Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 07:44 AM EDT

PDB ID	:	2QKM
Title	:	The crystal structure of fission yeast mRNA decapping enzyme Dcp1-Dcp2 complex
Authors	:	She, M.; Song, H.
Deposited on	:	2007-07-11
Resolution	:	2.80 Å(reported)

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

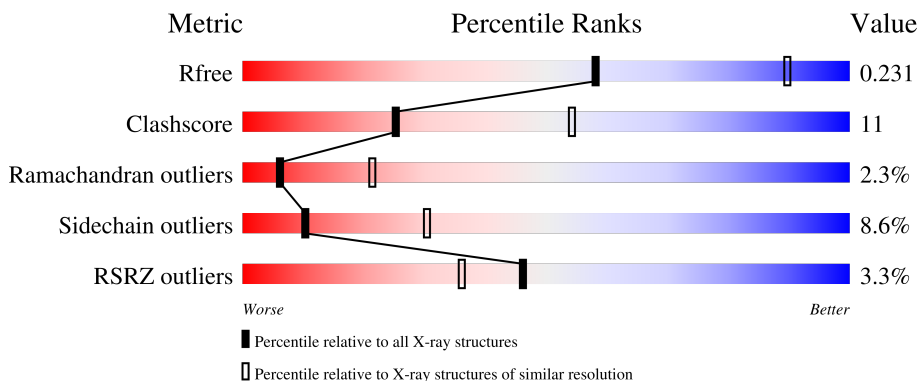|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.231
Clashscore		11
Ramachandran outliers		2.3%
Sidechain outliers		8.6%
RSRZ outliers		3.3%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	127	2% 71% 25% • •
1	C	127	72% 23% • •
1	E	127	2% 83% 13% • •
1	G	127	4% 69% 27% • •
2	B	266	70% 27% •

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Mol	Chain	Length	Quality of chain
2	D	266	8% 51% 19% 6% 24%
2	F	266	67% 27% 5%
2	H	266	6% 48% 20% 29%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11874 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 SPBC3B9.21 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			1034	666	181	184	3			
1	C	123	Total	C	N	O	S	0	0	0
			1026	660	179	184	3			
1	E	123	Total	C	N	O	S	0	0	0
			1034	666	181	184	3			
1	G	127	Total	C	N	O	S	0	0	0
			1060	681	186	190	3			

- Molecule 2 is a protein called SPAC19A8.12 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	266	Total	C	N	O	S	0	0	0
			2175	1392	373	397	13			
2	D	202	Total	C	N	O	S	0	0	0
			1670	1076	280	302	12			
2	F	262	Total	C	N	O	S	0	0	0
			2143	1372	367	391	13			
2	H	190	Total	C	N	O	S	0	0	0
			1562	1005	263	282	12			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	27	Total	O	0	0
			27	27		
4	C	8	Total	O	0	0
			8	8		
4	D	5	Total	O	0	0
			5	5		
4	E	8	Total	O	0	0
			8	8		
4	F	24	Total	O	0	0
			24	24		
4	G	16	Total	O	0	0
			16	16		
4	H	12	Total	O	0	0
			12	12		

3 Residue-property plots ⓘ

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

• Molecule 1: SPBC3B9.21 protein
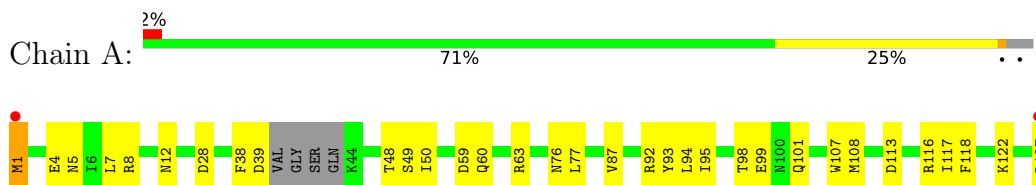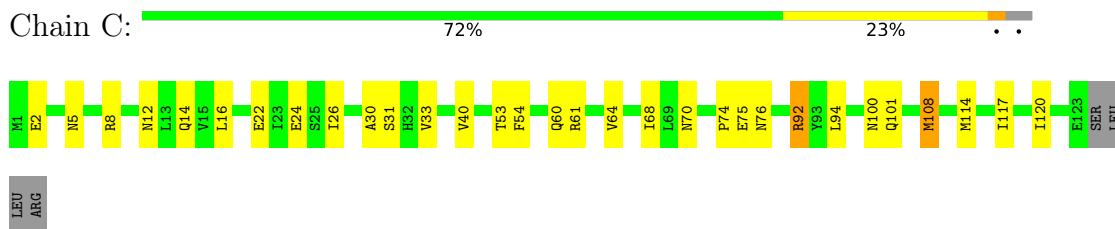
• Molecule 1: SPBC3B9.21 protein

• Molecule 1: SPBC3B9.21 protein
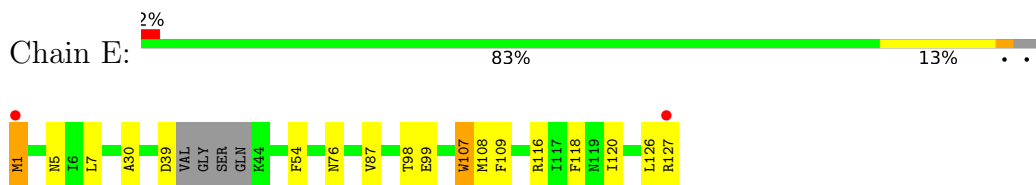
• Molecule 1: SPBC3B9.21 protein
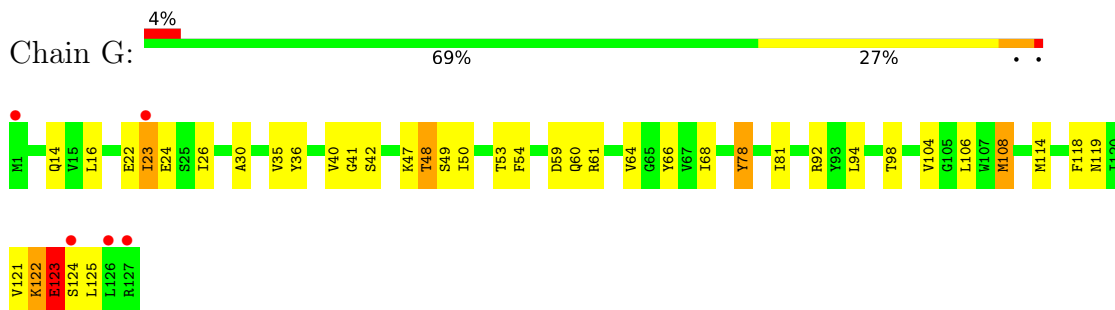
• Molecule 2: SPAC19A8.12 protein

• Molecule 2: SPAC19A8.12 protein

Chain D:

• Molecule 2: SPAC19A8.12 protein

Chain F:

• Molecule 2: SPAC19A8.12 protein

Chain H:
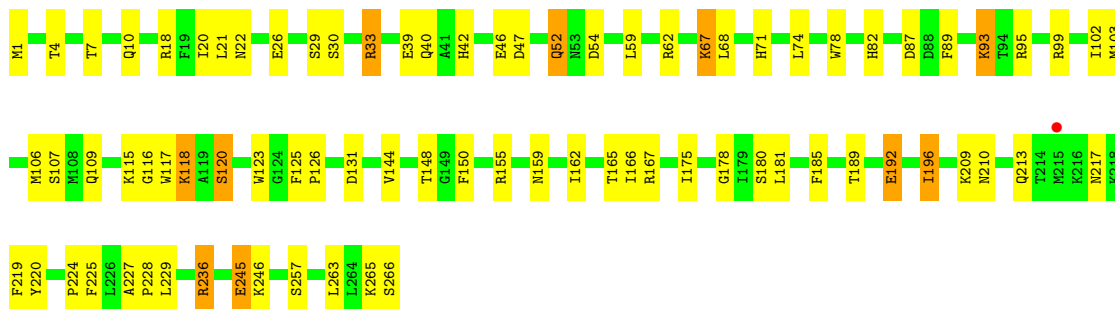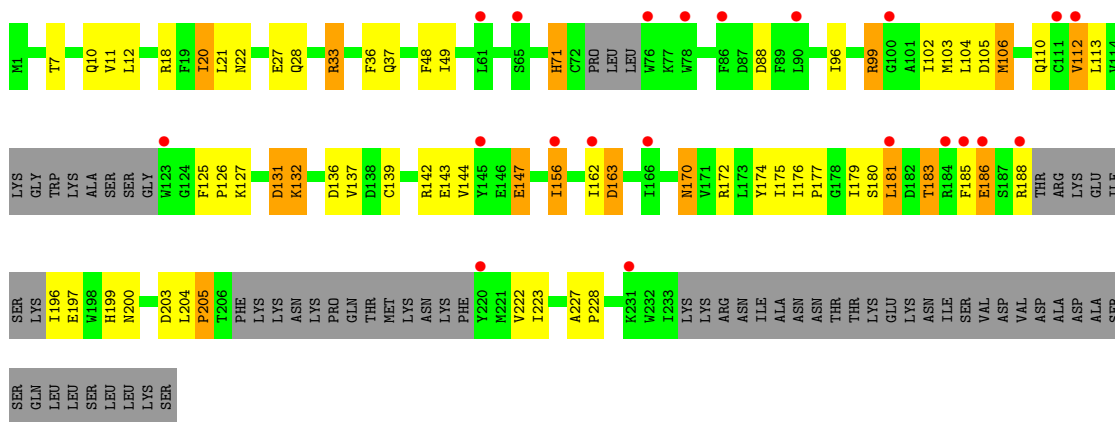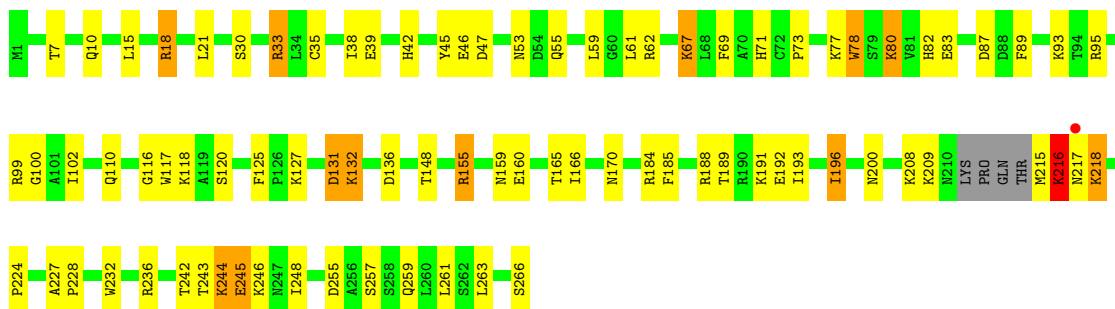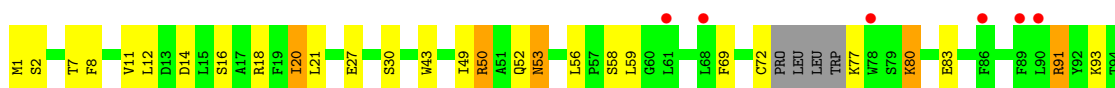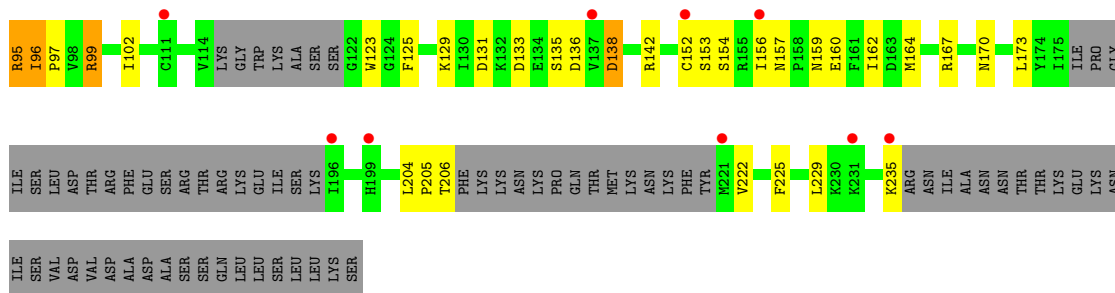
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.29Å 161.44Å 91.39Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 90.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.80) 99.9 (90.61-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.95 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.289 0.229 , 0.231	Depositor DCC
R_{free} test set	2438 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.8	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/1058	0.63	0/1432
1	C	0.47	0/1051	0.62	0/1426
1	E	0.48	0/1058	0.62	0/1432
1	G	0.46	0/1085	0.62	0/1470
2	B	0.52	0/2225	0.66	0/2999
2	D	0.44	0/1710	0.54	0/2308
2	F	0.52	0/2191	0.65	0/2951
2	H	0.66	1/1597 (0.1%)	0.56	0/2151
All	All	0.52	1/11975 (0.0%)	0.62	0/16169

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	235	LYS	C-O	19.61	1.60	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1034	0	1026	22	0
1	C	1026	0	1012	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1034	0	1026	12	0
1	G	1060	0	1052	29	0
2	B	2175	0	2179	52	0
2	D	1670	0	1629	45	0
2	F	2143	0	2143	63	0
2	H	1562	0	1534	32	0
3	B	31	0	12	0	0
3	F	31	0	12	0	0
4	A	8	0	0	0	0
4	B	27	0	0	4	0
4	C	8	0	0	1	0
4	D	5	0	0	0	0
4	E	8	0	0	0	0
4	F	24	0	0	1	0
4	G	16	0	0	1	0
4	H	12	0	0	1	0
All	All	11874	0	11625	250	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 11.

All (250) 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)
2:F:218:LYS:H	2:F:218:LYS:HD2	1.06	1.08
2:B:117:TRP:O	2:B:118:LYS:HB2	1.49	1.07
2:H:50:ARG:HH22	2:H:58:SER:HB2	1.14	1.04
2:F:53:ASN:HD21	2:F:55:GLN:HB2	1.29	0.96
1:G:81:ILE:HD13	1:G:121:VAL:HG11	1.48	0.93
1:A:8:ARG:HE	2:B:74:LEU:HD11	1.33	0.91
2:F:218:LYS:HD2	2:F:218:LYS:N	1.80	0.90
2:D:196:ILE:HG13	2:D:197:GLU:H	1.36	0.89
1:C:60:GLN:O	1:C:61:ARG:HB2	1.74	0.85
2:D:183:THR:HB	2:D:185:PHE:CE1	2.12	0.85
2:B:159:ASN:HB3	2:B:246:LYS:O	1.80	0.81
1:A:12:ASN:HD21	2:B:22:ASN:HD21	1.29	0.81
1:G:30:ALA:HB3	1:G:54:PHE:HB3	1.63	0.80
2:B:67:LYS:HE2	2:F:266:SER:O	1.81	0.80
1:G:48:THR:HG22	1:G:50:ILE:H	1.47	0.79
1:G:60:GLN:O	1:G:61:ARG:HB2	1.84	0.77
1:C:117:ILE:HA	1:C:120:ILE:HG22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:53:ASN:ND2	2:F:55:GLN:HB2	2.01	0.75
1:G:23:ILE:HG13	1:G:24:GLU:H	1.51	0.75
1:G:60:GLN:HA	4:G:129:HOH:O	1.87	0.75
1:G:16:LEU:HB3	1:G:23:ILE:HD13	1.66	0.75
2:F:35:CYS:O	2:F:39:GLU:HG3	1.87	0.74
2:B:213:GLN:HG3	4:B:279:HOH:O	1.88	0.74
2:H:95:ARG:HE	2:H:95:ARG:HA	1.52	0.73
2:F:15:LEU:HD11	2:F:45:TYR:HB2	1.70	0.73
2:H:91:ARG:HH21	2:H:129:LYS:HE3	1.54	0.73
1:E:5:ASN:HD21	1:G:49:SER:HB3	1.53	0.72
2:F:100:GLY:HA3	2:F:127:LYS:HB3	1.72	0.72
2:B:40:GLN:HE22	2:B:167:ARG:HE	1.37	0.71
2:F:216:LYS:O	2:F:216:LYS:HG2	1.89	0.71
1:G:123:GLU:H	1:G:123:GLU:CD	1.93	0.70
2:D:196:ILE:HG13	2:D:197:GLU:N	2.06	0.70
2:F:42:HIS:HE1	2:F:59:LEU:O	1.74	0.70
2:D:103:MET:HB2	2:D:112:VAL:HG13	1.73	0.69
2:D:179:ILE:O	2:D:181:LEU:N	2.25	0.69
2:B:263:LEU:O	2:F:67:LYS:HD2	1.92	0.68
2:B:266:SER:OXT	2:F:71:HIS:NE2	2.27	0.68
1:G:23:ILE:O	1:G:59:ASP:HA	1.93	0.67
2:F:148:THR:HG22	2:F:196:ILE:CD1	2.25	0.67
2:F:232:TRP:CD1	2:F:248:ILE:HG22	2.29	0.67
1:G:48:THR:CG2	1:G:50:ILE:H	2.08	0.66
2:B:144:VAL:O	2:B:148:THR:HB	1.96	0.65
2:B:7:THR:H	2:B:10:GLN:HE21	1.45	0.64
2:F:148:THR:HG22	2:F:196:ILE:HD12	1.80	0.64
2:B:162:ILE:HG13	2:B:175:ILE:HD11	1.79	0.64
1:G:94:LEU:HB3	1:G:106:LEU:HB2	1.80	0.63
2:B:117:TRP:O	2:B:118:LYS:CB	2.32	0.63
2:H:72:CYS:SG	2:H:77:LYS:HD3	2.39	0.63
2:H:131:ASP:HB2	2:H:142:ARG:NH2	2.14	0.62
2:B:42:HIS:HD2	4:B:271:HOH:O	1.81	0.62
1:A:50:ILE:HD13	1:A:77:LEU:HB2	1.80	0.62
2:D:99:ARG:HB2	2:D:139:CYS:SG	2.40	0.61
2:D:105:ASP:O	2:D:106:MET:HB2	2.00	0.61
2:B:42:HIS:HE1	2:B:59:LEU:O	1.83	0.61
2:D:103:MET:HB2	2:D:112:VAL:CG1	2.31	0.61
2:H:14:ASP:OD2	2:H:18:ARG:HD2	2.01	0.60
1:C:16:LEU:HD12	1:C:26:ILE:HD11	1.82	0.60
1:G:35:VAL:O	1:G:48:THR:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:GLU:HB3	2:D:33:ARG:HG3	1.83	0.60
1:A:8:ARG:NE	2:B:74:LEU:HD11	2.12	0.59
2:F:62:ARG:NH1	2:F:87:ASP:OD1	2.35	0.59
2:D:147:GLU:HA	2:D:188:ARG:HH11	1.67	0.59
2:D:205:PRO:HG2	2:D:223:ILE:HD11	1.84	0.59
2:H:50:ARG:HB2	4:H:267:HOH:O	2.02	0.59
2:B:148:THR:HG22	2:B:150:PHE:H	1.68	0.59
2:D:125:PHE:CE1	2:D:222:VAL:HG13	2.37	0.59
1:C:108:MET:HG2	4:C:128:HOH:O	2.02	0.58
2:D:7:THR:H	2:D:10:GLN:HE21	1.49	0.58
1:E:107:TRP:CZ3	1:E:109:PHE:HA	2.39	0.57
1:G:23:ILE:O	1:G:24:GLU:HB3	2.04	0.57
2:B:67:LYS:HD2	2:F:263:LEU:O	2.04	0.57
1:E:116:ARG:O	1:E:120:ILE:HG13	2.05	0.57
2:H:50:ARG:HH22	2:H:58:SER:CB	2.04	0.57
2:B:185:PHE:HB3	2:B:196:ILE:HG12	1.86	0.57
1:A:76:ASN:OD1	2:B:18:ARG:NH2	2.37	0.57
2:F:218:LYS:H	2:F:218:LYS:CD	1.96	0.57
2:H:80:LYS:HA	2:H:83:GLU:HB2	1.87	0.57
2:B:115:LYS:HG2	2:B:116:GLY:O	2.04	0.56
1:A:59:ASP:HB3	1:A:63:ARG:H	1.70	0.56
1:C:30:ALA:HB3	1:C:54:PHE:HB3	1.87	0.56
2:H:135:SER:HB2	2:H:138:ASP:HB2	1.86	0.56
2:H:204:LEU:O	2:H:206:THR:N	2.38	0.56
2:D:185:PHE:O	2:D:186:GLU:HG3	2.05	0.55
2:B:148:THR:HG23	2:B:185:PHE:CD2	2.42	0.55
2:H:102:ILE:HG12	2:H:125:PHE:CD2	2.42	0.55
1:C:117:ILE:HA	1:C:120:ILE:CG2	2.36	0.55
1:A:87:VAL:HA	1:A:95:ILE:O	2.06	0.55
1:E:1:MET:N	2:F:77:LYS:HE3	2.22	0.54
2:F:165:THR:HG22	2:F:170:ASN:OD1	2.08	0.54
2:B:148:THR:HG23	2:B:185:PHE:HD2	1.72	0.54
1:A:48:THR:HG22	1:A:49:SER:N	2.23	0.54
2:B:118:LYS:C	2:B:120:SER:H	2.11	0.54
2:F:110:GLN:HG2	2:F:200:ASN:ND2	2.22	0.54
2:F:257:SER:O	2:F:261:LEU:HB2	2.07	0.54
1:G:121:VAL:O	1:G:122:LYS:HB2	2.07	0.53
2:H:173:LEU:HD12	2:H:225:PHE:CE2	2.43	0.53
2:B:107:SER:OG	2:B:109:GLN:HG2	2.09	0.53
2:H:157:ASN:HD22	2:H:160:GLU:HG2	1.72	0.53
2:F:33:ARG:HD3	2:F:33:ARG:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ASP:HB2	2:D:142:ARG:NH1	2.24	0.53
2:H:8:PHE:HD1	2:H:56:LEU:HD22	1.72	0.53
2:H:99:ARG:HG2	2:H:136:ASP:O	2.07	0.53
2:F:218:LYS:N	2:F:218:LYS:CD	2.56	0.53
1:C:76:ASN:HD21	2:D:18:ARG:HH12	1.57	0.53
2:F:160:GLU:OE1	2:F:236:ARG:NH1	2.42	0.53
2:B:95:ARG:CZ	2:B:165:THR:HG21	2.39	0.52
2:D:20:ILE:HG22	2:D:21:LEU:H	1.74	0.52
2:F:248:ILE:N	2:F:248:ILE:HD12	2.25	0.52
1:E:30:ALA:HB3	1:E:54:PHE:HB3	1.91	0.52
1:C:22:GLU:O	1:C:60:GLN:HG2	2.10	0.52
1:C:70:ASN:H	1:C:76:ASN:HD22	1.57	0.52
2:F:46:GLU:HB3	2:F:224:PRO:HG3	1.91	0.52
2:B:71:HIS:NE2	2:F:266:SER:OXT	2.43	0.52
1:A:59:ASP:HB2	1:A:63:ARG:HB2	1.92	0.51
1:A:87:VAL:HG12	1:A:118:PHE:CE1	2.45	0.51
2:D:172:ARG:HD3	2:D:174:TYR:CZ	2.46	0.51
2:B:89:PHE:CZ	2:B:93:LYS:HG2	2.45	0.51
2:H:69:PHE:HD2	2:H:77:LYS:HG2	1.76	0.51
1:A:28:ASP:OD2	1:A:116:ARG:HD2	2.11	0.51
2:B:30:SER:HB2	2:D:36:PHE:HE1	1.76	0.51
2:F:227:ALA:HB3	2:F:228:PRO:HD3	1.93	0.51
1:C:92:ARG:HA	1:C:114:MET:SD	2.51	0.50
2:F:155:ARG:HA	2:F:155:ARG:HH11	1.76	0.50
2:B:185:PHE:CB	2:B:196:ILE:HG12	2.41	0.50
1:A:113:ASP:O	1:A:117:ILE:HG12	2.12	0.50
1:G:16:LEU:CB	1:G:23:ILE:HD13	2.39	0.50
2:B:227:ALA:HB3	2:B:228:PRO:HD3	1.93	0.50
2:F:78:TRP:HE1	2:F:83:GLU:HB3	1.76	0.50
2:H:69:PHE:CD2	2:H:77:LYS:HG2	2.47	0.50
1:G:92:ARG:NH2	1:G:108:MET:O	2.45	0.49
2:B:266:SER:OXT	2:F:71:HIS:CE1	2.65	0.49
2:F:7:THR:H	2:F:10:GLN:HE21	1.60	0.49
1:G:66:TYR:O	1:G:78:TYR:HA	2.12	0.49
1:E:5:ASN:ND2	1:G:49:SER:HB3	2.24	0.49
2:D:227:ALA:HB3	2:D:228:PRO:HD3	1.94	0.49
1:A:48:THR:HG22	1:A:49:SER:H	1.77	0.48
2:F:116:GLY:O	2:F:118:LYS:N	2.40	0.48
2:B:102:ILE:HG12	2:B:125:PHE:CD2	2.48	0.48
1:C:2:GLU:HA	1:C:5:ASN:HD22	1.78	0.48
1:A:87:VAL:HG12	1:A:118:PHE:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ASP:HB2	2:D:142:ARG:CZ	2.44	0.48
2:F:80:LYS:HA	2:F:83:GLU:HG2	1.96	0.48
1:A:94:LEU:CD1	1:A:118:PHE:HD1	2.26	0.48
2:D:113:LEU:HD11	2:D:204:LEU:HD11	1.95	0.48
2:D:185:PHE:HB3	2:D:196:ILE:HD11	1.96	0.48
1:C:74:PRO:HG3	2:D:48:PHE:HB3	1.93	0.48
1:G:23:ILE:HG13	1:G:24:GLU:N	2.24	0.48
1:G:40:VAL:HG13	1:G:41:GLY:H	1.78	0.48
1:C:33:VAL:HG22	1:C:108:MET:HA	1.96	0.47
2:D:11:VAL:HG13	2:D:49:ILE:HD13	1.96	0.47
2:H:72:CYS:SG	2:H:77:LYS:HB2	2.53	0.47
2:F:215:MET:O	2:F:217:ASN:N	2.43	0.47
2:H:20:ILE:HG22	2:H:21:LEU:H	1.79	0.47
1:A:93:TYR:HB2	1:A:95:ILE:HD11	1.96	0.47
2:B:33:ARG:HG3	4:B:284:HOH:O	2.14	0.47
1:C:117:ILE:CA	1:C:120:ILE:HG22	2.42	0.47
2:D:162:ILE:HG23	2:D:175:ILE:HD11	1.97	0.47
2:D:102:ILE:HG12	2:D:125:PHE:CD2	2.49	0.47
2:D:143:GLU:O	2:D:147:GLU:HB2	2.14	0.47
2:F:62:ARG:NH2	4:F:271:HOH:O	2.47	0.47
2:B:217:ASN:HB3	2:B:219:PHE:CE1	2.50	0.47
2:D:163:ASP:HB3	2:D:172:ARG:HG3	1.97	0.47
2:D:33:ARG:O	2:D:37:GLN:HG2	2.14	0.46
2:B:192:GLU:H	2:B:192:GLU:HG3	1.27	0.46
2:D:147:GLU:HA	2:D:188:ARG:NH1	2.30	0.46
2:F:78:TRP:CE3	2:F:82:HIS:CE1	3.03	0.46
2:F:191:LYS:H	2:F:191:LYS:HG2	1.46	0.46
2:F:131:ASP:O	2:F:132:LYS:C	2.54	0.46
1:A:5:ASN:N	1:A:5:ASN:HD22	2.12	0.46
2:B:106:MET:HA	2:B:178:GLY:HA2	1.96	0.46
2:D:104:LEU:HB2	2:D:177:PRO:HA	1.97	0.46
2:D:99:ARG:NH2	2:D:170:ASN:HB3	2.31	0.46
1:G:119:ASN:O	1:G:123:GLU:HA	2.16	0.46
2:F:155:ARG:HA	2:F:155:ARG:NH1	2.31	0.45
2:D:7:THR:HG23	2:D:10:GLN:HE21	1.81	0.45
2:F:42:HIS:CE1	2:F:59:LEU:O	2.63	0.45
2:B:1:MET:N	4:B:280:HOH:O	2.48	0.45
2:H:11:VAL:HG13	2:H:49:ILE:HD13	1.99	0.45
2:B:62:ARG:HD2	2:B:87:ASP:OD2	2.16	0.45
2:B:236:ARG:NE	2:B:245:GLU:HB3	2.31	0.45
2:H:59:LEU:HD12	2:H:59:LEU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:ARG:HD3	2:F:33:ARG:H	1.82	0.45
2:B:46:GLU:HB3	2:B:224:PRO:HG3	1.97	0.45
1:C:76:ASN:HD21	2:D:18:ARG:NH1	2.15	0.45
2:F:245:GLU:HB2	2:F:246:LYS:H	1.51	0.45
2:H:225:PHE:O	2:H:229:LEU:HB2	2.17	0.44
2:D:28:GLN:OE1	2:D:28:GLN:HA	2.17	0.44
2:D:132:LYS:HD2	2:D:132:LYS:HA	1.75	0.44
2:F:38:ILE:CD1	2:F:69:PHE:HE1	2.31	0.44
2:F:159:ASN:HD21	2:H:159:ASN:HA	1.82	0.44
2:H:96:ILE:HA	2:H:97:PRO:HD3	1.86	0.44
2:F:102:ILE:HG23	2:F:125:PHE:CE2	2.53	0.44
1:E:98:THR:HG22	1:E:99:GLU:H	1.83	0.44
1:G:92:ARG:HA	1:G:114:MET:SD	2.57	0.44
1:A:98:THR:HG22	1:A:99:GLU:N	2.32	0.43
1:G:53:THR:O	1:G:68:ILE:HA	2.17	0.43
1:C:53:THR:O	1:C:68:ILE:HA	2.18	0.43
2:F:117:TRP:HD1	2:F:192:GLU:O	2.01	0.43
1:G:118:PHE:CZ	1:G:122:LYS:HG2	2.54	0.43
2:H:12:LEU:O	2:H:16:SER:HB2	2.18	0.43
2:B:39:GLU:OE2	2:B:95:ARG:HD3	2.18	0.43
2:D:137:VAL:HG13	2:D:156:ILE:HD12	2.00	0.43
2:F:30:SER:HB3	2:F:33:ARG:HB2	2.01	0.43
2:D:126:PRO:HB2	2:D:144:VAL:HG12	1.99	0.43
1:C:16:LEU:HD12	1:C:26:ILE:CD1	2.48	0.43
2:B:103:MET:CE	2:B:126:PRO:HG2	2.48	0.42
2:H:152:CYS:C	2:H:154:SER:H	2.23	0.42
2:B:20:ILE:HG13	2:B:21:LEU:N	2.34	0.42
2:B:67:LYS:CE	2:F:266:SER:O	2.60	0.42
2:B:93:LYS:HD2	2:B:95:ARG:HG2	2.01	0.42
2:B:107:SER:OG	2:B:109:GLN:CG	2.67	0.42
2:F:82:HIS:HA	2:H:43:TRP:CZ3	2.54	0.42
2:F:21:LEU:HD13	2:F:73:PRO:HD2	2.01	0.42
1:A:1:MET:O	1:A:4:GLU:HG2	2.20	0.42
1:A:118:PHE:CZ	1:A:122:LYS:HE3	2.54	0.42
2:B:225:PHE:C	2:B:228:PRO:HD2	2.39	0.42
1:C:94:LEU:HA	1:C:94:LEU:HD12	1.81	0.42
1:C:108:MET:HG2	1:C:108:MET:H	1.56	0.42
1:E:39:ASP:OD2	1:E:39:ASP:N	2.53	0.42
2:F:89:PHE:O	2:F:93:LYS:HB2	2.20	0.42
2:D:131:ASP:O	2:D:132:LYS:C	2.58	0.42
2:D:110:GLN:HA	2:D:199:HIS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:H3	2:F:77:LYS:HE3	1.85	0.41
2:F:95:ARG:NH1	2:F:165:THR:HG21	2.35	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.97	0.41
2:D:12:LEU:HD12	2:D:71:HIS:CD2	2.55	0.41
2:F:192:GLU:HG2	2:F:193:ILE:N	2.36	0.41
2:H:157:ASN:ND2	2:H:160:GLU:HG2	2.34	0.41
2:B:30:SER:HB2	2:D:36:PHE:CE1	2.55	0.41
1:E:76:ASN:OD1	2:F:18:ARG:NH2	2.54	0.41
1:G:16:LEU:CB	1:G:23:ILE:CD1	2.99	0.41
1:G:36:TYR:CZ	1:G:47:LYS:HD3	2.56	0.41
2:F:185:PHE:HB3	2:F:196:ILE:HG12	2.02	0.41
1:A:99:GLU:C	1:A:101:GLN:H	2.24	0.41
2:B:4:THR:HG22	2:B:52:GLN:HB2	2.01	0.41
2:D:20:ILE:O	2:D:22:ASN:N	2.49	0.41
1:A:113:ASP:OD2	1:A:116:ARG:NH2	2.50	0.41
2:B:95:ARG:NE	2:B:165:THR:HG21	2.36	0.41
1:E:87:VAL:HG12	1:E:118:PHE:CE1	2.56	0.41
2:F:165:THR:CG2	2:F:170:ASN:OD1	2.69	0.40
1:G:40:VAL:HG13	1:G:41:GLY:N	2.36	0.40
2:F:244:LYS:O	2:F:244:LYS:HD2	2.21	0.40
2:H:8:PHE:CD1	2:H:56:LEU:HD22	2.53	0.40
1:C:8:ARG:HG2	1:C:12:ASN:ND2	2.37	0.40
2:D:200:ASN:HB2	2:D:203:ASP:HB3	2.04	0.40
1:E:1:MET:H1	2:F:77:LYS:HE3	1.86	0.40
2:F:110:GLN:HG2	2:F:200:ASN:HD22	1.83	0.40
2:F:136:ASP:CG	2:H:164:MET:HA	2.42	0.40
1:G:16:LEU:HD12	1:G:26:ILE:HD11	2.03	0.40
2:H:52:GLN:O	2:H:53:ASN:CB	2.69	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	119/127 (94%)	114 (96%)	5 (4%)	0	100	100
1	C	121/127 (95%)	109 (90%)	10 (8%)	2 (2%)	9	29
1	E	119/127 (94%)	111 (93%)	8 (7%)	0	100	100
1	G	125/127 (98%)	108 (86%)	12 (10%)	5 (4%)	3	9
2	B	264/266 (99%)	243 (92%)	16 (6%)	5 (2%)	8	26
2	D	192/266 (72%)	160 (83%)	27 (14%)	5 (3%)	5	18
2	F	258/266 (97%)	237 (92%)	15 (6%)	6 (2%)	6	21
2	H	180/266 (68%)	143 (79%)	28 (16%)	9 (5%)	2	6
All	All	1378/1572 (88%)	1225 (89%)	121 (9%)	32 (2%)	6	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	LYS
2	B	245	GLU
2	D	106	MET
2	D	132	LYS
2	F	61	LEU
2	F	132	LYS
2	F	209	LYS
1	G	23	ILE
1	G	122	LYS
1	G	123	GLU
2	D	180	SER
2	H	7	THR
2	H	30	SER
2	H	53	ASN
2	H	133	ASP
2	H	153	SER
2	B	123	TRP
2	B	209	LYS
2	F	243	THR
1	G	42	SER
2	H	162	ILE
2	H	205	PRO
2	B	220	TYR
2	D	186	GLU
2	F	216	LYS
2	H	27	GLU
1	C	75	GLU

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Mol	Chain	Res	Type
2	D	205	PRO
2	F	242	THR
1	G	22	GLU
2	H	123	TRP
1	C	100	ASN

5.3.2 Protein sidechains ⓘ

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	116/119 (98%)	107 (92%)	9 (8%)	12	35
1	C	115/119 (97%)	107 (93%)	8 (7%)	15	40
1	E	116/119 (98%)	110 (95%)	6 (5%)	23	55
1	G	119/119 (100%)	109 (92%)	10 (8%)	11	31
2	B	242/242 (100%)	217 (90%)	25 (10%)	7	21
2	D	184/242 (76%)	167 (91%)	17 (9%)	9	27
2	F	238/242 (98%)	216 (91%)	22 (9%)	9	27
2	H	172/242 (71%)	157 (91%)	15 (9%)	10	30
All	All	1302/1444 (90%)	1190 (91%)	112 (9%)	10	30

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	38	PHE
1	A	39	ASP
1	A	60	GLN
1	A	92	ARG
1	A	107	TRP
1	A	108	MET
1	A	127	ARG
2	B	26	GLU

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Mol	Chain	Res	Type
2	B	29	SER
2	B	33	ARG
2	B	47	ASP
2	B	52	GLN
2	B	54	ASP
2	B	67	LYS
2	B	78	TRP
2	B	82	HIS
2	B	93	LYS
2	B	99	ARG
2	B	120	SER
2	B	131	ASP
2	B	155	ARG
2	B	166	ILE
2	B	180	SER
2	B	181	LEU
2	B	189	THR
2	B	192	GLU
2	B	196	ILE
2	B	210	ASN
2	B	229	LEU
2	B	236	ARG
2	B	257	SER
2	B	265	LYS
1	C	14	GLN
1	C	24	GLU
1	C	31	SER
1	C	40	VAL
1	C	64	VAL
1	C	92	ARG
1	C	101	GLN
1	C	108	MET
2	D	20	ILE
2	D	33	ARG
2	D	71	HIS
2	D	88	ASP
2	D	96	ILE
2	D	99	ARG
2	D	112	VAL
2	D	127	LYS
2	D	131	ASP
2	D	136	ASP

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Mol	Chain	Res	Type
2	D	147	GLU
2	D	156	ILE
2	D	163	ASP
2	D	170	ASN
2	D	176	ILE
2	D	181	LEU
2	D	183	THR
1	E	1	MET
1	E	7	LEU
1	E	107	TRP
1	E	108	MET
1	E	126	LEU
1	E	127	ARG
2	F	18	ARG
2	F	33	ARG
2	F	47	ASP
2	F	67	LYS
2	F	78	TRP
2	F	80	LYS
2	F	99	ARG
2	F	120	SER
2	F	131	ASP
2	F	155	ARG
2	F	166	ILE
2	F	184	ARG
2	F	188	ARG
2	F	189	THR
2	F	196	ILE
2	F	208	LYS
2	F	216	LYS
2	F	218	LYS
2	F	244	LYS
2	F	245	GLU
2	F	255	ASP
2	F	259	GLN
1	G	14	GLN
1	G	48	THR
1	G	64	VAL
1	G	78	TYR
1	G	98	THR
1	G	104	VAL
1	G	108	MET

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Mol	Chain	Res	Type
1	G	123	GLU
1	G	124	SER
1	G	125	LEU
2	H	1	MET
2	H	2	SER
2	H	20	ILE
2	H	50	ARG
2	H	80	LYS
2	H	91	ARG
2	H	93	LYS
2	H	95	ARG
2	H	96	ILE
2	H	99	ARG
2	H	138	ASP
2	H	156	ILE
2	H	167	ARG
2	H	170	ASN
2	H	222	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	82	ASN
1	A	100	ASN
2	B	5	ASN
2	B	10	GLN
2	B	22	ASN
2	B	40	GLN
2	B	42	HIS
2	B	82	HIS
2	B	217	ASN
2	B	247	ASN
1	C	5	ASN
1	C	14	GLN
1	C	43	GLN
1	C	76	ASN
1	C	86	ASN
2	D	10	GLN
2	D	37	GLN
2	D	42	HIS
2	D	55	GLN

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Mol	Chain	Res	Type
2	D	71	HIS
1	E	9	ASN
1	E	12	ASN
2	F	5	ASN
2	F	10	GLN
2	F	22	ASN
2	F	28	GLN
2	F	42	HIS
2	F	53	ASN
2	F	200	ASN
2	F	210	ASN
2	F	241	ASN
1	G	60	GLN
1	G	82	ASN
2	H	37	GLN
2	H	82	HIS
2	H	110	GLN
2	H	170	ASN
2	H	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	ATP	F	267	-	26,33,33	0.88	1 (3%)	31,52,52	1.57	5 (16%)
3	ATP	B	267	-	26,33,33	0.98	1 (3%)	31,52,52	1.54	7 (22%)

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
3	ATP	F	267	-	-	8/18/38/38	0/3/3/3
3	ATP	B	267	-	-	8/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	267	ATP	C5-C4	2.68	1.48	1.40
3	F	267	ATP	C5-C4	2.33	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	267	ATP	PA-O3A-PB	-4.28	118.14	132.83
3	F	267	ATP	N3-C2-N1	-3.74	122.84	128.68
3	B	267	ATP	PB-O3B-PG	-3.64	120.34	132.83
3	B	267	ATP	N3-C2-N1	-3.51	123.20	128.68
3	F	267	ATP	PB-O3B-PG	-3.21	121.83	132.83
3	B	267	ATP	PA-O3A-PB	-2.81	123.18	132.83
3	B	267	ATP	C3'-C2'-C1'	2.65	104.97	100.98
3	F	267	ATP	C4-C5-N7	-2.59	106.70	109.40
3	B	267	ATP	C4-C5-N7	-2.40	106.89	109.40
3	F	267	ATP	C2-N1-C6	2.16	122.45	118.75
3	B	267	ATP	C2'-C3'-C4'	2.07	106.66	102.64
3	B	267	ATP	C2-N1-C6	2.06	122.28	118.75

There are no chirality outliers.

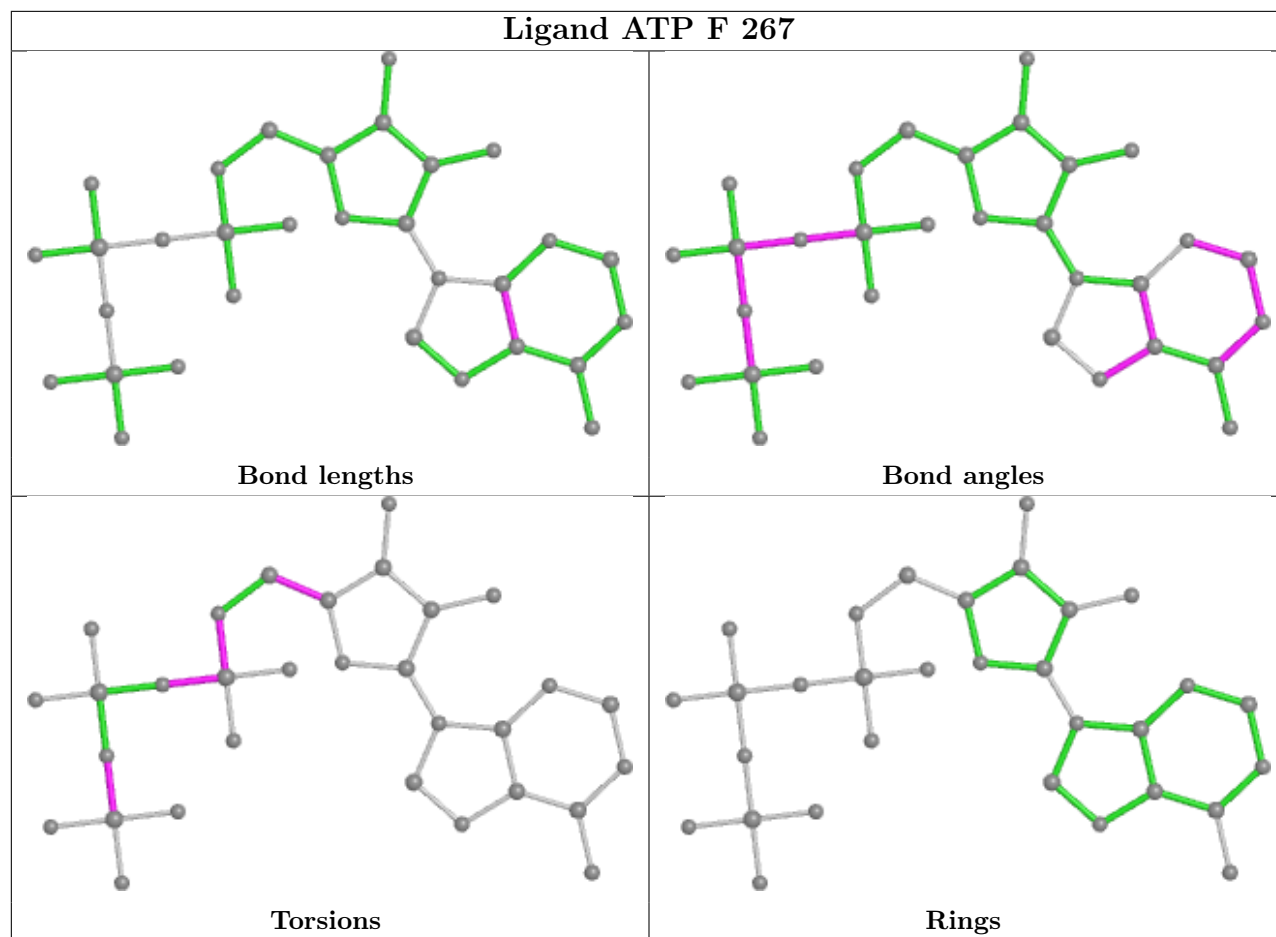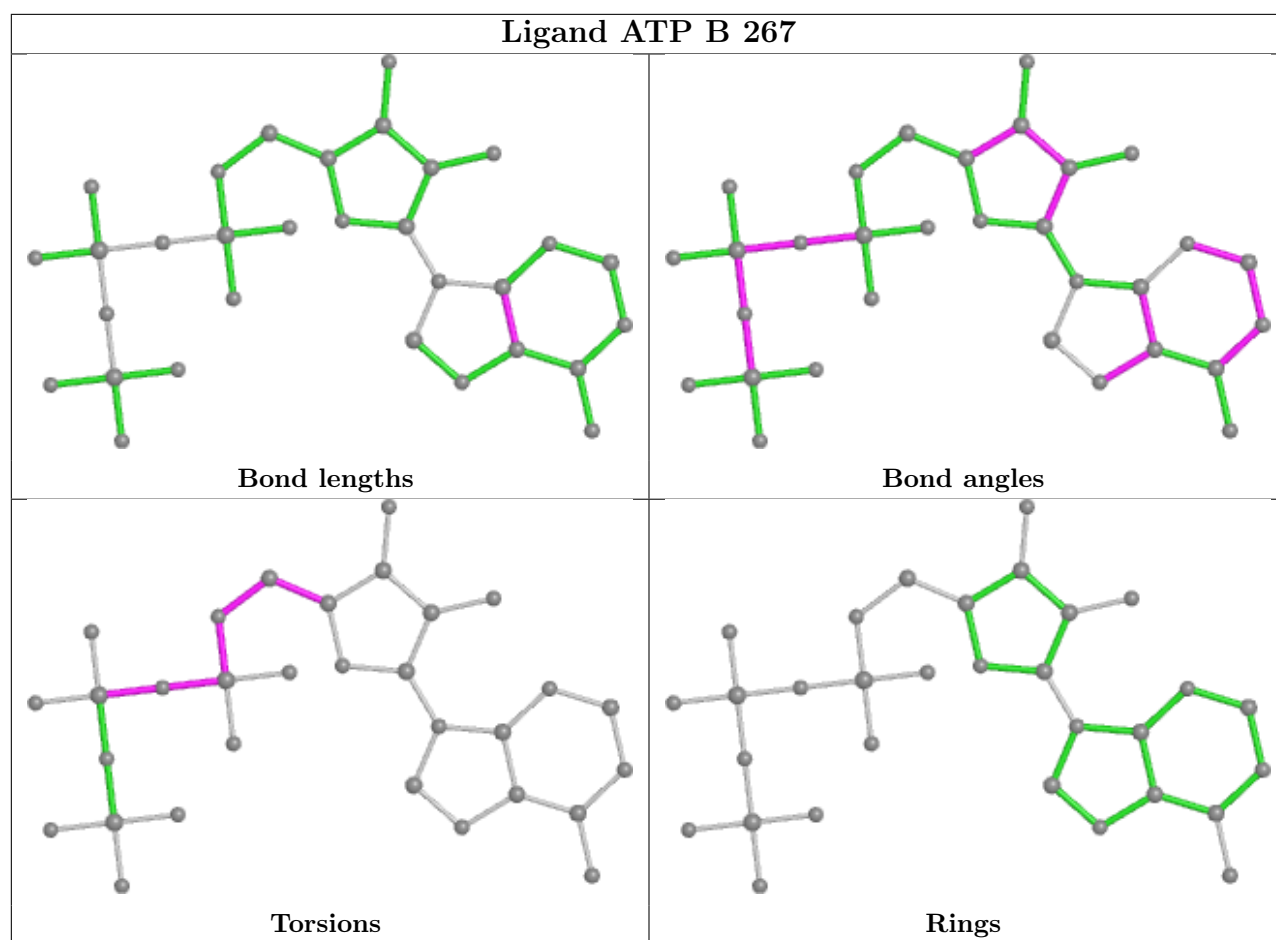All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	267	ATP	C5'-O5'-PA-O1A
3	F	267	ATP	C5'-O5'-PA-O2A
3	F	267	ATP	C5'-O5'-PA-O3A
3	F	267	ATP	C3'-C4'-C5'-O5'
3	B	267	ATP	O4'-C4'-C5'-O5'
3	F	267	ATP	O4'-C4'-C5'-O5'
3	B	267	ATP	C3'-C4'-C5'-O5'
3	B	267	ATP	PA-O3A-PB-O2B
3	F	267	ATP	PB-O3A-PA-O1A
3	B	267	ATP	C4'-C5'-O5'-PA
3	F	267	ATP	C5'-O5'-PA-O1A
3	F	267	ATP	PB-O3A-PA-O2A
3	B	267	ATP	PB-O3A-PA-O1A
3	B	267	ATP	PB-O3A-PA-O2A
3	F	267	ATP	PB-O3B-PG-O2G
3	B	267	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 F 267

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 267

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	123/127 (96%)	0.24	2 (1%)	72	66	38, 48, 73, 94	0
1	C	123/127 (96%)	0.24	0	100	100	43, 55, 75, 101	0
1	E	123/127 (96%)	0.20	2 (1%)	72	66	38, 48, 73, 95	0
1	G	127/127 (100%)	0.32	5 (3%)	39	29	42, 56, 85, 101	0
2	B	266/266 (100%)	0.28	1 (0%)	92	91	28, 41, 62, 76	0
2	D	202/266 (75%)	0.74	21 (10%)	6	3	48, 79, 107, 114	0
2	F	262/266 (98%)	0.21	1 (0%)	92	91	29, 41, 60, 76	0
2	H	190/266 (71%)	0.58	15 (7%)	12	7	54, 83, 108, 114	0
All	All	1416/1572 (90%)	0.36	47 (3%)	46	36	28, 52, 91, 114	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	186	GLU	6.3
2	H	111	CYS	5.5
2	D	188	ARG	5.1
2	D	123	TRP	4.8
2	D	185	PHE	4.6
1	G	126	LEU	4.5
2	D	86	PHE	4.4
2	D	184	ARG	4.0
1	E	1	MET	3.9
2	D	78	TRP	3.9
2	F	217	ASN	3.3
2	H	90	LEU	3.2
2	D	181	LEU	3.2
2	D	100	GLY	3.2
1	A	127	ARG	3.1
2	H	68	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	76	TRP	3.0
2	H	221	MET	3.0
2	D	90	LEU	2.9
2	H	137	VAL	2.9
2	D	145	TYR	2.9
2	H	78	TRP	2.8
2	D	111	CYS	2.7
2	D	166	ILE	2.6
1	G	127	ARG	2.6
2	H	196	ILE	2.5
2	B	215	MET	2.5
1	A	1	MET	2.5
1	E	127	ARG	2.5
2	H	156	ILE	2.5
2	H	89	PHE	2.4
2	D	220	TYR	2.4
2	H	86	PHE	2.4
2	H	231	LYS	2.4
2	D	231	LYS	2.3
1	G	23	ILE	2.3
2	D	65	SER	2.3
2	H	235	LYS	2.3
2	H	152	CYS	2.3
2	D	156	ILE	2.2
1	G	124	SER	2.2
2	H	61	LEU	2.1
2	H	199	HIS	2.1
1	G	1	MET	2.1
2	D	112	VAL	2.1
2	D	162	ILE	2.0
2	D	61	LEU	2.0

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

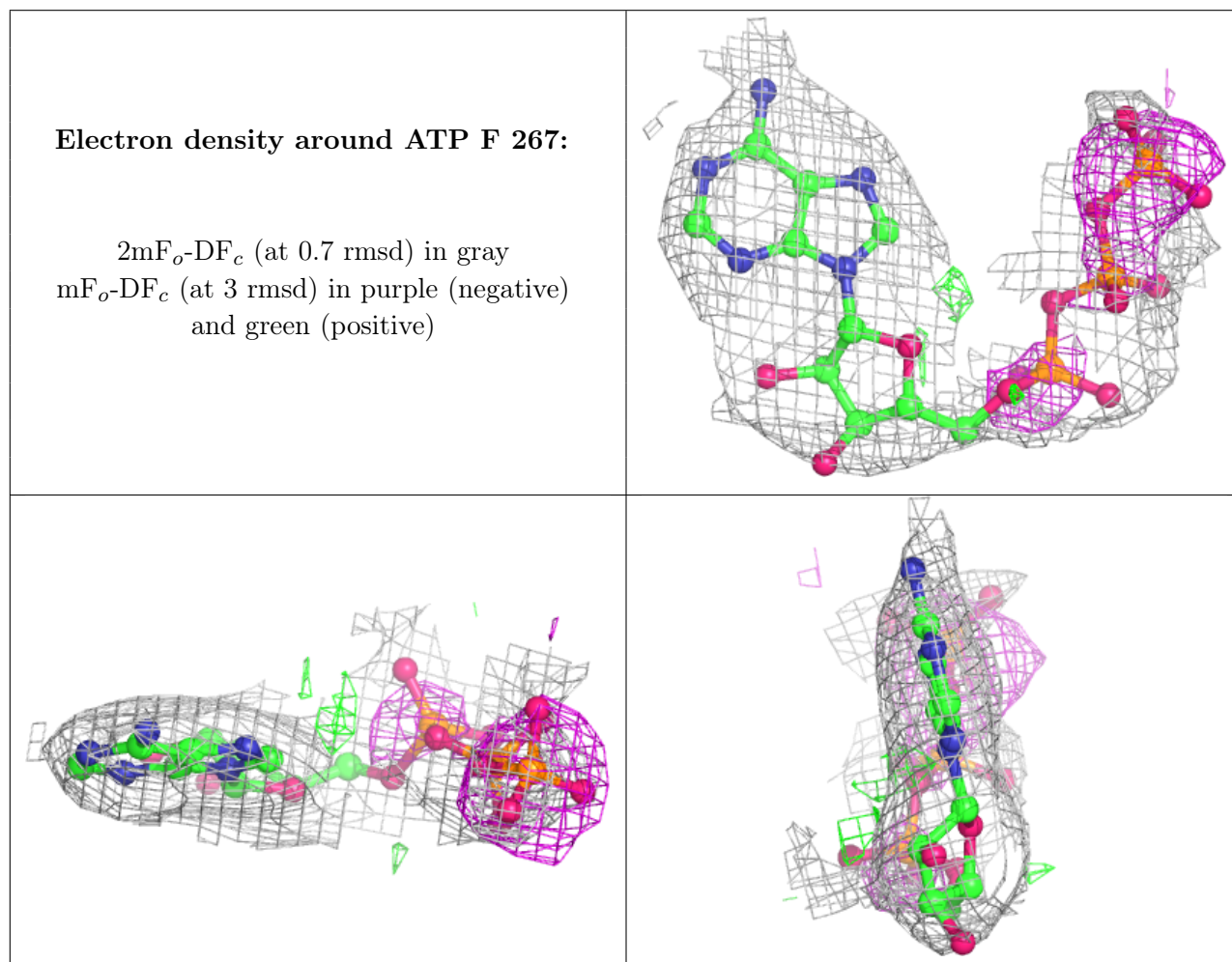There are no non-standard protein/DNA/RNA residues in this entry.

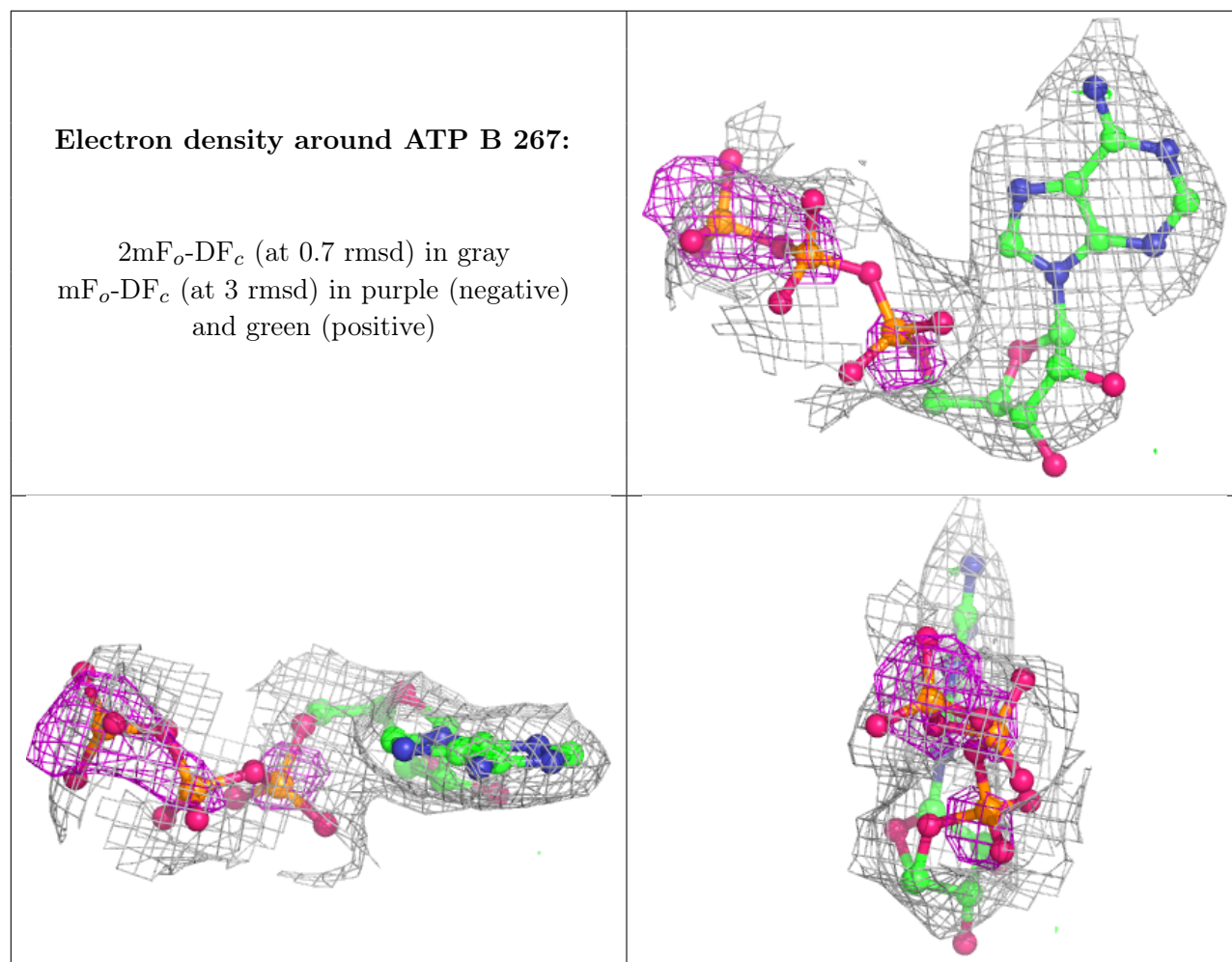## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	ATP	F	267	31/31	0.75	0.25	93,100,122,123	0
3	ATP	B	267	31/31	0.79	0.24	102,107,121,121	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 F 267:

$2mF_o$-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 B 267:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.