ILE:HG13	2:B:265:LEU:HD23	1.86	0.58
2:B:343:ARG:HG2	2:B:343:ARG:HH21	1.70	0.57
3:C:155:VAL:HG21	3:C:180:PRO:CG	2.35	0.57
1:A:12:CYS:HB3	1:A:78:ILE:HD13	1.86	0.57
6:F:6:ARG:HB3	6:F:7:PRO:HD3	1.87	0.57
1:A:359:LYS:N	1:A:360:PRO:HD3	2.19	0.57
3:C:183:THR:HG22	3:C:185:TRP:H	1.68	0.57
3:C:256:SER:HB2	3:C:372:VAL:HG13	1.87	0.57
1:A:174:VAL:HG11	1:A:192:HIS:ND1	2.18	0.57
1:A:384:LEU:HD11	1:A:414:PHE:CE1	2.40	0.57
3:C:76:ALA:HB2	3:C:93:LEU:HD11	1.87	0.57
1:A:216:PRO:HG2	1:A:260:ASN:HB2	1.87	0.56
5:E:60:ILE:CD1	5:E:116:ILE:HG21	2.35	0.56
2:B:140:ILE:HD13	2:B:174:SER:HB3	1.88	0.56
1:A:301:ASP:HB2	1:A:339:LEU:HD11	1.87	0.56
4:D:205:PRO:HB3	4:D:209:LEU:HD12	1.88	0.56
7:G:15:ASP:O	7:G:18:GLU:HB2	2.04	0.56
2:B:151:LEU:HD13	2:B:300:HIS:HD2	1.69	0.56
2:B:279:ALA:HB1	2:B:320:GLU:HG2	1.85	0.56
2:B:173:PHE:N	2:B:173:PHE:CD2	2.74	0.56
2:B:177:HIS:O	2:B:178:LEU:HD12	2.06	0.55
7:G:44:SER:O	7:G:48:GLN:N	2.34	0.55
5:E:74:TYR:CE1	5:E:137:ARG:HD2	2.41	0.55
1:A:135:ASN:HB2	11:D:444:HOH:O	2.07	0.55
5:E:152:GLN:HB3	5:E:155:LYS:HZ1	1.70	0.55
1:A:309:ILE:CA	1:A:312:ARG:HH11	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ILE:O	2:B:143:VAL:HG22	2.06	0.55
6:F:142:ILE:O	6:F:146:ILE:HG13	2.06	0.55
3:C:144:THR:H	6:F:28:GLN:HE21	1.54	0.55
5:E:153:ASN:OD1	5:E:154:ASP:N	2.39	0.55
1:A:384:LEU:CD2	1:A:414:PHE:HE1	2.15	0.55
2:B:173:PHE:N	2:B:173:PHE:HD2	2.05	0.55
2:B:174:SER:C	2:B:175:LEU:HD23	2.28	0.55
3:C:156:LEU:HD11	3:C:183:THR:HG21	1.89	0.55
2:B:184:ILE:HD12	2:B:188:ASP:HB2	1.88	0.54
1:A:76:TRP:O	1:A:79:ARG:HD2	2.07	0.54
1:A:257:THR:HG22	1:A:258:GLY:N	2.23	0.54
3:C:19:ASP:OD1	3:C:21:THR:HB	2.08	0.54
2:B:146:LEU:HD12	2:B:169:VAL:HB	1.89	0.54
4:D:269:LYS:HE2	6:F:145:GLU:HB2	1.89	0.54
5:E:78:CYS:O	5:E:82:LEU:HB2	2.08	0.54
4:D:248:ARG:HD3	4:D:248:ARG:C	2.28	0.54
1:A:239:VAL:HG13	5:E:4:TYR:CE2	2.43	0.54
1:A:160:GLU:OE2	1:A:160:GLU:HA	2.08	0.53
4:D:199:LEU:N	4:D:199:LEU:HD12	2.23	0.53
1:A:343:VAL:HG22	1:A:363:ILE:HD11	1.90	0.53
5:E:60:ILE:CD1	5:E:116:ILE:HD13	2.39	0.53
2:B:330:LEU:O	2:B:332:GLY:N	2.41	0.53
6:F:45:GLU:HB3	7:G:24:PHE:CD2	2.44	0.53
1:A:349:LEU:O	1:A:353:LEU:HB2	2.08	0.53
2:B:163:VAL:HG21	2:B:181:ARG:NH2	2.23	0.53
2:B:182:LEU:HD13	2:B:184:ILE:HG23	1.91	0.53
5:E:112:PRO:O	5:E:114:ASN:N	2.42	0.53
1:A:152:SER:C	1:A:154:THR:N	2.61	0.53
1:A:216:PRO:HB2	1:A:219:GLN:HB2	1.89	0.53
1:A:258:GLY:O	1:A:266:GLU:HA	2.08	0.53
2:B:336:LYS:CG	2:B:339:LYS:HE3	2.39	0.53
9:A:1002:C69:OAA	9:A:1002:C69:CAG	2.57	0.53
3:C:98:ALA:O	3:C:115:SER:HB2	2.09	0.53
5:E:123:LYS:O	5:E:127:GLU:HG3	2.08	0.52
1:A:348:LYS:HE2	1:A:352:GLU:OE2	2.09	0.52
2:B:158:ASP:HA	2:B:304:SER:O	2.10	0.52
4:D:61:LEU:N	4:D:61:LEU:HD12	2.24	0.52
5:E:95:MET:HE3	5:E:95:MET:HA	1.92	0.52
1:A:239:VAL:HG11	5:E:48:TYR:CD1	2.44	0.52
4:D:53:THR:O	4:D:54:LYS:HD2	2.10	0.52
5:E:15:LEU:HD21	5:E:63:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:95:MET:HA	5:E:95:MET:CE	2.40	0.52
5:E:95:MET:HG2	5:E:141:GLY:O	2.09	0.52
7:G:87:LYS:HD3	7:G:87:LYS:N	2.25	0.52
4:D:141:ARG:HG2	4:D:141:ARG:NH1	2.24	0.52
5:E:16:ILE:HG23	5:E:16:ILE:O	2.09	0.52
2:B:173:PHE:HD2	2:B:173:PHE:H	1.56	0.52
1:A:115:PRO:HD3	9:A:1002:C69:CAB	2.32	0.52
2:B:287:GLN:NE2	2:B:298:TYR:OH	2.42	0.52
2:B:330:LEU:C	2:B:332:GLY:H	2.12	0.52
1:A:126:THR:OG1	9:A:1002:C69:H10	2.09	0.51
1:A:272:GLY:H	1:A:274:GLU:CD	2.13	0.51
3:C:167:ARG:HG2	3:C:197:GLU:HG3	1.92	0.51
2:B:146:LEU:HD23	2:B:302:VAL:HG11	1.92	0.51
5:E:95:MET:HG3	5:E:141:GLY:CA	2.40	0.51
1:A:55:VAL:CG2	1:A:58:LEU:HD12	2.41	0.51
1:A:301:ASP:HB2	1:A:339:LEU:CD1	2.40	0.51
3:C:332:ILE:HA	3:C:346:CYS:O	2.11	0.51
7:G:100:LYS:HA	7:G:100:LYS:HE2	1.92	0.51
5:E:152:GLN:O	5:E:155:LYS:HD2	2.10	0.51
6:F:145:GLU:O	6:F:149:MET:HG3	2.10	0.51
2:B:200:ARG:HD3	11:B:502:HOH:O	2.11	0.51
4:D:263:HIS:HD2	4:D:266:MET:HE3	1.75	0.51
3:C:125:PHE:CE1	3:C:127:GLN:HA	2.45	0.51
4:D:6:VAL:HG13	4:D:245:HIS:HE1	1.76	0.51
3:C:14:HIS:H	3:C:331:GLN:NE2	2.08	0.51
4:D:233:ASN:O	4:D:237:ARG:HB2	2.11	0.51
4:D:62:LYS:NZ	4:D:148:ASP:OD2	2.44	0.51
1:A:351:GLU:C	1:A:353:LEU:H	2.15	0.50
2:B:218:GLU:HG2	8:B:401:ATP:C5	2.46	0.50
3:C:284:ARG:HB2	11:C:464:HOH:O	2.12	0.50
1:A:69:LYS:CB	1:A:72:TYR:HB2	2.41	0.50
3:C:90:LEU:HD23	3:C:90:LEU:C	2.30	0.50
4:D:228:PHE:H	4:D:231:HIS:CD2	2.24	0.50
7:G:42:VAL:HG12	7:G:57:ALA:HB3	1.93	0.50
4:D:212:THR:O	4:D:212:THR:HG22	2.10	0.50
2:B:326:LEU:CD1	2:B:337:LEU:HD12	2.37	0.50
7:G:51:MET:HB3	7:G:86:PHE:CZ	2.46	0.50
2:B:153:THR:HA	2:B:169:VAL:O	2.10	0.50
3:C:16:TRP:CZ2	3:C:23:ILE:HD12	2.47	0.50
2:B:13:ASN:OD1	2:B:14:GLY:N	2.45	0.49
2:B:357:GLY:O	2:B:360:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:GLY:C	3:C:58:ILE:HG13	2.33	0.49
1:A:194:PRO:O	1:A:195:ILE:HD12	2.12	0.49
2:B:153:THR:HG22	2:B:154:GLY:N	2.27	0.49
3:C:119:VAL:HG22	3:C:120:ILE:N	2.27	0.49
3:C:119:VAL:HG23	3:C:137:ILE:O	2.13	0.49
7:G:68:SER:CB	7:G:71:VAL:HG12	2.41	0.49
1:A:239:VAL:HG23	1:A:240:LYS:N	2.27	0.49
5:E:15:LEU:CD2	5:E:63:GLU:HG3	2.42	0.49
3:C:126:GLU:CB	3:C:131:TRP:HZ3	2.25	0.49
5:E:105:ILE:CD1	5:E:130:ARG:NH1	2.75	0.49
1:A:328:PHE:CZ	8:A:1001:ATP:H2	2.31	0.49
3:C:103:ARG:NH1	11:C:410:HOH:O	2.46	0.49
3:C:151:HIS:CB	3:C:156:LEU:HB2	2.43	0.49
2:B:182:LEU:HG	2:B:281:LEU:HD12	1.94	0.49
2:B:205:ASN:HB3	2:B:208:ALA:HB3	1.94	0.49
2:B:313:LEU:HB3	2:B:314:PRO:HD3	1.93	0.49
3:C:62:PRO:HG2	3:C:108:GLU:OE2	2.12	0.49
1:A:30:ILE:HD13	1:A:375:TYR:OH	2.13	0.49
1:A:180:VAL:HG22	1:A:185:VAL:HG22	1.95	0.49
1:A:309:ILE:HA	1:A:312:ARG:CD	2.41	0.49
2:B:163:VAL:CG2	2:B:181:ARG:HH21	2.24	0.49
3:C:183:THR:HG23	3:C:185:TRP:H	1.75	0.49
4:D:202:HIS:HE1	4:D:218:ASP:O	1.96	0.49
5:E:153:ASN:O	5:E:155:LYS:HG3	2.13	0.48
1:A:328:PHE:CE1	8:A:1001:ATP:H2	2.31	0.48
1:A:384:LEU:HD11	1:A:414:PHE:HE1	1.77	0.48
2:B:111:GLU:HG3	2:B:140:ILE:HA	1.94	0.48
2:B:177:HIS:O	2:B:179:THR:N	2.46	0.48
5:E:60:ILE:HD12	5:E:116:ILE:HD13	1.95	0.48
6:F:130:LYS:HA	6:F:130:LYS:HE2	1.96	0.48
1:A:135:ASN:OD1	1:A:397:LYS:CE	2.61	0.48
6:F:121:PHE:O	6:F:125:GLN:HG3	2.14	0.48
1:A:239:VAL:HG11	5:E:48:TYR:HD1	1.78	0.48
1:A:384:LEU:HD22	1:A:384:LEU:O	2.13	0.48
4:D:67:LEU:HD13	4:D:120:CYS:O	2.13	0.48
3:C:14:HIS:HA	3:C:24:ALA:O	2.14	0.47
8:B:401:ATP:O2B	8:B:401:ATP:O3G	2.32	0.47
5:E:71:ILE:O	5:E:75:ILE:HG13	2.13	0.47
5:E:10:ASP:HB3	5:E:12:ASP:OD1	2.13	0.47
5:E:86:ASN:O	5:E:87:SER:HB3	2.15	0.47
2:B:108:LEU:N	2:B:108:LEU:HD13	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:LEU:CD1	6:F:35:LYS:HE3	2.44	0.47
5:E:146:GLU:O	5:E:146:GLU:HG2	2.15	0.47
2:B:166:ILE:HD13	2:B:282:LEU:HA	1.95	0.47
4:D:65:LYS:HA	4:D:65:LYS:HD3	1.70	0.47
1:A:30:ILE:HD13	1:A:375:TYR:CZ	2.50	0.47
1:A:230:ARG:NH1	1:A:230:ARG:HG2	2.29	0.47
1:A:311:VAL:C	1:A:314:PRO:HD2	2.34	0.47
2:B:308:THR:HA	2:B:313:LEU:CD2	2.45	0.47
2:B:341:LYS:O	2:B:341:LYS:HG3	2.15	0.47
5:E:10:ASP:HB2	5:E:13:THR:OG1	2.15	0.47
1:A:206:GLN:NE2	1:A:209:ARG:HH11	2.11	0.47
5:E:150:ASP:C	5:E:152:GLN:N	2.68	0.47
6:F:87:CYS:O	6:F:91:MET:HG2	2.14	0.47
7:G:50:ASN:HA	7:G:51:MET:CE	2.44	0.47
2:B:177:HIS:C	2:B:179:THR:H	2.18	0.46
7:G:50:ASN:HA	7:G:51:MET:HE3	1.97	0.46
1:A:223:THR:HG23	1:A:256:TYR:CE2	2.50	0.46
2:B:347:PRO:HA	2:B:348:PRO:HD3	1.83	0.46
4:D:220:ILE:N	4:D:220:ILE:HD12	2.31	0.46
4:D:223:ILE:HD12	4:D:223:ILE:N	2.30	0.46
5:E:35:GLU:HG2	5:E:40:ASP:HB3	1.96	0.46
3:C:249:ALA:HB1	3:C:332:ILE:HG22	1.98	0.46
5:E:20:ALA:HB3	5:E:22:LEU:HD21	1.97	0.46
2:B:156:VAL:HG22	2:B:302:VAL:CG1	2.46	0.46
2:B:306:GLY:HA2	2:B:309:MET:CE	2.46	0.46
9:A:1002:C69:OAW	9:A:1002:C69:CAP	2.56	0.46
3:C:130:ASP:O	3:C:131:TRP:HB3	2.15	0.46
5:E:9:MET:HG2	5:E:62:ASN:HB3	1.97	0.46
7:G:11:PHE:CE1	7:G:12:ARG:HG3	2.50	0.46
7:G:83:LEU:HD22	7:G:128:TRP:CD2	2.50	0.46
7:G:62:PRO:HA	7:G:63:PRO:HD3	1.67	0.46
1:A:239:VAL:HG13	5:E:4:TYR:CZ	2.50	0.46
2:B:184:ILE:HD12	2:B:185:ALA:N	2.31	0.46
1:A:84:GLU:H	1:A:84:GLU:CD	2.19	0.46
3:C:151:HIS:CE1	3:C:152:PRO:HG2	2.51	0.46
7:G:68:SER:HB3	7:G:71:VAL:CG1	2.45	0.46
1:A:230:ARG:HG2	1:A:230:ARG:HH11	1.81	0.45
2:B:227:ILE:HD11	2:B:263:GLU:OE2	2.15	0.45
3:C:7:LEU:O	3:C:352:GLY:HA3	2.16	0.45
5:E:165:LYS:HB2	11:E:204:HOH:O	2.14	0.45
6:F:102:PHE:HB2	11:F:221:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:N	1:A:18:LYS:HD3	2.31	0.45
1:A:55:VAL:HG13	1:A:55:VAL:O	2.15	0.45
4:D:147:ARG:HB2	4:D:150:GLU:HB2	1.96	0.45
4:D:67:LEU:O	4:D:72:ALA:HB2	2.16	0.45
7:G:66:THR:O	7:G:72:LYS:HE3	2.16	0.45
1:A:206:GLN:NE2	1:A:209:ARG:NH1	2.53	0.45
1:A:260:ASN:O	1:A:264:LYS:N	2.49	0.45
1:A:283:PHE:CE1	1:A:334:ARG:HG3	2.52	0.45
1:A:296:ILE:HG23	1:A:297:SER:N	2.32	0.45
2:B:224:GLY:O	2:B:316:ARG:HD3	2.16	0.45
4:D:171:ASP:O	4:D:174:ASP:HB2	2.15	0.45
5:E:5:HIS:HD2	5:E:65:ASP:OD2	1.99	0.45
5:E:138:GLN:OE1	5:E:138:GLN:HA	2.16	0.45
4:D:118:ARG:HD3	4:D:118:ARG:C	2.37	0.45
5:E:105:ILE:HD13	5:E:130:ARG:NH1	2.32	0.45
1:A:336:GLN:OE1	1:A:366:GLN:HA	2.16	0.45
4:D:75:LEU:HD23	4:D:75:LEU:C	2.37	0.45
5:E:168:PHE:CD2	5:E:169:MET:HE2	2.52	0.45
6:F:2:THR:OG1	6:F:3:ALA:N	2.48	0.45
1:A:55:VAL:HG21	1:A:58:LEU:HD12	1.98	0.45
5:E:88:LYS:O	5:E:92:GLU:HG3	2.17	0.45
2:B:156:VAL:HG22	2:B:302:VAL:HG13	1.99	0.45
4:D:141:ARG:HB3	4:D:155:GLU:CG	2.45	0.45
4:D:141:ARG:HD2	4:D:141:ARG:O	2.17	0.45
5:E:20:ALA:HB3	5:E:22:LEU:CD2	2.46	0.45
1:A:398:LYS:O	1:A:402:GLU:HG3	2.17	0.45
3:C:342:CYS:O	3:C:359:VAL:HG21	2.17	0.44
1:A:330:ASP:OD1	1:A:333:ARG:NH1	2.50	0.44
2:B:343:ARG:HG2	2:B:343:ARG:NH2	2.33	0.44
3:C:57:GLY:O	3:C:58:ILE:HG12	2.16	0.44
3:C:254:THR:HG1	3:C:372:VAL:HG22	1.81	0.44
4:D:141:ARG:HD2	4:D:141:ARG:C	2.37	0.44
5:E:56:LYS:HG3	5:E:170:ASN:ND2	2.33	0.44
3:C:102:VAL:HA	3:C:112:ALA:O	2.18	0.44
4:D:6:VAL:HG11	4:D:118:ARG:HG3	1.99	0.44
7:G:86:PHE:C	7:G:87:LYS:HD3	2.38	0.44
2:B:346:ASP:OD1	2:B:346:ASP:N	2.51	0.44
3:C:54:GLN:HB3	11:C:457:HOH:O	2.18	0.44
3:C:84:ARG:NH2	11:C:449:HOH:O	2.51	0.44
3:C:131:TRP:HE3	3:C:131:TRP:O	2.00	0.44
4:D:67:LEU:HD23	4:D:144:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:14:LYS:O	5:E:15:LEU:HD23	2.16	0.44
5:E:60:ILE:HD12	5:E:116:ILE:CG2	2.47	0.44
3:C:57:GLY:HA3	3:C:102:VAL:HG12	1.99	0.44
1:A:289:ASN:ND2	1:A:291:ASP:H	2.14	0.44
1:A:374:ARG:NH1	8:A:1001:ATP:N7	2.66	0.44
5:E:113:LEU:HA	11:E:219:HOH:O	2.17	0.44
3:C:27:PRO:HG2	3:C:29:ASN:ND2	2.33	0.44
3:C:344:GLN:HA	3:C:357:TRP:O	2.17	0.44
5:E:35:GLU:OE1	5:E:36:THR:N	2.51	0.44
1:A:343:VAL:HG12	1:A:344:ASP:N	2.32	0.44
3:C:48:LEU:HD12	3:C:48:LEU:N	2.33	0.44
7:G:64:ILE:HG23	7:G:149:LYS:HB3	2.00	0.44
2:B:15:THR:HG22	2:B:15:THR:O	2.17	0.44
2:B:353:MET:O	2:B:356:LEU:HB3	2.17	0.44
3:C:33:HIS:HD2	11:C:401:HOH:O	2.00	0.44
4:D:95:LEU:HD11	4:D:116:LEU:HG	1.99	0.44
1:A:134:PHE:HA	4:D:256:LYS:HD3	2.00	0.43
1:A:309:ILE:HG23	1:A:310:ASP:N	2.33	0.43
4:D:75:LEU:HD13	4:D:123:SER:N	2.33	0.43
3:C:209:CYS:SG	3:C:251:THR:HA	2.58	0.43
2:B:182:LEU:HG	2:B:281:LEU:CD1	2.48	0.43
2:B:306:GLY:HA2	2:B:309:MET:HE1	2.00	0.43
2:B:326:LEU:HD23	2:B:326:LEU:C	2.39	0.43
3:C:118:ARG:HH11	3:C:118:ARG:HG3	1.82	0.43
5:E:133:LEU:O	5:E:137:ARG:HG3	2.18	0.43
5:E:141:GLY:HA3	11:E:202:HOH:O	2.18	0.43
2:B:155:VAL:HG21	2:B:286:ILE:HD11	1.99	0.43
5:E:105:ILE:O	5:E:106:PRO:C	2.56	0.43
1:A:219:GLN:OE1	1:A:260:ASN:HA	2.18	0.43
2:B:194:ILE:HG12	2:B:213:VAL:CG2	2.40	0.43
2:B:337:LEU:HD23	2:B:337:LEU:C	2.39	0.43
5:E:150:ASP:C	5:E:152:GLN:H	2.22	0.43
7:G:44:SER:O	7:G:48:GLN:CB	2.66	0.43
7:G:149:LYS:HD3	11:G:204:HOH:O	2.19	0.43
3:C:174:LYS:HB3	3:C:174:LYS:HE2	1.81	0.43
6:F:73:SER:HB3	6:F:112:TYR:CG	2.54	0.43
3:C:69:THR:O	3:C:76:ALA:HA	2.18	0.43
6:F:153:VAL:O	6:F:156:ARG:HG2	2.18	0.43
7:G:51:MET:CE	7:G:51:MET:N	2.82	0.43
1:A:69:LYS:HB2	1:A:72:TYR:HB2	2.00	0.43
1:A:393:VAL:HG23	1:A:394:CYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:HB3	1:A:158:VAL:CG1	2.49	0.42
1:A:343:VAL:CG1	1:A:363:ILE:HG13	2.47	0.42
2:B:318:GLU:O	2:B:322:LYS:HG3	2.19	0.42
3:C:287:VAL:CG2	3:C:366:LEU:HD11	2.49	0.42
3:C:144:THR:N	6:F:28:GLN:HE21	2.16	0.42
4:D:68:GLN:HA	4:D:72:ALA:HB3	2.01	0.42
1:A:152:SER:O	1:A:154:THR:N	2.52	0.42
3:C:178:GLU:O	3:C:179:ARG:C	2.58	0.42
3:C:264:ASP:O	3:C:265:CYS:HB2	2.20	0.42
4:D:41:VAL:HG21	4:D:117:LYS:HE3	2.01	0.42
4:D:279:ARG:HG3	4:D:279:ARG:HH11	1.84	0.42
1:A:359:LYS:O	1:A:359:LYS:HG2	2.20	0.42
3:C:151:HIS:HB3	3:C:156:LEU:HB2	2.00	0.42
4:D:53:THR:C	4:D:54:LYS:HD2	2.40	0.42
5:E:82:LEU:HD13	5:E:95:MET:SD	2.59	0.42
5:E:149:PHE:CE2	5:E:156:PRO:HG3	2.55	0.42
1:A:311:VAL:O	1:A:314:PRO:HD2	2.20	0.42
2:B:281:LEU:O	2:B:281:LEU:HD23	2.19	0.42
2:B:334:VAL:HG23	2:B:335:GLU:N	2.34	0.42
3:C:250:VAL:HG22	3:C:251:THR:N	2.34	0.42
4:D:70:HIS:CE1	4:D:142:ALA:HB2	2.54	0.42
1:A:128:GLU:O	1:A:132:GLU:HB2	2.19	0.42
1:A:257:THR:HG22	1:A:258:GLY:H	1.85	0.42
1:A:329:ARG:NH1	11:A:1105:HOH:O	2.53	0.42
3:C:135:LYS:HE3	3:C:191:PHE:CE2	2.55	0.42
4:D:258:SER:OG	6:F:156:ARG:HD3	2.19	0.42
2:B:325:TYR:CZ	2:B:329:VAL:HG11	2.55	0.42
4:D:15:LEU:HD23	4:D:15:LEU:HA	1.76	0.42
7:G:84:ILE:HD12	7:G:84:ILE:N	2.34	0.42
1:A:12:CYS:HB3	1:A:78:ILE:CD1	2.50	0.42
5:E:88:LYS:H	5:E:153:ASN:ND2	2.18	0.42
3:C:48:LEU:N	3:C:48:LEU:CD1	2.83	0.42
1:A:390:PHE:O	1:A:394:CYS:HB2	2.20	0.42
4:D:198:VAL:HA	4:D:224:THR:O	2.20	0.42
2:B:332:GLY:O	2:B:334:VAL:N	2.53	0.41
5:E:111:PHE:CD2	5:E:112:PRO:O	2.73	0.41
1:A:11:ASP:HA	1:A:113:THR:OG1	2.20	0.41
2:B:153:THR:CG2	2:B:154:GLY:N	2.83	0.41
2:B:213:VAL:HA	2:B:216:ILE:HD12	2.02	0.41
2:B:306:GLY:O	2:B:309:MET:HE2	2.20	0.41
4:D:207:LEU:C	4:D:209:LEU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:248:ARG:HD3	4:D:248:ARG:O	2.19	0.41
5:E:60:ILE:CD1	5:E:116:ILE:CG2	2.98	0.41
1:A:191:LYS:HE2	1:A:191:LYS:HB2	1.90	0.41
3:C:90:LEU:HD23	3:C:91:VAL:C	2.41	0.41
4:D:130:GLN:HG3	4:D:134:GLU:OE1	2.20	0.41
5:E:86:ASN:O	5:E:87:SER:CB	2.69	0.41
6:F:31:GLU:OE2	6:F:32:ARG:NE	2.41	0.41
2:B:259:PHE:C	2:B:259:PHE:CD2	2.93	0.41
2:B:279:ALA:HB3	2:B:320:GLU:HG2	2.01	0.41
4:D:247:PHE:O	4:D:250:TYR:HB3	2.19	0.41
1:A:262:ILE:HG22	1:A:262:ILE:O	2.19	0.41
5:E:69:ILE:HG23	5:E:169:MET:HE1	2.03	0.41
6:F:86:LEU:HB3	6:F:149:MET:CE	2.51	0.41
2:B:308:THR:HA	2:B:313:LEU:HD23	2.02	0.41
4:D:186:LYS:HZ3	4:D:200:PHE:N	2.03	0.41
7:G:80:LEU:O	7:G:84:ILE:HD13	2.20	0.41
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.88	0.41
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.33	0.41
2:B:170:TYR:O	2:B:171:GLU:C	2.59	0.41
2:B:326:LEU:HD11	2:B:334:VAL:HG12	2.02	0.41
2:B:246:LEU:HB3	2:B:247:PRO:HD2	2.03	0.41
3:C:81:LEU:HD12	3:C:85:THR:O	2.21	0.41
3:C:157:LEU:O	3:C:168:ILE:HA	2.20	0.41
4:D:262:ILE:HD13	4:D:262:ILE:HA	1.90	0.41
1:A:305:GLN:O	1:A:312:ARG:NH2	2.52	0.41
2:B:165:HIS:CD2	2:B:181:ARG:HB2	2.56	0.41
2:B:274:GLU:OE1	2:B:274:GLU:HA	2.21	0.41
4:D:126:GLU:O	4:D:130:GLN:HB2	2.21	0.41
4:D:241:ILE:HA	4:D:244:ILE:HG22	2.02	0.41
5:E:77:GLU:HA	5:E:80:LYS:HD3	2.03	0.41
5:E:116:ILE:HG22	5:E:117:TYR:CD1	2.56	0.41
7:G:14:VAL:HG13	7:G:14:VAL:O	2.21	0.41
1:A:27:PRO:HG3	1:A:378:TRP:CD2	2.56	0.41
1:A:85:ASP:OD2	1:A:88:LEU:HD22	2.21	0.41
1:A:309:ILE:HA	1:A:312:ARG:HD2	2.03	0.41
4:D:134:GLU:HB2	4:D:136:LYS:HG3	2.01	0.41
1:A:335:LEU:HD23	1:A:367:VAL:CG2	2.45	0.40
2:B:151:LEU:HD13	2:B:300:HIS:CD2	2.52	0.40
1:A:343:VAL:O	1:A:347:LEU:HD13	2.20	0.40
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.35	0.40
3:C:106:PRO:HD2	3:C:154:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:HIS:O	4:D:203:ARG:CB	2.52	0.40
1:A:69:LYS:HB3	1:A:72:TYR:HB2	2.03	0.40
1:A:240:LYS:O	1:A:244:LYS:HG3	2.21	0.40
3:C:10:PRO:HG2	6:F:124:GLU:HG2	2.02	0.40
1:A:79:ARG:O	1:A:80:HIS:C	2.59	0.40
2:B:219:LYS:HG2	2:B:220:LEU:HD13	2.02	0.40
4:D:45:ILE:HA	4:D:56:MET:O	2.22	0.40
4:D:199:LEU:N	4:D:199:LEU:CD1	2.85	0.40
5:E:69:ILE:HG12	5:E:168:PHE:HE2	1.87	0.40
6:F:82:ILE:HG23	6:F:83:GLU:N	2.36	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	394/418 (94%)	367 (93%)	23 (6%)	4 (1%)	15 28
2	B	228/394 (58%)	205 (90%)	18 (8%)	5 (2%)	6 10
3	C	337/372 (91%)	314 (93%)	21 (6%)	2 (1%)	25 43
4	D	277/300 (92%)	266 (96%)	9 (3%)	2 (1%)	22 39
5	E	172/178 (97%)	160 (93%)	6 (4%)	6 (4%)	3 4
6	F	165/168 (98%)	157 (95%)	7 (4%)	1 (1%)	25 43
7	G	133/151 (88%)	117 (88%)	10 (8%)	6 (4%)	2 3
All	All	1706/1981 (86%)	1586 (93%)	94 (6%)	26 (2%)	10 18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	113	LEU

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Mol	Chain	Res	Type
5	E	153	ASN
1	A	52	MET
2	B	171	GLU
2	B	178	LEU
2	B	331	LYS
5	E	87	SER
6	F	102	PHE
7	G	48	GLN
2	B	333	ASP
4	D	203	ARG
7	G	22	ASN
7	G	27	GLU
7	G	88	ALA
5	E	49	PHE
5	E	151	PRO
7	G	23	LYS
2	B	359	ALA
3	C	58	ILE
4	D	208	GLU
5	E	112	PRO
1	A	352	GLU
1	A	412	PRO
1	A	194	PRO
7	G	63	PRO
3	C	179	ARG

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	349/363 (96%)	328 (94%)	21 (6%)	19	37
2	B	197/345 (57%)	183 (93%)	14 (7%)	14	28
3	C	290/313 (93%)	277 (96%)	13 (4%)	27	51
4	D	245/264 (93%)	236 (96%)	9 (4%)	34	60
5	E	155/159 (98%)	147 (95%)	8 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	154/155 (99%)	150 (97%)	4 (3%)	46	72
7	G	112/123 (91%)	105 (94%)	7 (6%)	18	34
All	All	1502/1722 (87%)	1426 (95%)	76 (5%)	24	45

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	88	LEU
1	A	89	MET
1	A	91	ARG
1	A	117	LEU
1	A	143	VAL
1	A	154	THR
1	A	156	ARG
1	A	172	ASP
1	A	191	LYS
1	A	192	HIS
1	A	230	ARG
1	A	251	LYS
1	A	260	ASN
1	A	289	ASN
1	A	310	ASP
1	A	312	ARG
1	A	343	VAL
1	A	353	LEU
1	A	384	LEU
1	A	401	GLU
2	B	108	LEU
2	B	111	GLU
2	B	173	PHE
2	B	175	LEU
2	B	182	LEU
2	B	184	ILE
2	B	220	LEU
2	B	240	LEU
2	B	257	GLU
2	B	290	ASP
2	B	298	TYR
2	B	320	GLU
2	B	331	LYS

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Mol	Chain	Res	Type
2	B	341	LYS
3	C	9	GLU
3	C	30	HIS
3	C	31	GLU
3	C	107	ASN
3	C	131	TRP
3	C	140	PRO
3	C	175	GLU
3	C	179	ARG
3	C	183	THR
3	C	201	SER
3	C	284	ARG
3	C	366	LEU
3	C	367	LYS
4	D	37	ASP
4	D	84	LEU
4	D	115	MET
4	D	116	LEU
4	D	141	ARG
4	D	172	ASP
4	D	207	LEU
4	D	245	HIS
4	D	281	ARG
5	E	10	ASP
5	E	25	ARG
5	E	82	LEU
5	E	95	MET
5	E	101	THR
5	E	133	LEU
5	E	146	GLU
5	E	166	ARG
6	F	85	ILE
6	F	101	PHE
6	F	152	SER
6	F	165	LEU
7	G	18	GLU
7	G	27	GLU
7	G	39	GLU
7	G	86	PHE
7	G	87	LYS
7	G	90	ASP
7	G	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	205	GLN
1	A	206	GLN
1	A	289	ASN
1	A	305	GLN
1	A	318	ASN
1	A	370	HIS
1	A	395	HIS
2	B	165	HIS
2	B	205	ASN
2	B	284	ASN
2	B	287	GLN
2	B	300	HIS
2	B	323	GLN
3	C	33	HIS
3	C	40	ASN
3	C	46	HIS
3	C	65	ASN
3	C	107	ASN
3	C	331	GLN
4	D	140	ASN
4	D	197	GLN
4	D	202	HIS
4	D	231	HIS
4	D	263	HIS
5	E	90	GLN
6	F	24	ASN
6	F	28	GLN
6	F	125	GLN
7	G	48	GLN
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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	ATP	A	1001	10	26,33,33	1.17	1 (3%)	31,52,52	1.61	4 (12%)
9	C69	A	1002	-	25,25,25	1.80	3 (12%)	33,35,35	2.54	9 (27%)
8	ATP	B	401	10	26,33,33	1.33	3 (11%)	31,52,52	2.14	11 (35%)

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
8	ATP	A	1001	10	-	7/18/38/38	0/3/3/3
9	C69	A	1002	-	-	8/12/25/25	0/3/3/3
8	ATP	B	401	10	-	2/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1002	C69	CAE-NAF	-7.41	1.34	1.43
8	B	401	ATP	C2-N1	3.54	1.40	1.33
8	A	1001	ATP	C2-N1	3.53	1.40	1.33
9	A	1002	C69	CAQ-NAF	-3.35	1.33	1.37
8	B	401	ATP	PG-O1G	3.31	1.61	1.50
8	B	401	ATP	O4'-C1'	2.29	1.44	1.41
9	A	1002	C69	CAH-CAG	2.05	1.53	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1002	C69	CAR-CAQ-NAF	7.85	117.51	112.14
9	A	1002	C69	CAQ-CAR-SAS	-6.85	101.74	107.60
8	A	1001	ATP	N3-C2-N1	-5.18	120.58	128.68
8	B	401	ATP	N3-C2-N1	-5.05	120.78	128.68
9	A	1002	C69	CAB-OAA-CAD	-5.04	109.92	117.53
8	B	401	ATP	O2G-PG-O3B	-4.04	91.09	104.64
8	B	401	ATP	PA-O3A-PB	-3.80	119.78	132.83
8	A	1001	ATP	O4'-C1'-C2'	-3.71	101.50	106.93
9	A	1002	C69	OAW-CAQ-NAF	-3.70	122.14	125.10
8	B	401	ATP	O3B-PG-O1G	-3.57	91.40	111.19
9	A	1002	C69	CAL-OAM-CAN	-3.53	109.85	117.51
8	B	401	ATP	PB-O3B-PG	-3.38	121.22	132.83
8	A	1001	ATP	PA-O3A-PB	-3.37	121.26	132.83
8	B	401	ATP	O3G-PG-O2G	3.28	120.18	107.64
9	A	1002	C69	OAA-CAD-CAC	-3.19	118.63	124.12
8	A	1001	ATP	PB-O3B-PG	-3.17	121.95	132.83
9	A	1002	C69	OAA-CAD-CAE	3.12	120.31	116.06
9	A	1002	C69	CAH-CAG-NAF	-2.99	110.23	113.49
8	B	401	ATP	O5'-PA-O1A	-2.98	97.42	109.07
8	B	401	ATP	O3G-PG-O1G	2.96	122.28	110.68
8	B	401	ATP	O2A-PA-O1A	2.64	125.30	112.24
9	A	1002	C69	CAE-NAF-CAG	2.36	121.71	118.81
8	B	401	ATP	O2A-PA-O5'	-2.15	97.75	107.75
8	B	401	ATP	O3G-PG-O3B	-2.11	97.56	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	ATP	PB-O3B-PG-O2G
8	A	1001	ATP	C5'-O5'-PA-O2A
9	A	1002	C69	CAD-CAE-NAF-CAQ
9	A	1002	C69	CAD-CAE-NAF-CAG
9	A	1002	C69	CAP-CAE-NAF-CAQ
9	A	1002	C69	CAP-CAE-NAF-CAG
9	A	1002	C69	CAO-CAN-OAM-CAL
9	A	1002	C69	CAC-CAN-OAM-CAL
9	A	1002	C69	CAC-CAD-OAA-CAB
9	A	1002	C69	CAE-CAD-OAA-CAB
8	A	1001	ATP	PB-O3B-PG-O1G
8	B	401	ATP	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
8	A	1001	ATP	C5'-O5'-PA-O3A
8	B	401	ATP	PB-O3B-PG-O2G
8	A	1001	ATP	PB-O3A-PA-O1A
8	A	1001	ATP	PB-O3A-PA-O2A
8	A	1001	ATP	C5'-O5'-PA-O1A

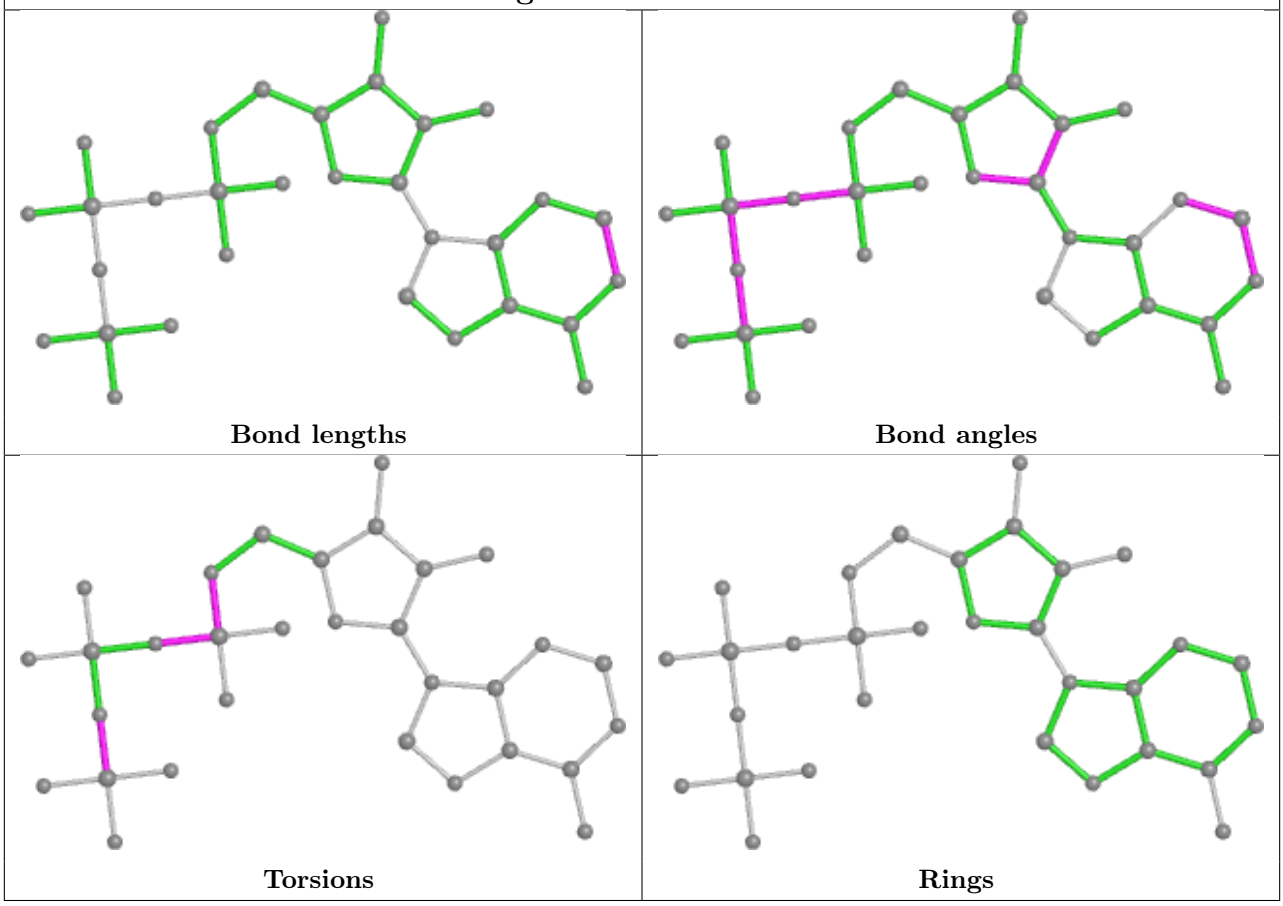
There are no ring outliers.

3 monomers are involved in 14 short contacts:

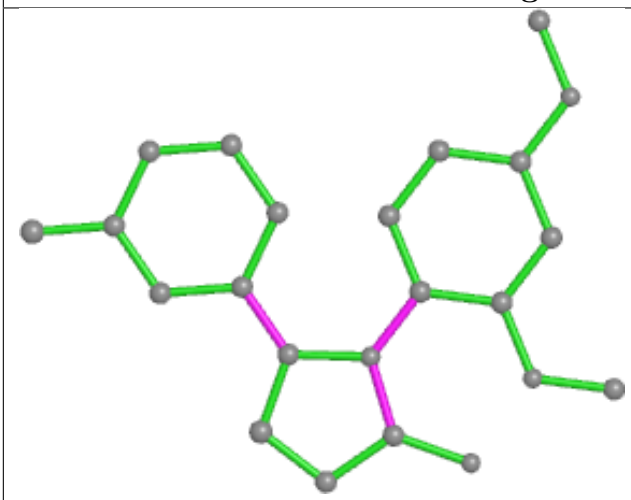
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	ATP	3	0
9	A	1002	C69	9	0
8	B	401	ATP	2	0

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.

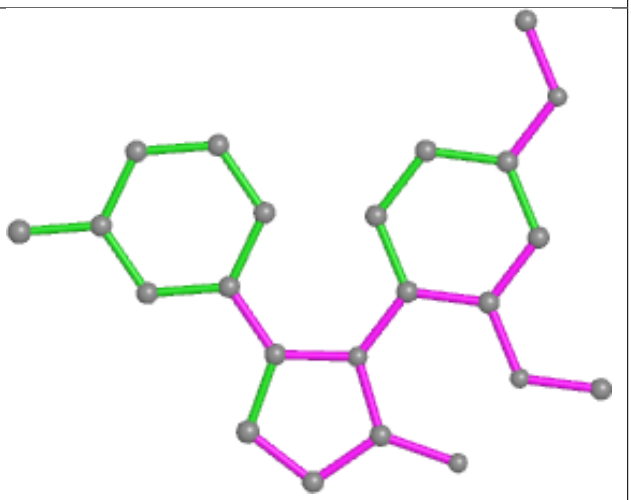
Ligand ATP A 1001



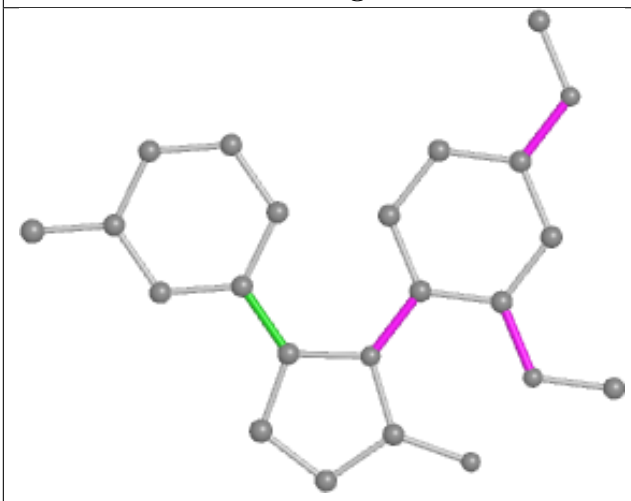
Ligand C69 A 1002



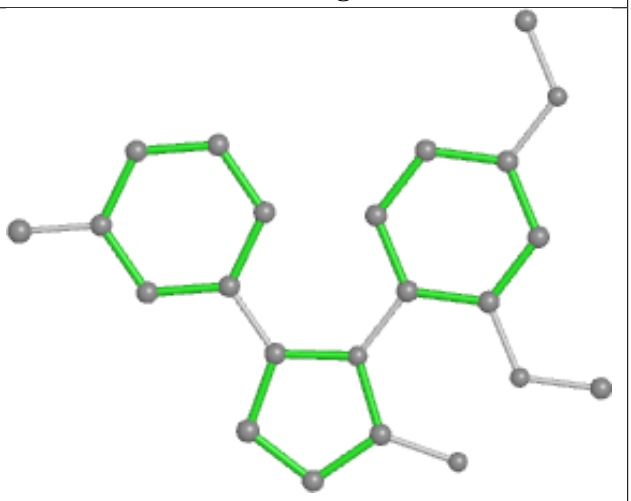
Bond lengths



Bond angles

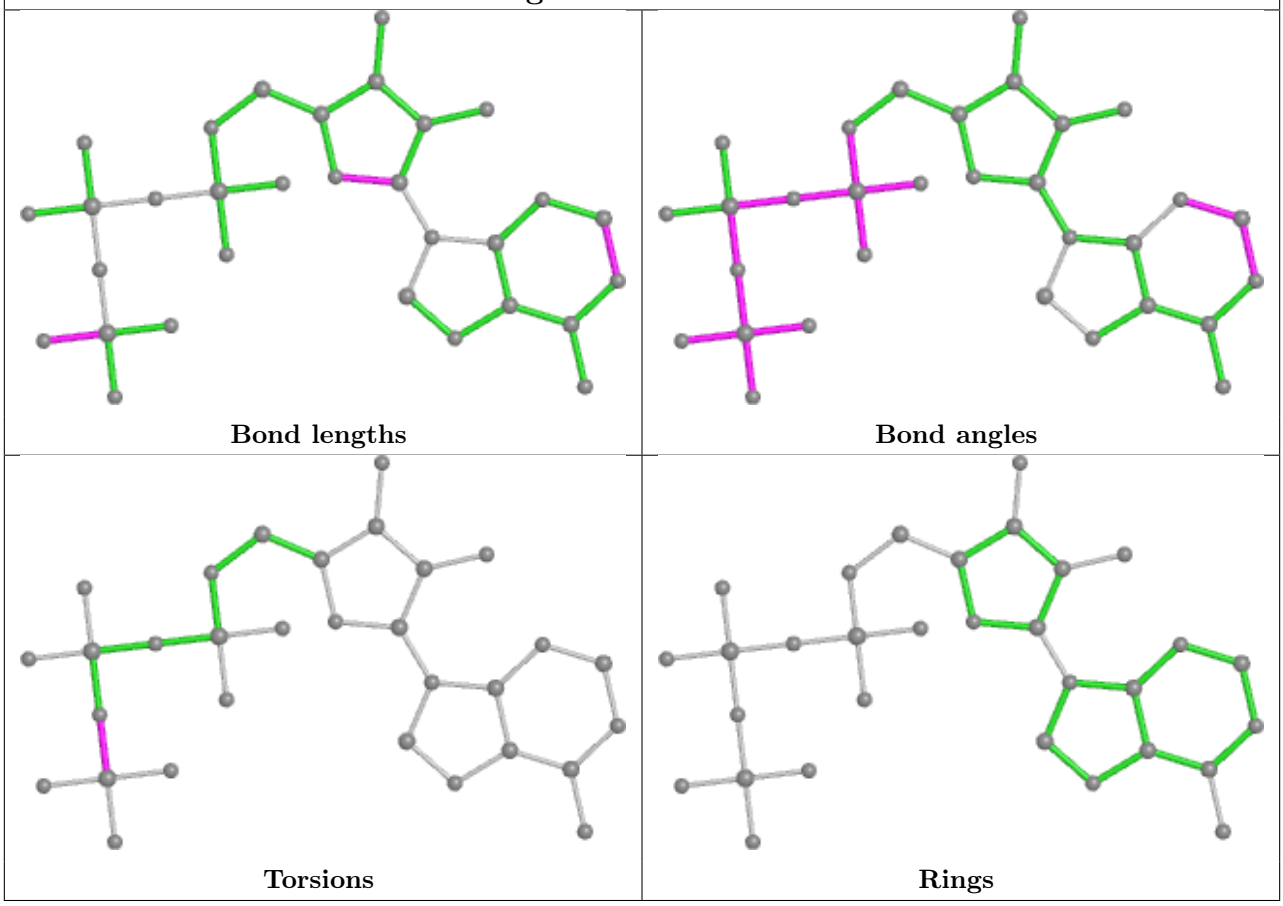


Torsions



Rings

Ligand ATP B 401



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	400/418 (95%)	0.10	12 (3%)	50	53	20, 40, 74, 93	0
2	B	236/394 (59%)	0.58	30 (12%)	3	3	26, 55, 94, 99	0
3	C	341/372 (91%)	-0.16	2 (0%)	89	90	25, 35, 63, 81	0
4	D	281/300 (93%)	-0.25	3 (1%)	80	82	19, 37, 63, 98	0
5	E	174/178 (97%)	-0.09	1 (0%)	89	90	30, 45, 68, 90	0
6	F	167/168 (99%)	-0.22	2 (1%)	79	80	18, 31, 44, 78	0
7	G	137/151 (90%)	0.20	8 (5%)	23	24	26, 52, 84, 94	0
All	All	1736/1981 (87%)	0.02	58 (3%)	46	50	18, 39, 82, 99	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	7.6
2	B	114	MET	6.2
1	A	52	MET	5.6
2	B	109	LEU	5.4
2	B	360	VAL	5.1
1	A	158	VAL	4.9
4	D	215	ALA	4.9
2	B	140	ILE	4.6
2	B	139	ALA	4.4
1	A	414	PHE	4.2
1	A	156	ARG	4.2
2	B	147	TYR	4.0
2	B	112	PRO	3.9
2	B	108	LEU	3.8
1	A	359	LYS	3.7
2	B	359	ALA	3.5
2	B	356	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
7	G	28	GLU	3.5
2	B	342	ILE	3.4
7	G	11	PHE	3.3
4	D	214	ALA	3.3
2	B	339	LYS	3.3
7	G	10	ARG	3.2
2	B	16	GLY	3.1
2	B	12	ASP	3.1
2	B	152	LEU	3.1
6	F	2	THR	3.1
2	B	345	GLU	3.0
2	B	173	PHE	3.0
5	E	154	ASP	3.0
2	B	178	LEU	3.0
2	B	176	PRO	3.0
2	B	349	ARG	3.0
2	B	17	PHE	2.8
2	B	174	SER	2.8
7	G	35	ALA	2.7
2	B	171	GLU	2.7
7	G	13	LYS	2.7
2	B	13	ASN	2.7
1	A	351	GLU	2.6
2	B	110	THR	2.6
2	B	299	LYS	2.5
1	A	352	GLU	2.5
6	F	3	ALA	2.5
3	C	369	LEU	2.4
4	D	107	ASP	2.4
2	B	111	GLU	2.4
1	A	292	PHE	2.3
2	B	340	PHE	2.3
7	G	50	ASN	2.3
7	G	120	ASN	2.3
1	A	159	GLY	2.3
2	B	154	GLY	2.3
7	G	37	PRO	2.2
3	C	127	GLN	2.1
1	A	347	LEU	2.1
2	B	15	THR	2.0
1	A	360	PRO	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)

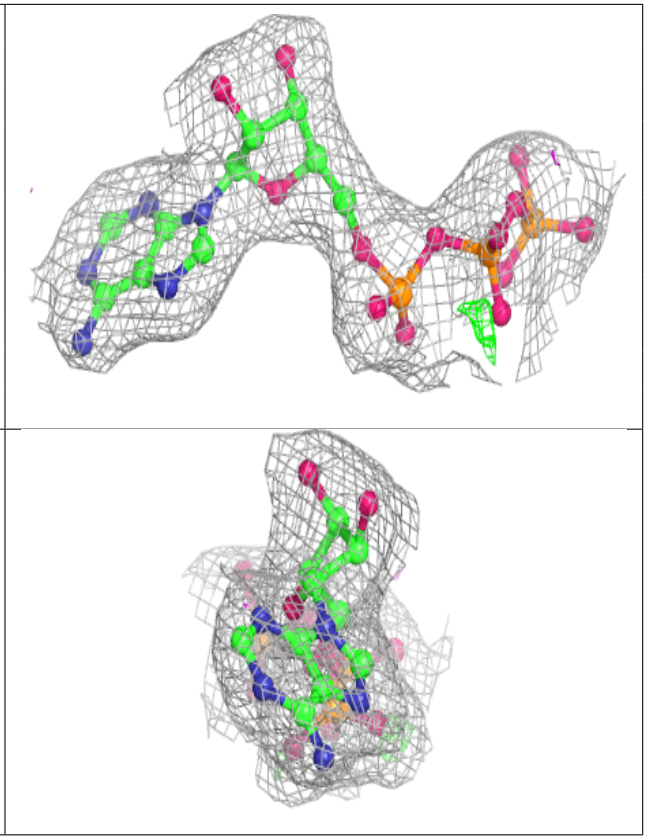
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CA	B	402	1/1	0.88	0.17	70,70,70,70	0
10	CA	A	1003	1/1	0.89	0.29	61,61,61,61	0
8	ATP	B	401	31/31	0.95	0.11	35,39,52,54	0
9	C69	A	1002	23/23	0.95	0.19	44,46,51,52	0
8	ATP	A	1001	31/31	0.97	0.16	31,38,41,43	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.

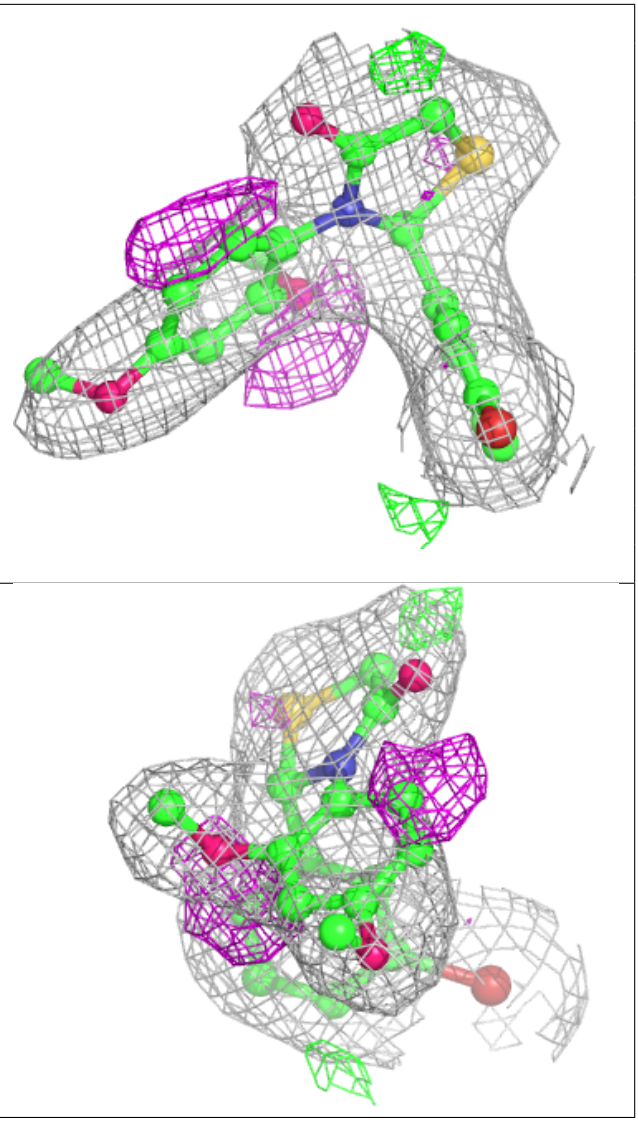
Electron density around ATP B 401:

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



Electron density around C69 A 1002:

$2mF_o$-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 1001:

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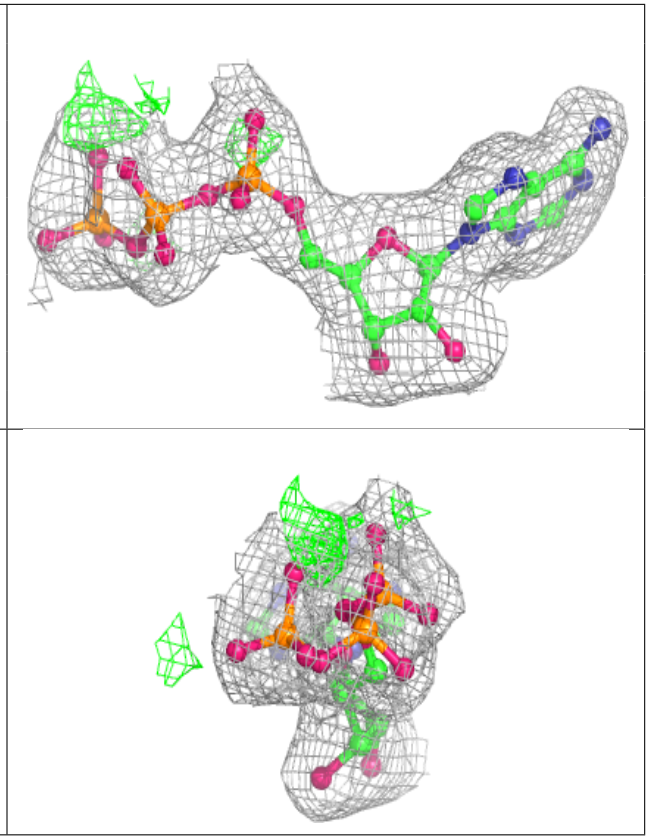
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.