



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:26 AM UTC

PDB ID : 4N1A / pdb_00004n1a
Title : Thermomonospora curvata EccC (ATPases 2 and 3) in complex with a signal sequence peptide
Authors : Dovala, D.L.; Bendebury, A.; Cox, J.S.; Stroud, R.M.; Rosenberg, O.S.
Deposited on : 2013-10-03
Resolution : 3.24 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

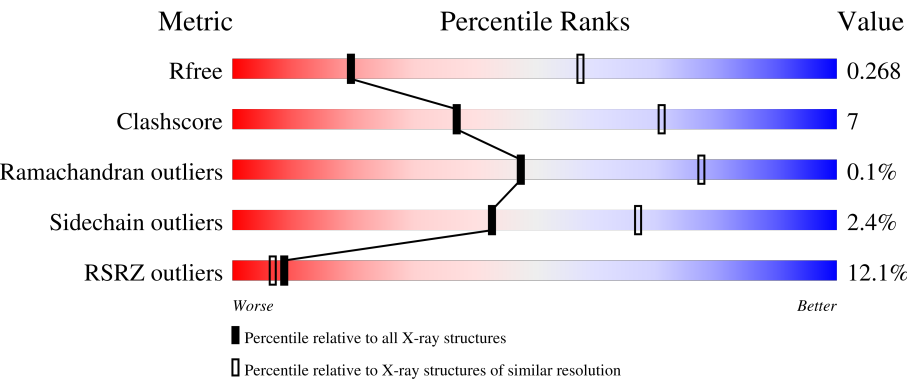
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.24 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}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	589	79% 14% 6%
1	B	589	77% 16% 6%
1	C	589	7% 78% 15% 6%
1	E	589	36% 77% 16% 6%
2	G	23	17% 13% 70%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	23	
2	J	23	
2	K	23	

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
4	MG	E	1401	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17460 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4298	2712	762	814	10			
1	B	553	Total	C	N	O	S	0	0	0
			4229	2671	738	810	10			
1	C	554	Total	C	N	O	S	0	0	0
			4247	2682	744	811	10			
1	E	555	Total	C	N	O	S	0	0	0
			4292	2709	759	814	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	727	MET	-	expression tag	UNP D1A4G7
A	728	HIS	-	expression tag	UNP D1A4G7
A	729	HIS	-	expression tag	UNP D1A4G7
A	730	HIS	-	expression tag	UNP D1A4G7
A	731	HIS	-	expression tag	UNP D1A4G7
A	732	HIS	-	expression tag	UNP D1A4G7
A	733	HIS	-	expression tag	UNP D1A4G7
A	734	HIS	-	expression tag	UNP D1A4G7
A	735	HIS	-	expression tag	UNP D1A4G7
A	736	GLY	-	expression tag	UNP D1A4G7
A	737	GLY	-	expression tag	UNP D1A4G7
A	738	SER	-	expression tag	UNP D1A4G7
A	739	GLU	-	expression tag	UNP D1A4G7
A	740	PHE	-	expression tag	UNP D1A4G7
A	741	SER	-	expression tag	UNP D1A4G7
A	742	ILE	-	expression tag	UNP D1A4G7
A	743	ASP	-	expression tag	UNP D1A4G7
A	744	GLY	-	expression tag	UNP D1A4G7
A	745	GLY	-	expression tag	UNP D1A4G7
A	746	SER	-	expression tag	UNP D1A4G7
A	747	LEU	-	expression tag	UNP D1A4G7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	748	GLU	-	expression tag	UNP D1A4G7
A	749	VAL	-	expression tag	UNP D1A4G7
A	750	LEU	-	expression tag	UNP D1A4G7
A	751	PHE	-	expression tag	UNP D1A4G7
A	752	GLN	-	expression tag	UNP D1A4G7
A	753	GLY	-	expression tag	UNP D1A4G7
A	754	PRO	-	expression tag	UNP D1A4G7
A	755	SER	-	expression tag	UNP D1A4G7
A	756	SER	-	expression tag	UNP D1A4G7
A	757	PRO	-	expression tag	UNP D1A4G7
A	758	SER	-	expression tag	UNP D1A4G7
B	727	MET	-	expression tag	UNP D1A4G7
B	728	HIS	-	expression tag	UNP D1A4G7
B	729	HIS	-	expression tag	UNP D1A4G7
B	730	HIS	-	expression tag	UNP D1A4G7
B	731	HIS	-	expression tag	UNP D1A4G7
B	732	HIS	-	expression tag	UNP D1A4G7
B	733	HIS	-	expression tag	UNP D1A4G7
B	734	HIS	-	expression tag	UNP D1A4G7
B	735	HIS	-	expression tag	UNP D1A4G7
B	736	GLY	-	expression tag	UNP D1A4G7
B	737	GLY	-	expression tag	UNP D1A4G7
B	738	SER	-	expression tag	UNP D1A4G7
B	739	GLU	-	expression tag	UNP D1A4G7
B	740	PHE	-	expression tag	UNP D1A4G7
B	741	SER	-	expression tag	UNP D1A4G7
B	742	ILE	-	expression tag	UNP D1A4G7
B	743	ASP	-	expression tag	UNP D1A4G7
B	744	GLY	-	expression tag	UNP D1A4G7
B	745	GLY	-	expression tag	UNP D1A4G7
B	746	SER	-	expression tag	UNP D1A4G7
B	747	LEU	-	expression tag	UNP D1A4G7
B	748	GLU	-	expression tag	UNP D1A4G7
B	749	VAL	-	expression tag	UNP D1A4G7
B	750	LEU	-	expression tag	UNP D1A4G7
B	751	PHE	-	expression tag	UNP D1A4G7
B	752	GLN	-	expression tag	UNP D1A4G7
B	753	GLY	-	expression tag	UNP D1A4G7
B	754	PRO	-	expression tag	UNP D1A4G7
B	755	SER	-	expression tag	UNP D1A4G7
B	756	SER	-	expression tag	UNP D1A4G7
B	757	PRO	-	expression tag	UNP D1A4G7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	758	SER	-	expression tag	UNP D1A4G7
C	727	MET	-	expression tag	UNP D1A4G7
C	728	HIS	-	expression tag	UNP D1A4G7
C	729	HIS	-	expression tag	UNP D1A4G7
C	730	HIS	-	expression tag	UNP D1A4G7
C	731	HIS	-	expression tag	UNP D1A4G7
C	732	HIS	-	expression tag	UNP D1A4G7
C	733	HIS	-	expression tag	UNP D1A4G7
C	734	HIS	-	expression tag	UNP D1A4G7
C	735	HIS	-	expression tag	UNP D1A4G7
C	736	GLY	-	expression tag	UNP D1A4G7
C	737	GLY	-	expression tag	UNP D1A4G7
C	738	SER	-	expression tag	UNP D1A4G7
C	739	GLU	-	expression tag	UNP D1A4G7
C	740	PHE	-	expression tag	UNP D1A4G7
C	741	SER	-	expression tag	UNP D1A4G7
C	742	ILE	-	expression tag	UNP D1A4G7
C	743	ASP	-	expression tag	UNP D1A4G7
C	744	GLY	-	expression tag	UNP D1A4G7
C	745	GLY	-	expression tag	UNP D1A4G7
C	746	SER	-	expression tag	UNP D1A4G7
C	747	LEU	-	expression tag	UNP D1A4G7
C	748	GLU	-	expression tag	UNP D1A4G7
C	749	VAL	-	expression tag	UNP D1A4G7
C	750	LEU	-	expression tag	UNP D1A4G7
C	751	PHE	-	expression tag	UNP D1A4G7
C	752	GLN	-	expression tag	UNP D1A4G7
C	753	GLY	-	expression tag	UNP D1A4G7
C	754	PRO	-	expression tag	UNP D1A4G7
C	755	SER	-	expression tag	UNP D1A4G7
C	756	SER	-	expression tag	UNP D1A4G7
C	757	PRO	-	expression tag	UNP D1A4G7
C	758	SER	-	expression tag	UNP D1A4G7
E	727	MET	-	expression tag	UNP D1A4G7
E	728	HIS	-	expression tag	UNP D1A4G7
E	729	HIS	-	expression tag	UNP D1A4G7
E	730	HIS	-	expression tag	UNP D1A4G7
E	731	HIS	-	expression tag	UNP D1A4G7
E	732	HIS	-	expression tag	UNP D1A4G7
E	733	HIS	-	expression tag	UNP D1A4G7
E	734	HIS	-	expression tag	UNP D1A4G7
E	735	HIS	-	expression tag	UNP D1A4G7

Continued on next page...

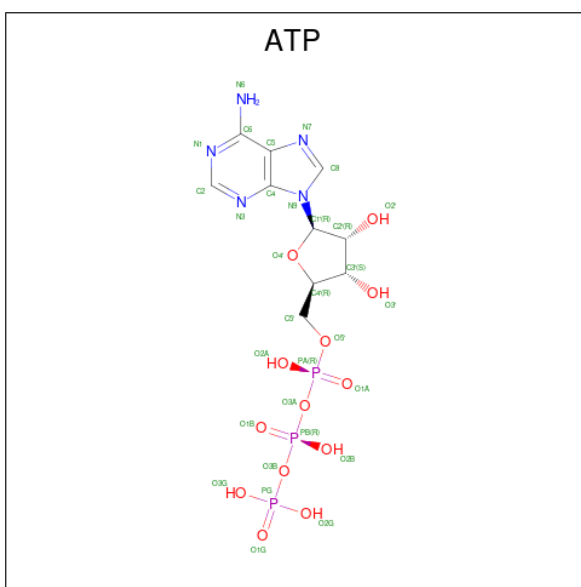
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	736	GLY	-	expression tag	UNP D1A4G7
E	737	GLY	-	expression tag	UNP D1A4G7
E	738	SER	-	expression tag	UNP D1A4G7
E	739	GLU	-	expression tag	UNP D1A4G7
E	740	PHE	-	expression tag	UNP D1A4G7
E	741	SER	-	expression tag	UNP D1A4G7
E	742	ILE	-	expression tag	UNP D1A4G7
E	743	ASP	-	expression tag	UNP D1A4G7
E	744	GLY	-	expression tag	UNP D1A4G7
E	745	GLY	-	expression tag	UNP D1A4G7
E	746	SER	-	expression tag	UNP D1A4G7
E	747	LEU	-	expression tag	UNP D1A4G7
E	748	GLU	-	expression tag	UNP D1A4G7
E	749	VAL	-	expression tag	UNP D1A4G7
E	750	LEU	-	expression tag	UNP D1A4G7
E	751	PHE	-	expression tag	UNP D1A4G7
E	752	GLN	-	expression tag	UNP D1A4G7
E	753	GLY	-	expression tag	UNP D1A4G7
E	754	PRO	-	expression tag	UNP D1A4G7
E	755	SER	-	expression tag	UNP D1A4G7
E	756	SER	-	expression tag	UNP D1A4G7
E	757	PRO	-	expression tag	UNP D1A4G7
E	758	SER	-	expression tag	UNP D1A4G7

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			56	35	12	9			
2	H	6	Total	C	N	O	0	0	0
			48	31	10	7			
2	J	7	Total	C	N	O	0	0	0
			50	32	9	9			
2	K	6	Total	C	N	O	0	0	0
			45	29	8	8			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		

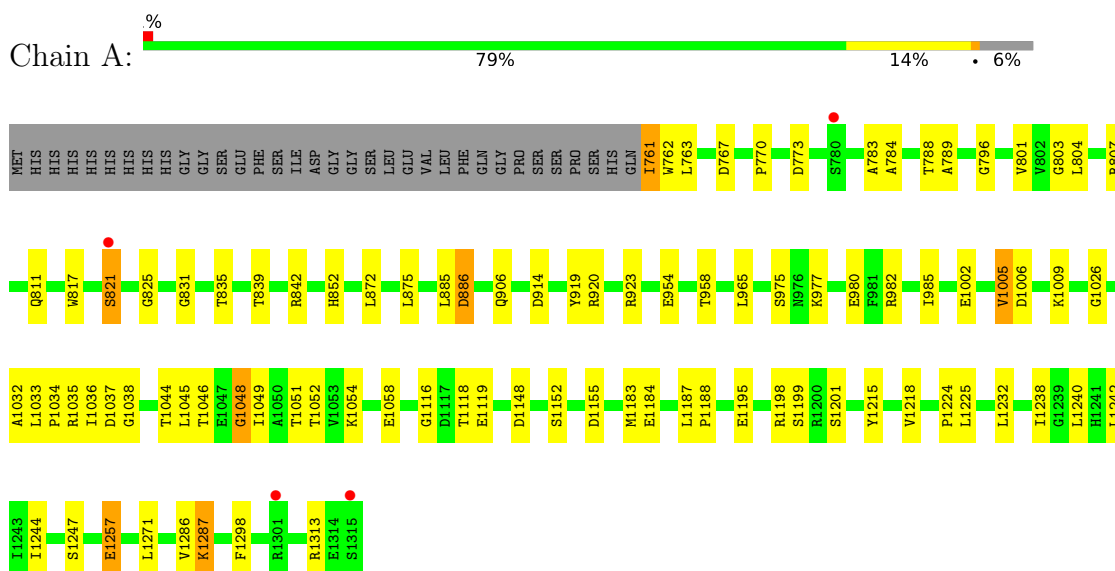
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

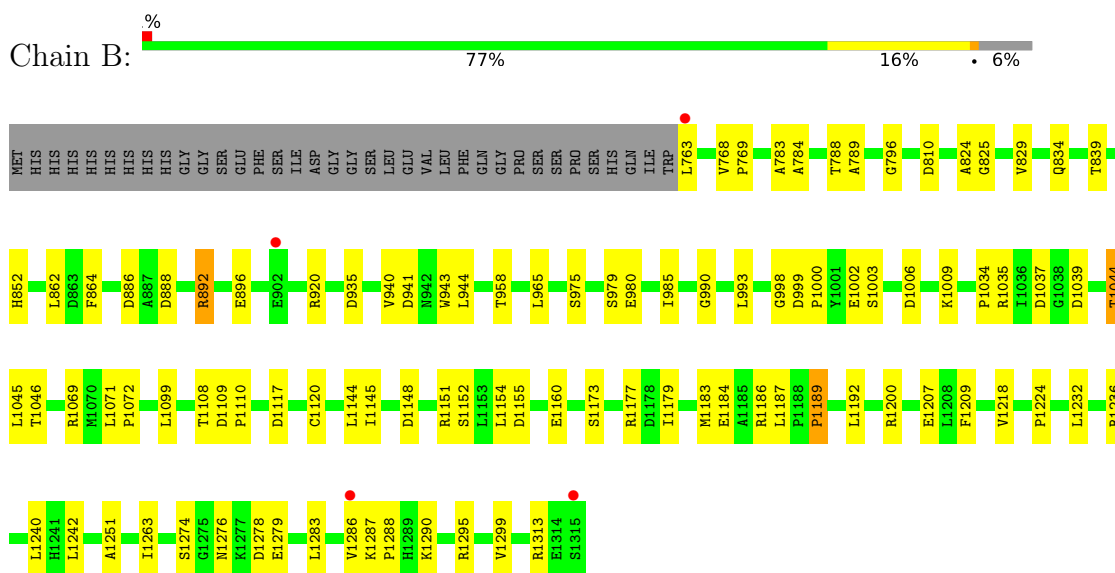
3 Residue-property plots

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.

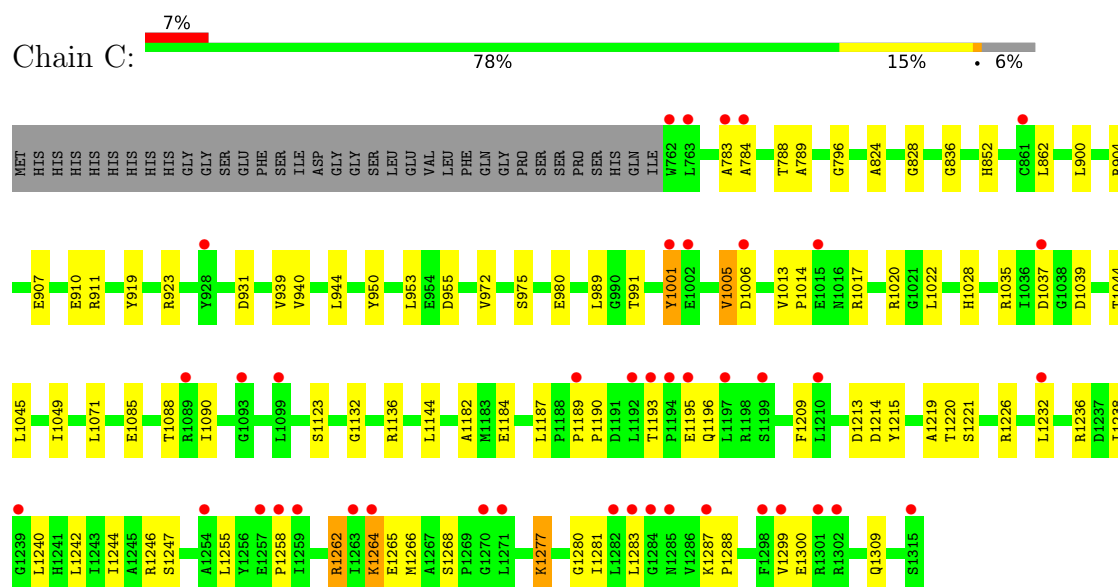
• Molecule 1: Cell divisionFtsK/SpoIIIE



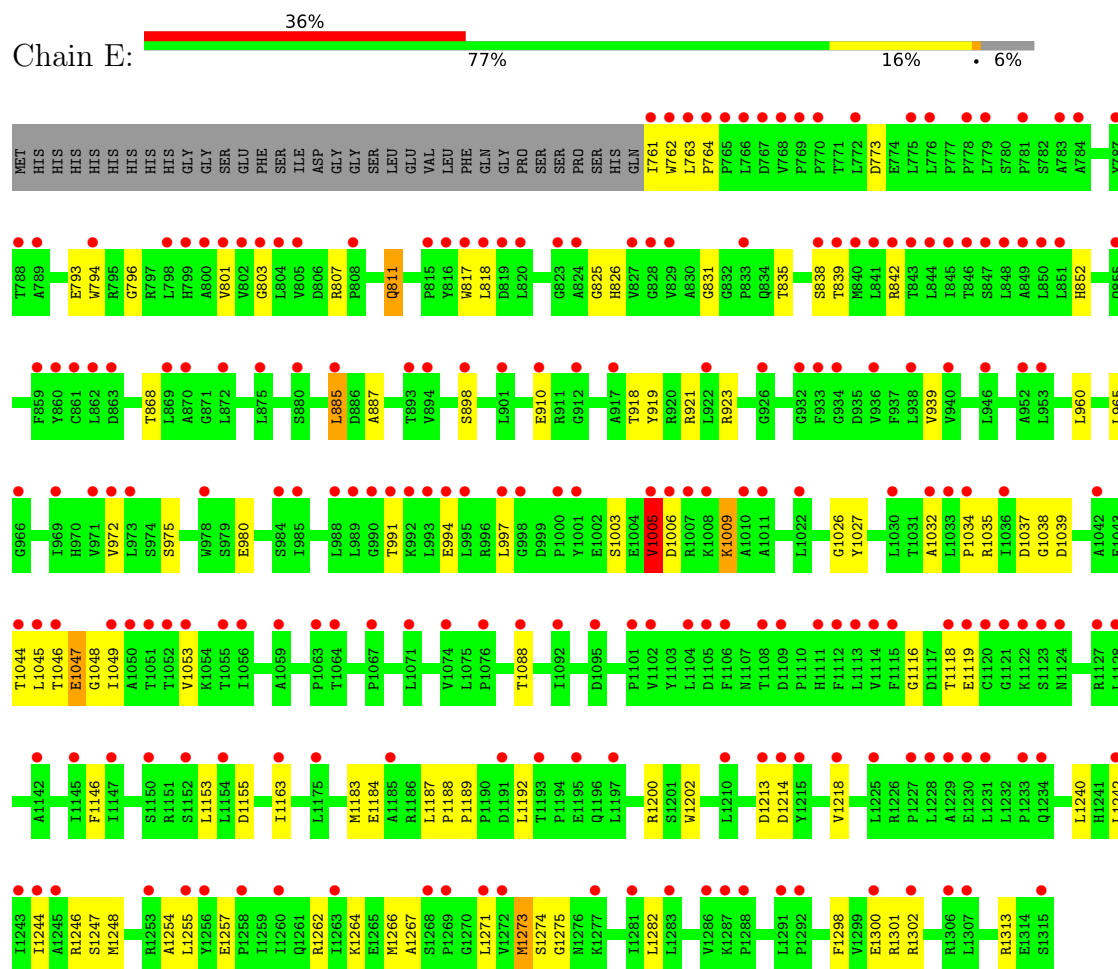
• Molecule 1: Cell divisionFtsK/SpoIIIE



• Molecule 1: Cell divisionFtsK/SpoIIIE

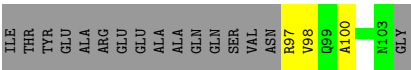


- Molecule 1: Cell divisionFtsK/SpoIIIE

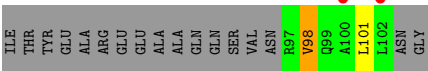


- Molecule 2: Uncharacterized protein

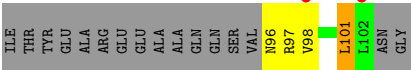




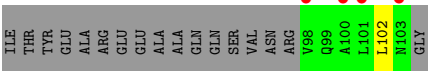
● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



● Molecule 2: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	216.15Å 216.15Å 186.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 3.24 49.15 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.15-3.24) 99.9 (49.15-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.266 0.229 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17460	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/4395	0.75	6/5984 (0.1%)
1	B	0.35	2/4324 (0.0%)	0.77	7/5895 (0.1%)
1	C	0.28	0/4344	0.75	3/5924 (0.1%)
1	E	0.40	1/4389 (0.0%)	0.81	8/5977 (0.1%)
2	G	0.25	0/55	0.67	0/73
2	H	0.23	0/47	0.90	0/62
2	J	0.29	0/49	0.69	0/66
2	K	0.27	0/44	0.65	0/59
All	All	0.35	3/17647 (0.0%)	0.77	24/24040 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	768	VAL	C-N	5.57	1.40	1.33
1	E	1273	MET	C-O	-5.52	1.17	1.24
1	B	769	PRO	C-O	-5.25	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	885	LEU	N-CA-C	7.29	119.23	111.28
1	E	1273	MET	N-CA-C	7.22	121.22	109.59
1	A	1048	GLY	N-CA-C	-6.80	104.06	112.77
1	B	768	VAL	CA-C-N	-6.59	113.60	120.38
1	B	768	VAL	C-N-CA	-6.59	113.60	120.38
1	C	1265	GLU	N-CA-C	-6.27	104.89	112.54
1	B	1232	LEU	CA-C-N	-6.12	113.50	119.87
1	B	1232	LEU	C-N-CA	-6.12	113.50	119.87
1	B	998	GLY	N-CA-C	-6.08	102.09	111.64
1	A	885	LEU	N-CA-C	5.75	117.63	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1257	GLU	CA-C-N	5.71	126.97	119.84
1	A	1257	GLU	C-N-CA	5.71	126.97	119.84
1	E	764	PRO	O-C-N	5.71	123.83	121.15
1	E	1188	PRO	CA-C-N	5.58	123.68	119.66
1	E	1188	PRO	C-N-CA	5.58	123.68	119.66
1	C	1013	VAL	CA-C-N	5.53	125.54	119.90
1	C	1013	VAL	C-N-CA	5.53	125.54	119.90
1	E	1254	ALA	N-CA-C	-5.39	106.38	113.17
1	E	1257	GLU	CA-C-N	5.34	126.52	119.84
1	E	1257	GLU	C-N-CA	5.34	126.52	119.84
1	A	1287	LYS	CA-C-N	5.12	125.12	119.90
1	A	1287	LYS	C-N-CA	5.12	125.12	119.90
1	B	1189	PRO	CA-C-N	5.04	126.14	119.84
1	B	1189	PRO	C-N-CA	5.04	126.14	119.84

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	4298	0	4268	51	0
1	B	4229	0	4164	58	0
1	C	4247	0	4175	61	0
1	E	4292	0	4257	75	0
2	G	56	0	62	2	0
2	H	48	0	56	2	0
2	J	50	0	51	3	0
2	K	45	0	49	1	0
3	A	62	0	24	1	0
3	B	62	0	24	3	0
3	C	62	0	24	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
All	All	17460	0	17154	244	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 7.

All (244) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1035:ARG:NH2	1:E:1037:ASP:OD2	1.80	1.13
1:E:1044:THR:HA	1:E:1047:GLU:OE2	1.56	0.98
1:C:1264:LYS:NZ	1:C:1268:SER:O	2.01	0.93
1:E:763:LEU:HD21	1:E:811:GLN:HA	1.57	0.86
1:E:1044:THR:CA	1:E:1047:GLU:OE2	2.24	0.85
1:E:1035:ARG:NH2	1:E:1039:ASP:HB3	1.94	0.82
1:C:1001:TYR:HD1	1:C:1001:TYR:H	1.29	0.81
1:B:1035:ARG:NH1	1:B:1039:ASP:HB3	1.94	0.81
1:E:1006:ASP:HB3	1:E:1009:LYS:HG3	1.61	0.81
1:E:1300:GLU:OE2	1:E:1302:ARG:NE	2.14	0.80
1:E:997:LEU:HD12	1:E:1003:SER:HB2	1.63	0.79
1:C:1226:ARG:HG3	1:C:1226:ARG:HH11	1.48	0.78
1:B:975:SER:OG	1:B:980:GLU:OE2	2.01	0.77
1:E:1035:ARG:NH2	1:E:1037:ASP:CG	2.43	0.75
1:E:1184:GLU:HA	1:E:1187:LEU:HD23	1.68	0.75
2:G:97:ARG:NH1	2:G:100:ALA:HB2	2.03	0.74
1:A:1035:ARG:NH1	1:A:1044:THR:O	2.21	0.73
1:E:1009:LYS:NZ	1:E:1026:GLY:O	2.22	0.73
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.22	0.72
1:E:761:ILE:HG23	1:E:762:TRP:H	1.55	0.72
1:E:1271:LEU:HD11	1:E:1273:MET:HE3	1.70	0.71
1:E:994:GLU:OE2	1:E:1003:SER:OG	2.07	0.69
1:E:1035:ARG:NH2	1:E:1039:ASP:CB	2.55	0.68
1:E:1242:LEU:HD23	1:E:1244:ILE:HD11	1.76	0.67
1:C:1035:ARG:HH11	1:C:1037:ASP:HB3	1.59	0.67
1:E:1035:ARG:CZ	1:E:1039:ASP:HB3	2.25	0.66
1:E:825:GLY:HA3	1:E:965:LEU:HD11	1.78	0.66
1:A:1184:GLU:HA	1:A:1187:LEU:HD23	1.78	0.65
1:C:1277:LYS:HZ2	1:C:1280:GLY:H	1.42	0.65
1:E:1035:ARG:HH21	1:E:1037:ASP:CG	2.03	0.65
1:E:839:THR:HG22	1:E:842:ARG:HH21	1.61	0.64
1:A:839:THR:HG22	1:A:842:ARG:HH21	1.60	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1183:MET:HE2	1:B:1240:LEU:HB2	1.79	0.64
1:C:950:TYR:HB3	1:C:953:LEU:HD13	1.79	0.64
1:E:1035:ARG:CZ	1:E:1037:ASP:OD2	2.46	0.63
1:A:1009:LYS:NZ	1:A:1026:GLY:O	2.29	0.63
2:G:97:ARG:HH11	2:G:100:ALA:HB2	1.62	0.63
1:E:975:SER:OG	1:E:980:GLU:OE1	2.17	0.62
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.32	0.62
1:A:977:LYS:HB3	1:A:1002:GLU:OE2	1.99	0.61
1:A:1242:LEU:HD23	1:A:1244:ILE:HD11	1.81	0.61
1:C:1232:LEU:HD11	1:C:1262:ARG:HB2	1.83	0.61
1:E:1006:ASP:CB	1:E:1009:LYS:HG3	2.30	0.61
1:E:997:LEU:CD1	1:E:1003:SER:HB2	2.30	0.61
1:A:1183:MET:HE2	1:A:1240:LEU:HB2	1.82	0.60
1:B:1184:GLU:HA	1:B:1187:LEU:HD23	1.84	0.60
1:A:1006:ASP:OD2	1:A:1009:LYS:HG3	2.02	0.60
1:A:825:GLY:HA3	1:A:965:LEU:HD11	1.82	0.59
1:C:1035:ARG:NH1	1:C:1039:ASP:HB3	2.17	0.59
1:C:1226:ARG:NH1	1:C:1258:PRO:HG2	2.18	0.59
1:B:824:ALA:HA	1:B:990:GLY:HA3	1.83	0.58
1:C:1277:LYS:HZ3	1:C:1280:GLY:HA2	1.69	0.58
1:C:910:GLU:HB2	1:E:1266:MET:HG2	1.84	0.58
1:B:1034:PRO:HD2	1:B:1045:LEU:HD11	1.85	0.58
1:B:1108:THR:O	1:B:1236:ARG:NH1	2.35	0.58
1:E:919:TYR:CZ	1:E:923:ARG:HD2	2.39	0.58
1:A:831:GLY:HA3	1:A:835:THR:HG21	1.85	0.57
1:E:1035:ARG:HH21	1:E:1039:ASP:CB	2.17	0.57
1:E:1044:THR:CB	1:E:1047:GLU:OE2	2.52	0.57
1:A:1036:ILE:HG12	1:A:1052:THR:HG23	1.85	0.57
1:A:761:ILE:HG23	1:A:762:TRP:H	1.69	0.56
1:A:975:SER:OG	1:A:980:GLU:OE1	2.24	0.56
1:E:1005:VAL:HG13	1:E:1006:ASP:H	1.70	0.56
1:E:1049:ILE:O	1:E:1053:VAL:HG23	2.04	0.56
1:C:1264:LYS:HD2	1:C:1283:LEU:HD22	1.86	0.56
1:C:1277:LYS:NZ	1:C:1280:GLY:H	2.04	0.56
1:B:839:THR:HG21	3:B:1401:ATP:N7	2.20	0.56
1:C:1226:ARG:HH12	1:C:1258:PRO:HG2	1.70	0.56
1:E:1183:MET:HE2	1:E:1240:LEU:HB2	1.88	0.55
1:A:919:TYR:CZ	1:A:923:ARG:HD2	2.41	0.55
1:A:839:THR:HG23	3:A:1401:ATP:O1A	2.07	0.54
1:B:1035:ARG:HH12	1:B:1039:ASP:HB3	1.72	0.54
1:C:1266:MET:HA	1:E:910:GLU:HG2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1155:ASP:OD2	1:E:1313:ARG:NH2	2.40	0.54
1:E:831:GLY:HA3	1:E:835:THR:HG21	1.88	0.54
1:C:1035:ARG:NH2	1:C:1044:THR:O	2.40	0.54
1:E:1248:MET:HG3	1:E:1275:GLY:HA2	1.90	0.54
1:E:796:GLY:HA2	1:E:852:HIS:CD2	2.44	0.53
1:E:1118:THR:HG22	1:E:1119:GLU:HG3	1.90	0.53
1:C:1220:THR:OG1	1:C:1221:SER:N	2.40	0.53
1:E:1035:ARG:NH1	1:E:1048:GLY:HA3	2.24	0.53
1:C:919:TYR:CZ	1:C:923:ARG:HD2	2.45	0.52
1:C:1071:LEU:HD13	1:C:1309:GLN:HB2	1.92	0.51
1:A:1045:LEU:O	1:A:1049:ILE:HG13	2.11	0.51
1:B:1283:LEU:HB3	1:B:1299:VAL:HG21	1.92	0.51
1:A:1155:ASP:OD1	1:A:1313:ARG:NH2	2.44	0.51
1:E:1271:LEU:HB3	1:E:1298:PHE:HA	1.93	0.51
1:B:1200:ARG:NH2	1:B:1207:GLU:OE1	2.41	0.50
1:E:773:ASP:N	1:E:773:ASP:OD1	2.44	0.50
1:C:1246:ARG:NH1	1:C:1247:SER:O	2.45	0.50
1:C:1144:LEU:HD23	1:C:1209:PHE:HB2	1.93	0.50
1:C:1236:ARG:NH2	1:E:910:GLU:OE2	2.41	0.50
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.47	0.49
1:C:1014:PRO:HB2	1:C:1017:ARG:HB3	1.92	0.49
1:B:862:LEU:HB2	1:B:940:VAL:HG12	1.94	0.49
1:E:1267:ALA:HB1	1:E:1301:ARG:HD2	1.93	0.49
1:C:1005:VAL:HG13	1:C:1006:ASP:H	1.78	0.49
1:C:1017:ARG:NH1	1:C:1017:ARG:HB2	2.27	0.49
1:B:1144:LEU:HD23	1:B:1209:PHE:HB2	1.93	0.49
1:E:1037:ASP:OD1	1:E:1038:GLY:N	2.45	0.49
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	1.94	0.49
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.45	0.49
1:B:1276:ASN:ND2	1:B:1278:ASP:OD2	2.46	0.49
1:E:1246:ARG:HH11	1:E:1246:ARG:HG2	1.78	0.49
1:E:838:SER:HB3	1:E:868:THR:HG21	1.95	0.48
1:C:939:VAL:HG22	1:C:972:VAL:HB	1.95	0.48
1:E:839:THR:HG22	1:E:842:ARG:NH2	2.29	0.48
1:A:821:SER:HB3	1:A:920:ARG:HH12	1.78	0.48
1:A:1271:LEU:HB3	1:A:1298:PHE:HA	1.96	0.48
1:B:864:PHE:H	1:B:941:ASP:HB3	1.78	0.48
1:B:1035:ARG:HH11	1:B:1039:ASP:HB3	1.74	0.48
1:C:783:ALA:HA	1:C:784:ALA:HA	1.51	0.48
1:E:1035:ARG:HH21	1:E:1039:ASP:HB2	1.78	0.48
1:A:1118:THR:HG22	1:A:1119:GLU:HG3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:GLU:OE1	1:A:1198:ARG:NH1	2.46	0.48
1:B:1155:ASP:OD2	1:B:1313:ARG:NH2	2.47	0.47
1:B:825:GLY:H	1:B:965:LEU:HD21	1.79	0.47
1:B:958:THR:HG23	1:B:985:ILE:HB	1.95	0.47
1:E:1009:LYS:HE2	1:E:1009:LYS:HB3	1.62	0.47
1:A:1224:PRO:HG2	1:A:1225:LEU:HD12	1.96	0.47
1:E:1146:PHE:HD2	1:E:1153:LEU:HD23	1.79	0.47
1:A:788:THR:OG1	1:A:789:ALA:N	2.48	0.47
1:B:783:ALA:HA	1:B:784:ALA:HA	1.55	0.47
1:C:828:GLY:HA3	1:C:989:LEU:HD23	1.97	0.47
1:A:763:LEU:HD21	1:A:811:GLN:HA	1.97	0.47
1:C:836:GLY:HA2	3:C:1401:ATP:O1A	2.15	0.47
1:A:803:GLY:HA2	1:A:1032:ALA:HB2	1.95	0.47
1:A:886:ASP:OD1	1:A:886:ASP:N	2.47	0.47
1:C:788:THR:OG1	1:C:789:ALA:N	2.48	0.47
1:B:825:GLY:HA3	1:B:965:LEU:HD11	1.97	0.47
1:C:900:LEU:HD11	1:C:931:ASP:OD2	2.14	0.47
1:B:944:LEU:HB2	1:B:980:GLU:OE2	2.15	0.46
1:B:1035:ARG:NH1	1:B:1037:ASP:OD1	2.48	0.46
1:C:1283:LEU:HB3	1:C:1299:VAL:HG21	1.96	0.46
1:C:1123:SER:OG	3:C:1402:ATP:O1B	2.34	0.46
1:C:1226:ARG:HG3	1:C:1226:ARG:NH1	2.24	0.46
1:C:1277:LYS:NZ	1:C:1280:GLY:N	2.63	0.46
1:B:1290:LYS:H	1:B:1290:LYS:HD2	1.80	0.46
1:B:1251:ALA:N	1:B:1279:GLU:OE2	2.46	0.46
1:B:958:THR:HA	1:B:985:ILE:HD12	1.97	0.46
1:B:999:ASP:N	1:B:1000:PRO:HD3	2.31	0.46
1:C:862:LEU:HB2	1:C:940:VAL:HG12	1.97	0.46
1:E:1163:ILE:HB	2:K:102:LEU:HD21	1.98	0.46
1:E:1116:GLY:O	1:E:1247:SER:HA	2.16	0.45
1:E:803:GLY:HA2	1:E:1032:ALA:HB2	1.98	0.45
1:C:1213:ASP:OD1	1:C:1214:ASP:N	2.49	0.45
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.52	0.45
1:B:839:THR:HG22	3:B:1401:ATP:O1A	2.15	0.45
1:B:888:ASP:OD2	1:B:1295:ARG:NH1	2.49	0.45
1:E:1273:MET:O	1:E:1274:SER:C	2.59	0.45
1:A:767:ASP:OD1	1:A:767:ASP:N	2.36	0.45
1:C:1017:ARG:HB2	1:C:1017:ARG:HH11	1.81	0.45
1:C:1132:GLY:O	1:C:1136:ARG:HD3	2.17	0.45
1:B:1186:ARG:HH22	2:H:98:VAL:HG22	1.81	0.45
1:E:1262:ARG:O	1:E:1266:MET:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:GLN:NE2	3:B:1401:ATP:O3G	2.50	0.45
1:B:1242:LEU:HD23	1:B:1263:ILE:HD11	1.99	0.45
1:C:1215:TYR:CZ	1:C:1219:ALA:HB2	2.51	0.45
1:A:783:ALA:HA	1:A:784:ALA:HA	1.65	0.45
1:B:1186:ARG:NH2	2:H:98:VAL:HG22	2.32	0.44
1:A:773:ASP:OD1	1:A:773:ASP:N	2.46	0.44
1:C:1045:LEU:O	1:C:1049:ILE:HG13	2.18	0.44
1:B:979:SER:CB	1:B:1002:GLU:OE2	2.66	0.44
1:E:1035:ARG:NH2	1:E:1039:ASP:HB2	2.33	0.44
1:A:770:PRO:HG3	1:A:804:LEU:HG	2.00	0.44
1:B:892:ARG:NH2	1:B:1099:LEU:HG	2.32	0.44
1:B:1002:GLU:O	1:B:1003:SER:C	2.60	0.44
1:C:824:ALA:O	1:C:991:THR:OG1	2.34	0.44
1:B:1117:ASP:OD1	1:B:1120:CYS:HB3	2.18	0.43
1:E:918:THR:HG23	1:E:921:ARG:HH22	1.82	0.43
1:A:1187:LEU:HD13	1:A:1188:PRO:HD2	2.00	0.43
1:B:1145:ILE:HD12	1:B:1179:ILE:HD11	1.99	0.43
1:E:793:GLU:HG3	1:E:794:TRP:CD1	2.53	0.43
1:E:898:SER:HA	1:E:960:LEU:HD11	1.99	0.43
1:A:1215:TYR:HE2	1:A:1257:GLU:OE2	2.01	0.43
1:C:1226:ARG:NH1	1:C:1226:ARG:CG	2.81	0.43
1:B:999:ASP:N	1:B:1000:PRO:CD	2.81	0.43
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.52	0.43
1:C:1182:ALA:HB2	2:J:101:LEU:HD13	2.00	0.43
2:J:96:ASN:OD1	2:J:97:ARG:N	2.41	0.43
1:A:872:LEU:HB3	1:A:875:LEU:HD12	2.00	0.43
1:A:1035:ARG:NH1	1:A:1048:GLY:HA3	2.34	0.43
1:C:1277:LYS:HZ3	1:C:1280:GLY:CA	2.32	0.43
1:B:1006:ASP:HB3	1:B:1009:LYS:HB2	2.01	0.42
1:E:1044:THR:OG1	1:E:1047:GLU:OE2	2.36	0.42
1:B:788:THR:OG1	1:B:789:ALA:N	2.52	0.42
1:E:763:LEU:HD23	1:E:763:LEU:HA	1.82	0.42
1:A:807:ARG:NH2	1:B:810:ASP:OD1	2.52	0.42
1:C:1035:ARG:HH21	1:C:1045:LEU:HA	1.84	0.42
1:B:940:VAL:HG21	1:B:943:TRP:HE3	1.84	0.42
1:C:796:GLY:HA2	1:C:852:HIS:CD2	2.54	0.42
1:E:1264:LYS:HD2	1:E:1282:LEU:O	2.20	0.42
1:A:1187:LEU:HD22	1:A:1238:ILE:HG21	1.99	0.42
1:C:1242:LEU:HD23	1:C:1244:ILE:HD11	2.02	0.42
1:E:939:VAL:HG22	1:E:972:VAL:HB	2.00	0.42
1:C:904:ARG:HA	1:C:907:GLU:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ARG:O	2:J:101:LEU:HB2	2.20	0.42
1:E:1213:ASP:OD1	1:E:1214:ASP:N	2.53	0.42
1:B:892:ARG:NH1	1:B:896:GLU:OE1	2.53	0.42
1:B:979:SER:HB3	1:B:1002:GLU:OE2	2.19	0.42
1:E:818:LEU:HD13	1:E:991:THR:HG21	2.01	0.42
1:E:1189:PRO:HD2	1:E:1192:LEU:HD11	2.02	0.42
1:A:1005:VAL:HG13	1:A:1006:ASP:H	1.84	0.42
1:A:1054:LYS:HE3	1:A:1058:GLU:OE2	2.20	0.42
1:B:1287:LYS:HA	1:B:1288:PRO:HD3	1.84	0.42
1:C:1238:ILE:HG13	1:C:1240:LEU:H	1.85	0.42
1:A:914:ASP:OD1	1:A:914:ASP:N	2.53	0.41
1:C:1184:GLU:HA	1:C:1187:LEU:HG	2.02	0.41
1:E:807:ARG:HG2	1:E:1027:TYR:CD1	2.55	0.41
1:A:1033:LEU:HA	1:A:1034:PRO:HD3	1.83	0.41
1:E:918:THR:HG23	1:E:921:ARG:NH2	2.35	0.41
1:E:1200:ARG:HA	1:E:1202:TRP:CZ3	2.54	0.41
1:A:954:GLU:CD	1:A:982:ARG:HE	2.28	0.41
1:A:1287:LYS:HE3	1:A:1287:LYS:HB2	1.96	0.41
1:B:892:ARG:O	1:B:892:ARG:HD3	2.20	0.41
1:A:1232:LEU:HD23	1:A:1232:LEU:HA	1.91	0.41
1:B:1071:LEU:HA	1:B:1072:PRO:HD3	1.93	0.41
1:B:1173:SER:HB2	1:B:1224:PRO:HB3	2.02	0.41
1:C:919:TYR:OH	1:C:931:ASP:OD1	2.28	0.41
1:C:1020:ARG:HH21	1:C:1028:HIS:HB3	1.85	0.41
1:E:885:LEU:O	1:E:887:ALA:N	2.54	0.41
1:A:1116:GLY:O	1:A:1247:SER:HA	2.20	0.41
1:C:1085:GLU:HA	1:E:1088:THR:HG23	2.03	0.41
1:C:1193:THR:HG22	1:C:1195:GLU:H	1.85	0.41
1:A:958:THR:HG23	1:A:985:ILE:HB	2.02	0.41
1:C:944:LEU:HD22	1:C:980:GLU:OE2	2.21	0.41
1:E:826:HIS:CE1	1:E:965:LEU:HD13	2.56	0.41
1:A:1199:SER:OG	1:A:1201:SER:OG	2.36	0.41
1:C:975:SER:OG	1:C:980:GLU:OE1	2.36	0.41
1:C:1035:ARG:HD3	1:C:1037:ASP:HB3	2.03	0.41
1:C:1287:LYS:HA	1:C:1288:PRO:HD3	1.94	0.41
1:A:801:VAL:HB	1:A:817:TRP:CE2	2.56	0.40
1:C:904:ARG:NE	1:C:931:ASP:OD2	2.49	0.40
1:E:994:GLU:CD	1:E:1003:SER:OG	2.64	0.40
1:E:1255:LEU:HD13	1:E:1264:LYS:HE2	2.03	0.40
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.54	0.40
1:B:1109:ASP:HA	1:B:1110:PRO:HD3	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:801:VAL:HB	1:E:817:TRP:CE2	2.56	0.40
1:B:829:VAL:HG22	1:B:993:LEU:HB2	2.04	0.40
1:B:892:ARG:HD2	1:B:1069:ARG:O	2.21	0.40
1:B:1151:ARG:HB3	1:B:1154:LEU:HD21	2.04	0.40
1:A:1035:ARG:CZ	1:A:1048:GLY:HA3	2.51	0.40
1:C:1189:PRO:HA	1:C:1190:PRO:HD3	1.89	0.40
1:E:1034:PRO:HD2	1:E:1045:LEU:HD11	2.04	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	553/589 (94%)	535 (97%)	18 (3%)	0	100	100
1	B	551/589 (94%)	524 (95%)	26 (5%)	1 (0%)	43	72
1	C	552/589 (94%)	515 (93%)	37 (7%)	0	100	100
1	E	553/589 (94%)	536 (97%)	16 (3%)	1 (0%)	43	72
2	G	5/23 (22%)	5 (100%)	0	0	100	100
2	H	4/23 (17%)	4 (100%)	0	0	100	100
2	J	5/23 (22%)	5 (100%)	0	0	100	100
2	K	4/23 (17%)	2 (50%)	2 (50%)	0	100	100
All	All	2227/2448 (91%)	2126 (96%)	99 (4%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	886	ASP
1	E	1005	VAL

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	455/485 (94%)	446 (98%)	9 (2%)	48	69
1	B	445/485 (92%)	436 (98%)	9 (2%)	48	69
1	C	446/485 (92%)	432 (97%)	14 (3%)	35	62
1	E	454/485 (94%)	448 (99%)	6 (1%)	61	75
2	G	6/18 (33%)	5 (83%)	1 (17%)	2	10
2	H	5/18 (28%)	3 (60%)	2 (40%)	0	0
2	J	5/18 (28%)	3 (60%)	2 (40%)	0	0
2	K	5/18 (28%)	5 (100%)	0	100	100
All	All	1821/2012 (90%)	1778 (98%)	43 (2%)	43	67

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	761	ILE
1	A	821	SER
1	A	886	ASP
1	A	906	GLN
1	A	1005	VAL
1	A	1046	THR
1	A	1051	THR
1	A	1218	VAL
1	A	1286	VAL
1	B	763	LEU
1	B	892	ARG
1	B	1044	THR
1	B	1046	THR
1	B	1160	GLU
1	B	1177	ARG
1	B	1218	VAL
1	B	1274	SER
1	B	1286	VAL
1	C	911	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	955	ASP
1	C	1001	TYR
1	C	1005	VAL
1	C	1022	LEU
1	C	1088	THR
1	C	1090	ILE
1	C	1196	GLN
1	C	1255	LEU
1	C	1262	ARG
1	C	1264	LYS
1	C	1277	LYS
1	C	1281	ILE
1	C	1300	GLU
2	G	98	VAL
2	H	98	VAL
2	H	101	LEU
2	J	98	VAL
2	J	101	LEU
1	E	811	GLN
1	E	1005	VAL
1	E	1009	LYS
1	E	1046	THR
1	E	1047	GLU
1	E	1218	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	785	HIS
1	A	855	GLN
1	A	1016	ASN
1	B	785	HIS
1	B	1061	HIS
1	B	1141	GLN
1	B	1293	GLN
1	C	785	HIS
1	C	1289	HIS
2	G	99	GLN
2	H	99	GLN
1	E	855	GLN
1	E	877	HIS
1	E	1016	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1028	HIS
1	E	1261	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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$
3	ATP	B	1402	4	32,33,33	1.43	4 (12%)	48,52,52	1.76	9 (18%)
3	ATP	C	1402	4	32,33,33	1.40	4 (12%)	48,52,52	1.74	9 (18%)
3	ATP	A	1401	4	32,33,33	1.41	4 (12%)	48,52,52	1.75	8 (16%)
3	ATP	A	1402	4	32,33,33	1.39	4 (12%)	48,52,52	1.77	9 (18%)
3	ATP	C	1401	4	32,33,33	1.42	4 (12%)	48,52,52	1.75	9 (18%)
3	ATP	B	1401	4	32,33,33	1.40	4 (12%)	48,52,52	1.75	9 (18%)

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	B	1402	4	-	0/22/38/38	0/3/3/3
3	ATP	C	1402	4	-	0/22/38/38	0/3/3/3
3	ATP	A	1401	4	-	2/22/38/38	0/3/3/3
3	ATP	A	1402	4	-	0/22/38/38	0/3/3/3
3	ATP	C	1401	4	-	2/22/38/38	0/3/3/3
3	ATP	B	1401	4	-	1/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	ATP	C5-C4	4.77	1.47	1.39
3	B	1402	ATP	C5-C4	4.76	1.47	1.39
3	A	1402	ATP	C5-C4	4.76	1.47	1.39
3	C	1401	ATP	C5-C4	4.76	1.47	1.39
3	B	1401	ATP	C5-C4	4.73	1.47	1.39
3	C	1402	ATP	C5-C4	4.72	1.47	1.39
3	A	1402	ATP	C5-C6	2.77	1.48	1.41
3	A	1401	ATP	C5-C6	2.74	1.48	1.41
3	C	1401	ATP	C5-C6	2.74	1.48	1.41
3	B	1402	ATP	C5-C6	2.74	1.48	1.41
3	C	1402	ATP	C5-C6	2.72	1.48	1.41
3	B	1401	ATP	C5-C6	2.58	1.48	1.41
3	B	1401	ATP	C5-N7	-2.51	1.34	1.39
3	C	1402	ATP	C8-N7	2.39	1.36	1.31
3	C	1401	ATP	C8-N7	2.37	1.36	1.31
3	A	1401	ATP	C8-N7	2.33	1.36	1.31
3	B	1402	ATP	C8-N7	2.32	1.36	1.31
3	A	1402	ATP	C8-N7	2.30	1.36	1.31
3	C	1401	ATP	C5-N7	-2.28	1.34	1.39
3	A	1401	ATP	C5-N7	-2.27	1.34	1.39
3	A	1402	ATP	C5-N7	-2.25	1.35	1.39
3	B	1402	ATP	C5-N7	-2.23	1.35	1.39
3	C	1402	ATP	C5-N7	-2.22	1.35	1.39
3	B	1401	ATP	C8-N7	2.21	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	ATP	C5-C4-N3	-5.96	118.51	126.72
3	B	1402	ATP	C5-C4-N3	-5.91	118.58	126.72
3	A	1401	ATP	C5-C4-N3	-5.88	118.62	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1402	ATP	C5-C4-N3	-5.88	118.62	126.72
3	C	1401	ATP	C5-C4-N3	-5.87	118.64	126.72
3	B	1401	ATP	C5-C4-N3	-5.86	118.65	126.72
3	B	1401	ATP	N3-C4-N9	4.80	135.34	127.17
3	A	1401	ATP	N3-C4-N9	4.73	135.22	127.17
3	A	1402	ATP	N3-C4-N9	4.72	135.20	127.17
3	B	1402	ATP	N3-C4-N9	4.63	135.04	127.17
3	C	1401	ATP	N3-C4-N9	4.62	135.02	127.17
3	C	1402	ATP	N3-C4-N9	4.61	135.00	127.17
3	B	1402	ATP	C2-N3-C4	3.70	120.88	111.83
3	A	1402	ATP	C2-N3-C4	3.69	120.84	111.83
3	C	1401	ATP	C2-N3-C4	3.67	120.80	111.83
3	A	1401	ATP	C2-N3-C4	3.67	120.79	111.83
3	C	1402	ATP	C2-N3-C4	3.67	120.79	111.83
3	B	1401	ATP	C2-N3-C4	3.54	120.47	111.83
3	B	1402	ATP	C4-C5-N7	-3.52	106.55	110.58
3	C	1402	ATP	C4-C5-N7	-3.50	106.58	110.58
3	A	1402	ATP	C4-C5-N7	-3.50	106.58	110.58
3	A	1401	ATP	C4-C5-N7	-3.44	106.65	110.58
3	C	1401	ATP	C4-C5-N7	-3.42	106.67	110.58
3	B	1401	ATP	C4-C5-N7	-3.31	106.80	110.58
3	C	1401	ATP	N3-C2-N1	-3.17	123.79	128.58
3	B	1402	ATP	N3-C2-N1	-3.15	123.82	128.58
3	A	1401	ATP	N3-C2-N1	-3.14	123.82	128.58
3	C	1402	ATP	N3-C2-N1	-3.11	123.88	128.58
3	A	1402	ATP	N3-C2-N1	-3.06	123.95	128.58
3	B	1401	ATP	N3-C2-N1	-3.05	123.96	128.58
3	A	1401	ATP	C4-N9-C8	2.72	108.59	105.74
3	B	1401	ATP	C4-N9-C8	2.72	108.59	105.74
3	B	1401	ATP	C5-N7-C8	2.58	107.50	103.45
3	A	1401	ATP	C5-N7-C8	2.57	107.49	103.45
3	A	1402	ATP	C4-N9-C8	2.56	108.42	105.74
3	C	1402	ATP	C4-N9-C8	2.56	108.42	105.74
3	A	1402	ATP	C5-N7-C8	2.55	107.45	103.45
3	B	1402	ATP	C5-N7-C8	2.53	107.43	103.45
3	C	1402	ATP	C5-N7-C8	2.51	107.39	103.45
3	C	1401	ATP	C4-N9-C8	2.50	108.37	105.74
3	B	1402	ATP	C4-N9-C8	2.50	108.36	105.74
3	A	1402	ATP	C3'-C2'-C1'	2.49	106.17	101.46
3	C	1401	ATP	C3'-C2'-C1'	2.46	106.11	101.46
3	C	1401	ATP	C5-N7-C8	2.44	107.29	103.45
3	B	1402	ATP	C3'-C2'-C1'	2.39	105.98	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	ATP	C3'-C2'-C1'	2.35	105.90	101.46
3	C	1402	ATP	C3'-C2'-C1'	2.24	105.69	101.46
3	A	1401	ATP	C3'-C2'-C1'	2.11	105.46	101.46
3	B	1402	ATP	C6-C5-N7	2.07	136.08	132.09
3	B	1401	ATP	C2'-C1'-N9	-2.07	108.17	113.30
3	C	1402	ATP	C6-C5-N7	2.05	136.04	132.09
3	A	1402	ATP	C6-C5-N7	2.02	135.99	132.09
3	C	1401	ATP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

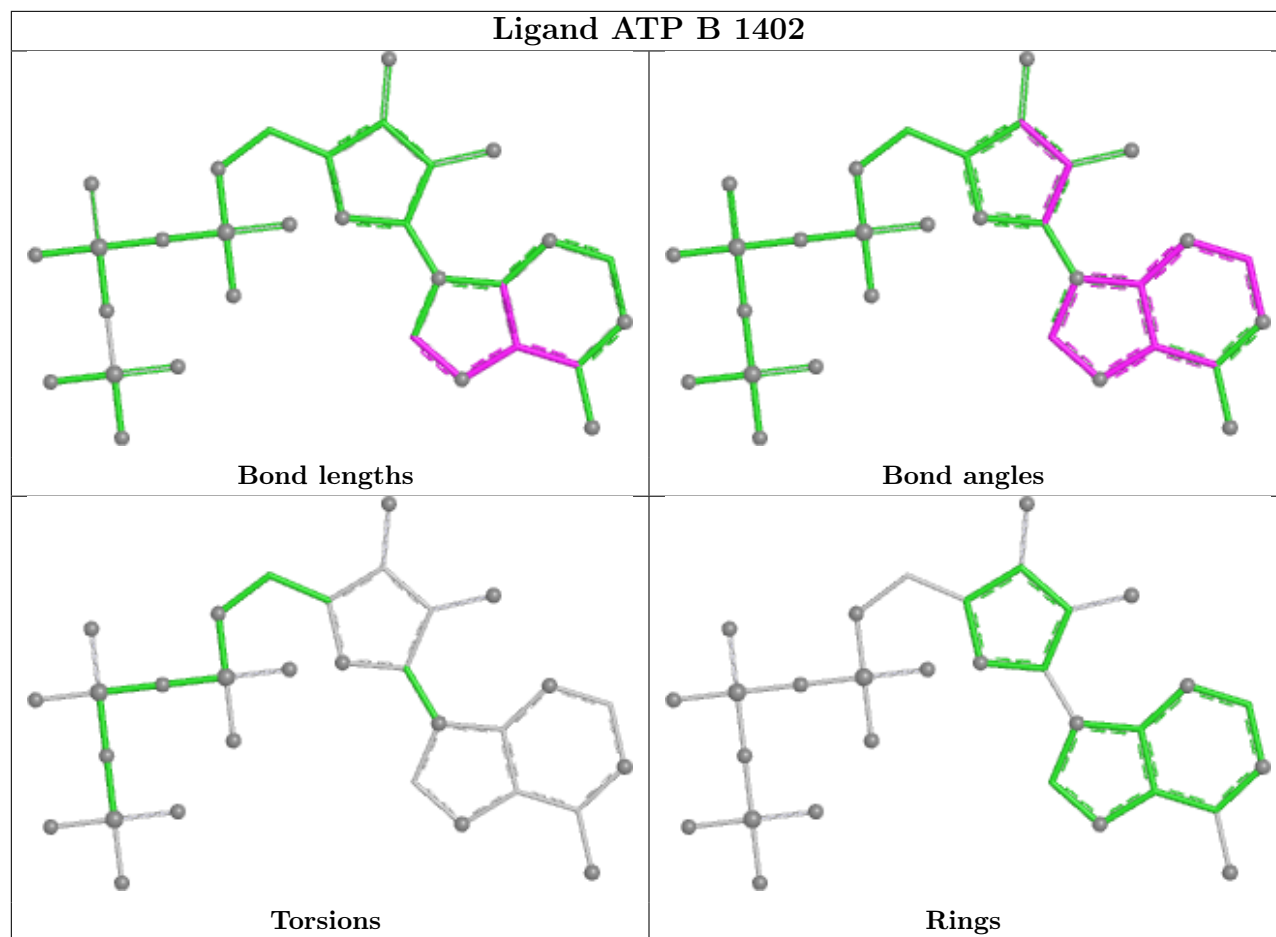
Mol	Chain	Res	Type	Atoms
3	A	1401	ATP	PA-O3A-PB-O1B
3	C	1401	ATP	PA-O3A-PB-O1B
3	A	1401	ATP	PA-O3A-PB-O2B
3	C	1401	ATP	PA-O3A-PB-O2B
3	B	1401	ATP	PA-O3A-PB-O2B

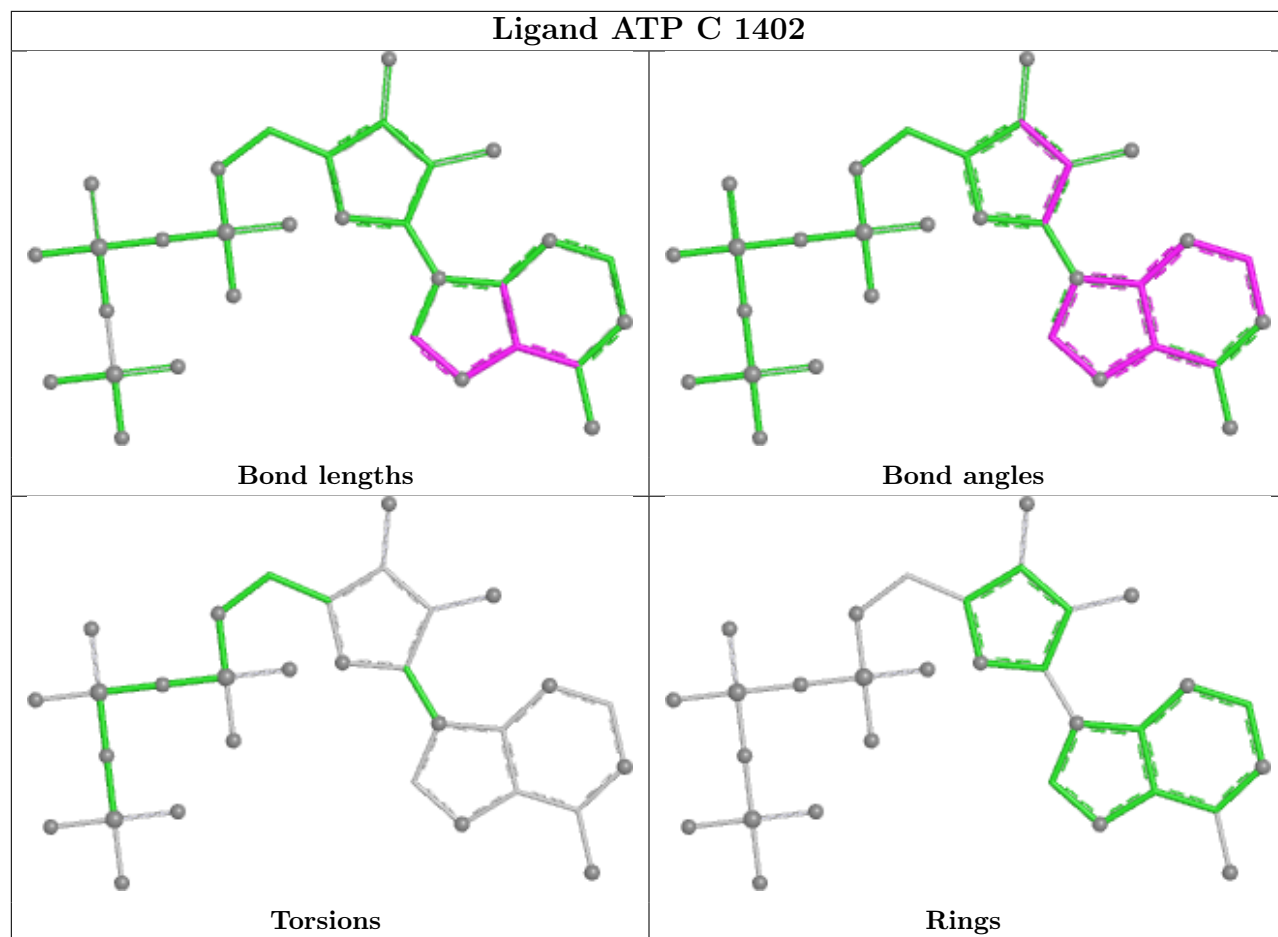
There are no ring outliers.

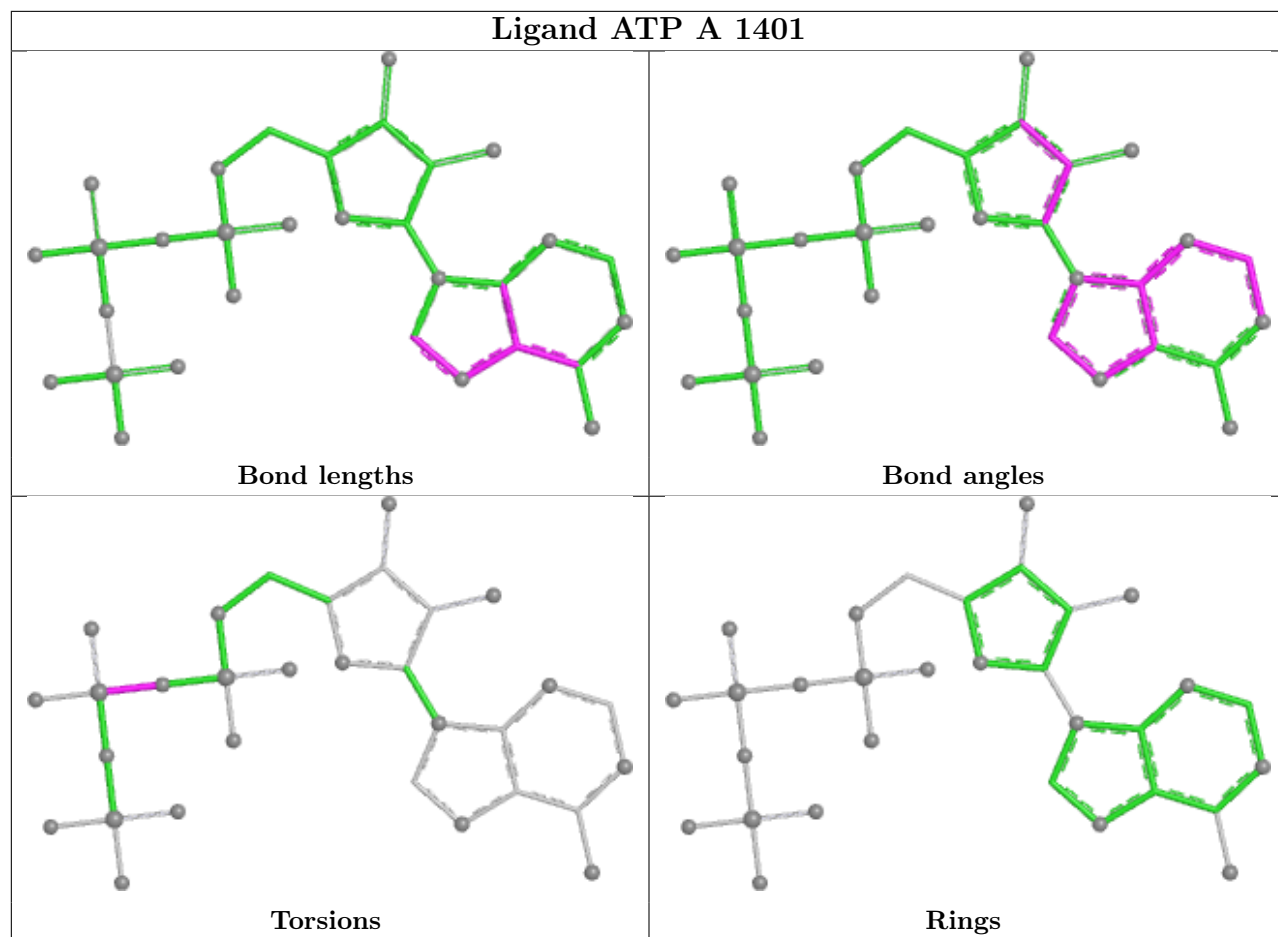
4 monomers are involved in 6 short contacts:

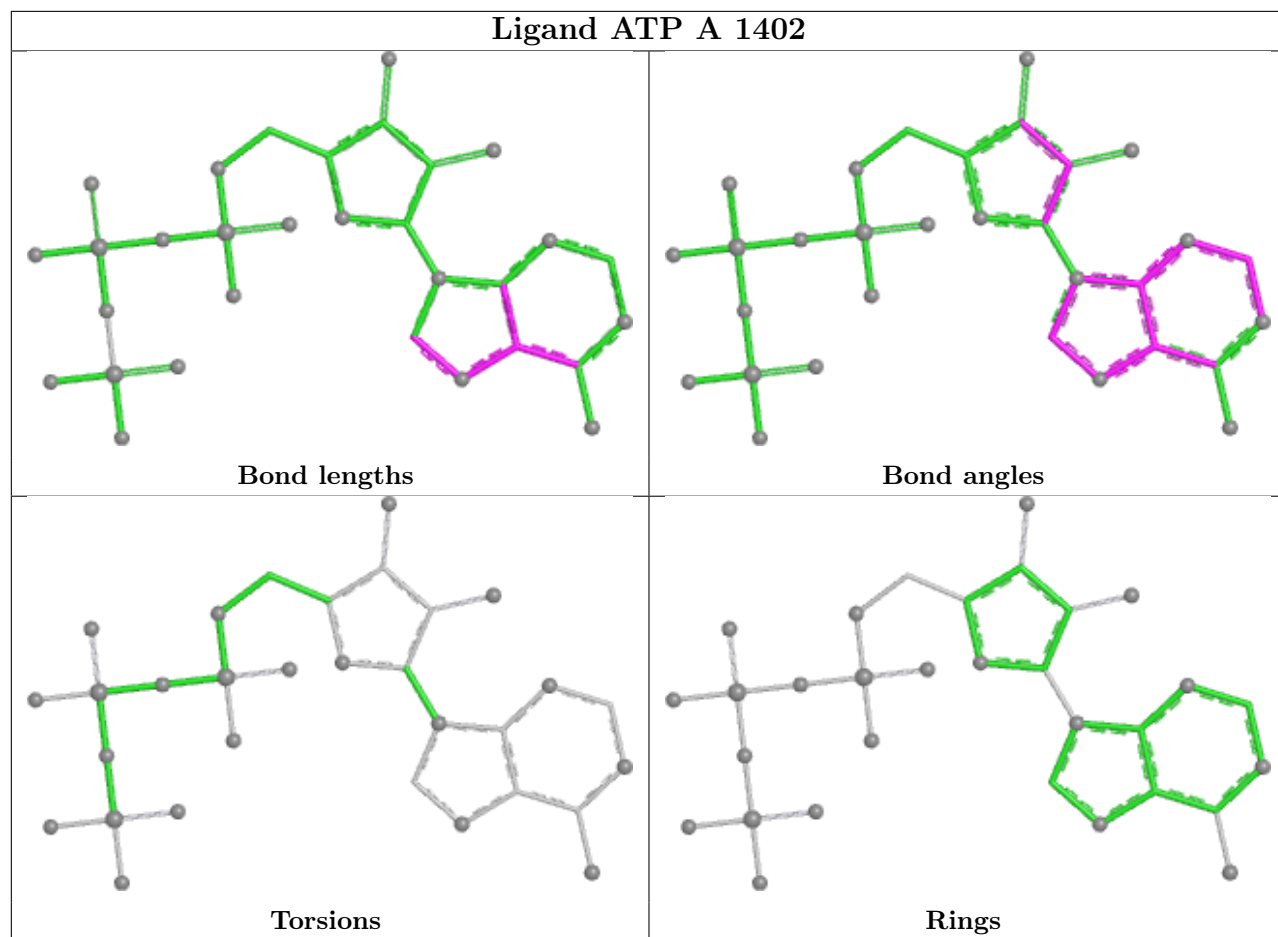
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1402	ATP	1	0
3	A	1401	ATP	1	0
3	C	1401	ATP	1	0
3	B	1401	ATP	3	0

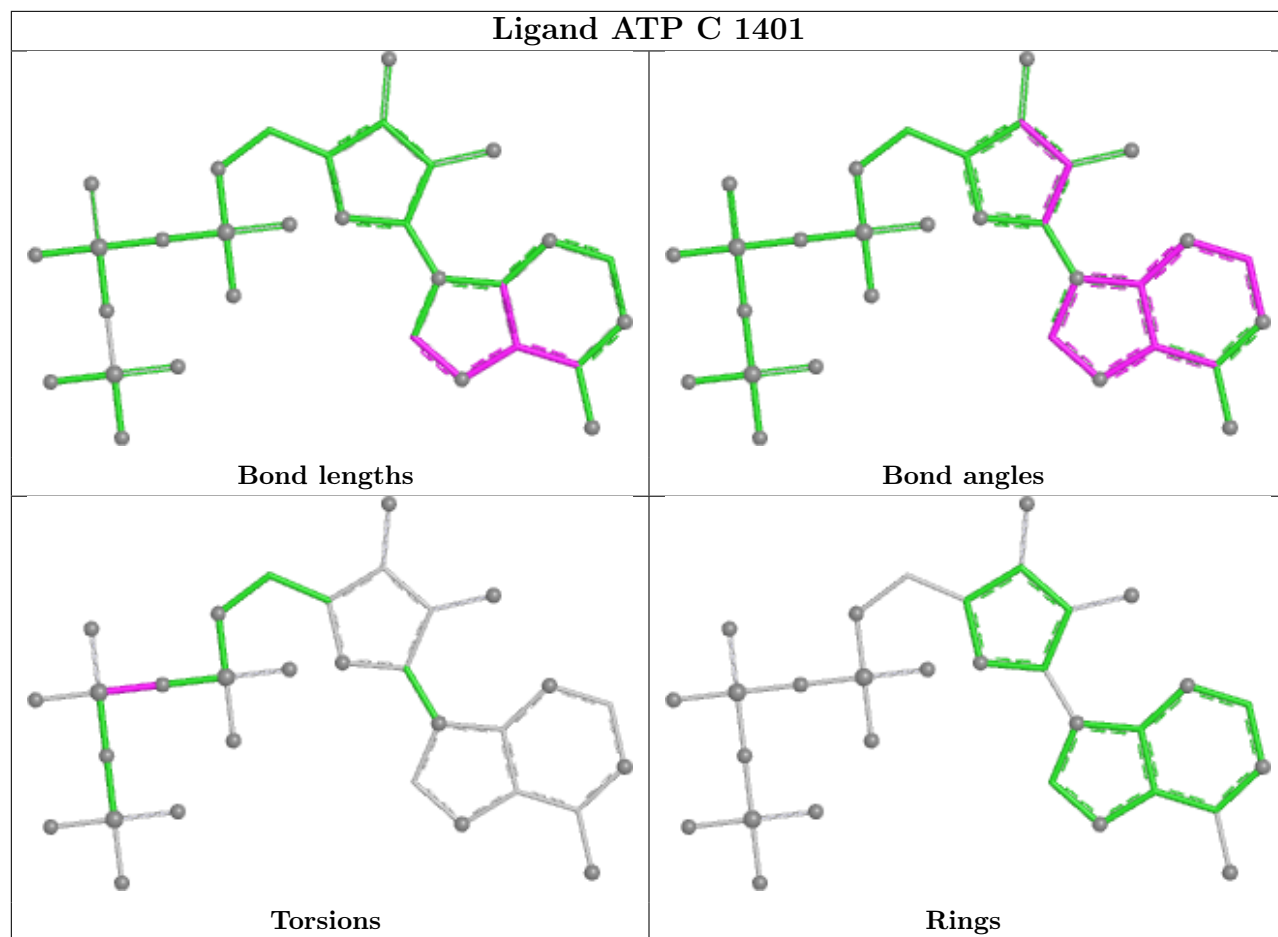
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

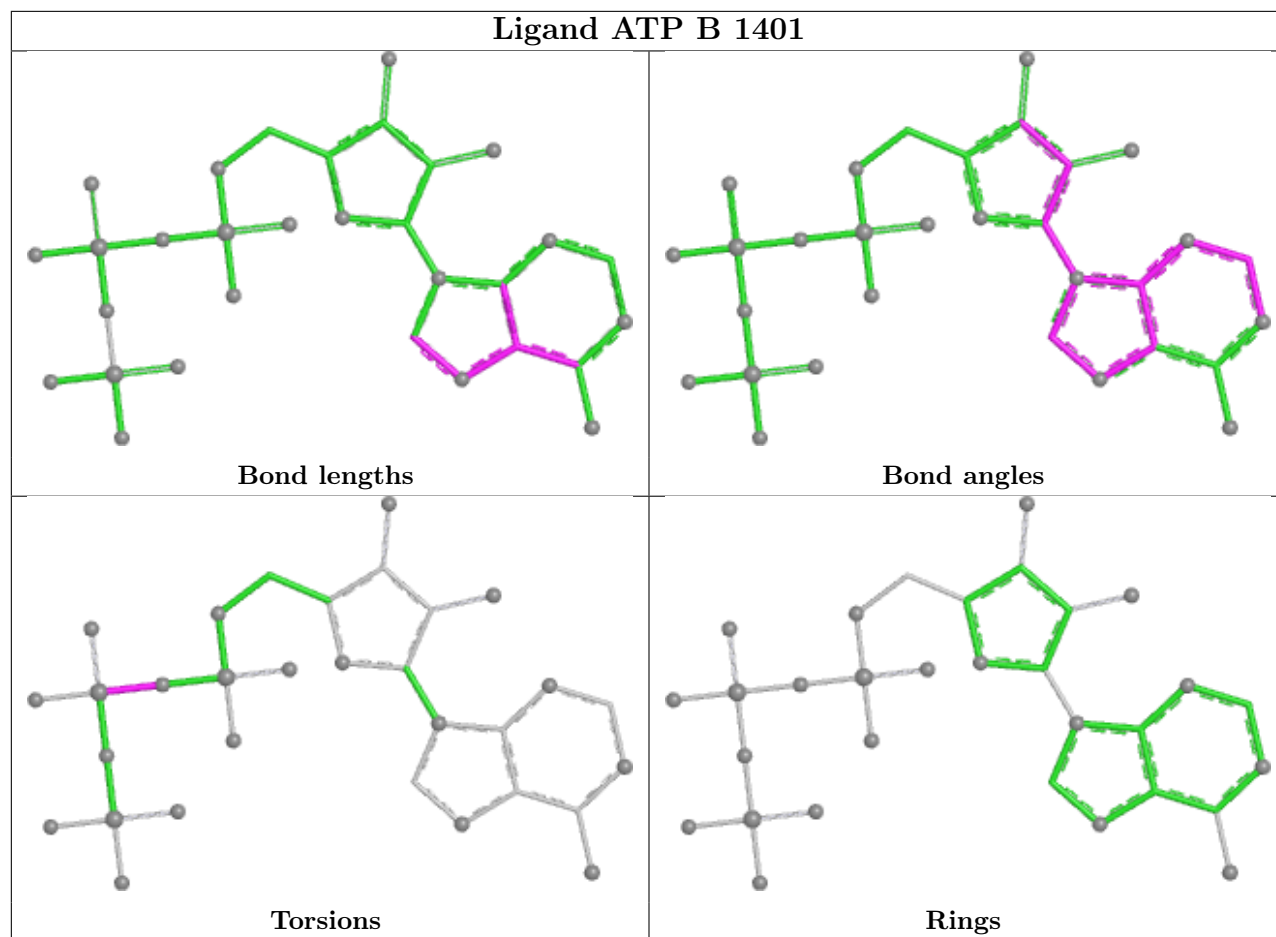












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/589 (94%)	-0.12	4 (0%) 84 70	25, 48, 78, 103	0
1	B	553/589 (93%)	0.03	4 (0%) 84 70	29, 55, 90, 122	0
1	C	554/589 (94%)	0.65	42 (7%) 20 14	43, 84, 137, 177	0
1	E	555/589 (94%)	1.91	214 (38%) 1 1	122, 187, 222, 279	0
2	G	7/23 (30%)	0.92	0 100 100	64, 66, 92, 95	0
2	H	6/23 (26%)	1.63	2 (33%) 1 1	96, 102, 122, 128	0
2	J	7/23 (30%)	1.47	2 (28%) 1 1	102, 110, 118, 124	0
2	K	6/23 (26%)	2.38	4 (66%) 0 0	136, 159, 170, 175	0
All	All	2243/2448 (91%)	0.63	272 (12%) 8 7	25, 72, 205, 279	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	845	ILE	7.3
1	E	844	LEU	6.8
1	E	841	LEU	6.2
1	E	846	THR	5.9
1	E	794	TRP	5.6
1	E	850	LEU	5.5
1	E	993	LEU	5.3
1	E	1045	LEU	5.2
1	E	848	LEU	5.2
1	E	1033	LEU	5.1
1	E	1123	SER	4.8
1	E	801	VAL	4.8
1	E	818	LEU	4.8
1	E	872	LEU	4.7
1	E	829	VAL	4.7
1	E	1111	HIS	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	820	LEU	4.7
1	C	762	TRP	4.6
1	E	1228	LEU	4.6
1	E	1121	GLY	4.5
1	E	816	TYR	4.5
1	E	849	ALA	4.3
1	E	843	THR	4.2
1	B	763	LEU	4.2
1	E	869	LEU	4.2
1	E	800	ALA	4.1
1	E	1281	ILE	4.0
1	E	840	MET	4.0
1	E	817	TRP	4.0
1	E	1263	ILE	4.0
1	E	1213	ASP	3.9
1	E	769	PRO	3.9
1	C	1270	GLY	3.9
1	E	1092	ILE	3.9
1	C	1264	LYS	3.9
1	E	997	LEU	3.9
1	E	1255	LEU	3.9
1	E	802	VAL	3.8
1	E	953	LEU	3.8
1	E	1105	ASP	3.8
1	E	994	GLU	3.8
2	K	98	VAL	3.7
1	C	1006	ASP	3.6
1	E	1253	ARG	3.6
1	E	1052	THR	3.6
1	E	1042	ALA	3.6
1	E	1114	VAL	3.6
1	E	839	THR	3.6
1	E	1056	ILE	3.6
1	E	1112	PHE	3.6
1	E	932	GLY	3.6
1	E	893	THR	3.6
1	C	763	LEU	3.6
1	E	827	VAL	3.6
1	E	851	LEU	3.6
1	E	1011	ALA	3.5
1	E	1231	LEU	3.5
1	E	1010	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	808	PRO	3.5
1	E	1193	THR	3.5
1	E	875	LEU	3.5
1	E	1197	LEU	3.4
1	C	1258	PRO	3.4
1	E	1113	LEU	3.4
1	A	1301	ARG	3.4
1	E	988	LEU	3.4
1	E	764	PRO	3.4
1	E	842	ARG	3.3
1	E	922	LEU	3.3
1	E	861	CYS	3.3
1	E	912	GLY	3.3
1	E	1000	PRO	3.3
1	E	1067	PRO	3.3
1	E	1244	ILE	3.3
2	H	100	ALA	3.3
1	E	804	LEU	3.3
1	E	894	VAL	3.3
1	E	1122	LYS	3.2
1	E	1106	PHE	3.2
1	E	870	ALA	3.2
1	E	799	HIS	3.2
1	E	766	LEU	3.1
1	E	989	LEU	3.1
1	E	1104	LEU	3.1
1	C	1194	PRO	3.1
1	C	1239	GLY	3.1
1	C	1037	ASP	3.1
1	E	781	PRO	3.1
1	C	1298	PHE	3.0
1	E	1119	GLU	3.0
1	E	1050	ALA	3.0
1	E	1101	PRO	3.0
1	E	1242	LEU	3.0
1	E	761	ILE	3.0
1	E	1034	PRO	3.0
1	E	1269	PRO	3.0
1	C	1259	ILE	3.0
1	E	998	GLY	3.0
1	E	1271	LEU	2.9
1	E	778	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	815	PRO	2.9
1	E	783	ALA	2.9
1	E	784	ALA	2.9
1	C	1284	GLY	2.9
1	E	823	GLY	2.9
1	E	1109	ASP	2.9
1	E	798	LEU	2.9
1	E	946	LEU	2.9
1	E	1030	LEU	2.9
1	E	1210	LEU	2.9
1	C	1257	GLU	2.9
1	E	885	LEU	2.9
1	E	985	ILE	2.9
1	E	1147	ILE	2.9
1	E	1291	LEU	2.9
1	E	770	PRO	2.8
1	C	1285	ASN	2.8
1	E	995	LEU	2.8
1	E	1152	SER	2.8
1	E	1064	THR	2.8
1	E	828	GLY	2.8
1	E	1260	ILE	2.8
1	E	847	SER	2.8
1	E	1268	SER	2.8
1	C	1089	ARG	2.8
1	E	1302	ARG	2.8
1	E	992	LYS	2.8
1	E	1046	THR	2.8
1	E	1001	TYR	2.7
1	E	768	VAL	2.7
1	E	1076	PRO	2.7
1	E	1258	PRO	2.7
1	C	1210	LEU	2.7
1	E	838	SER	2.7
1	E	880	SER	2.7
1	E	910	GLU	2.7
1	E	1088	THR	2.7
1	E	933	PHE	2.7
1	E	1049	ILE	2.7
1	E	1214	ASP	2.7
1	E	860	TYR	2.7
1	E	1059	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1272	VAL	2.7
1	E	1154	LEU	2.7
1	E	819	ASP	2.7
1	E	776	LEU	2.7
2	K	103	ASN	2.7
1	E	969	ILE	2.7
1	C	1199	SER	2.7
1	E	1286	VAL	2.7
1	B	902	GLU	2.6
1	E	1315	SER	2.6
1	E	1036	ILE	2.6
1	C	1254	ALA	2.6
1	E	917	ALA	2.6
1	E	1032	ALA	2.6
1	E	1283	LEU	2.6
1	A	1315	SER	2.6
1	C	1002	GLU	2.6
1	E	1256	TYR	2.6
1	E	1292	PRO	2.6
1	C	1271	LEU	2.6
1	C	1282	LEU	2.6
1	E	763	LEU	2.6
1	E	1128	LEU	2.6
2	K	101	LEU	2.6
1	E	1120	CYS	2.6
1	E	1063	PRO	2.6
1	E	966	GLY	2.6
1	E	775	LEU	2.6
1	C	1301	ARG	2.6
1	C	1189	PRO	2.5
1	E	1007	ARG	2.5
1	E	1163	ILE	2.5
1	E	1022	LEU	2.5
1	E	1218	VAL	2.5
1	E	789	ALA	2.5
1	E	940	VAL	2.5
1	E	1245	ALA	2.5
1	C	1099	LEU	2.5
1	E	772	LEU	2.5
1	E	901	LEU	2.5
1	E	1102	VAL	2.5
1	E	824	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	934	GLY	2.4
1	E	1053	VAL	2.4
1	E	1234	GLN	2.4
1	C	1015	GLU	2.4
1	E	779	LEU	2.4
1	E	991	THR	2.4
1	E	1055	THR	2.4
1	E	926	GLY	2.4
1	E	1005	VAL	2.4
1	E	1145	ILE	2.4
1	C	1001	TYR	2.4
1	C	1287	LYS	2.4
2	H	102	LEU	2.4
1	E	1108	THR	2.3
1	E	1095	ASP	2.3
1	E	1306	ARG	2.3
1	C	1315	SER	2.3
1	C	784	ALA	2.3
2	K	100	ALA	2.3
1	E	973	LEU	2.3
1	E	1071	LEU	2.3
1	E	1008	LYS	2.3
1	E	1277	LYS	2.3
1	E	1229	ALA	2.3
1	C	928	TYR	2.3
1	E	1124	ASN	2.3
1	E	859	PHE	2.3
1	E	1191	ASP	2.3
1	E	1233	PRO	2.3
1	B	1315	SER	2.3
1	E	898	SER	2.3
1	E	938	LEU	2.3
1	E	1288	PRO	2.3
1	C	783	ALA	2.3
1	E	762	TRP	2.3
1	E	1051	THR	2.3
1	E	767	ASP	2.3
1	E	1243	ILE	2.2
1	C	1283	LEU	2.2
1	E	787	TYR	2.2
1	E	1006	ASP	2.2
1	E	862	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1195	GLU	2.2
1	C	1232	LEU	2.2
1	E	1142	ALA	2.2
1	E	805	VAL	2.2
1	C	1192	LEU	2.2
1	C	1197	LEU	2.2
1	E	1175	LEU	2.2
1	C	1093	GLY	2.2
1	E	952	ALA	2.2
1	E	1287	LYS	2.2
1	E	1115	PHE	2.2
1	E	978	TRP	2.2
1	C	1299	VAL	2.2
1	C	1263	ILE	2.2
1	E	803	GLY	2.2
2	J	98	VAL	2.1
1	A	821	SER	2.1
1	E	1185	ALA	2.1
1	C	1302	ARG	2.1
1	E	1074	VAL	2.1
1	E	765	PRO	2.1
1	E	990	GLY	2.1
1	E	863	ASP	2.1
1	C	1193	THR	2.1
1	E	1225	LEU	2.1
1	E	1307	LEU	2.1
1	E	1127	ARG	2.1
1	E	833	PRO	2.1
1	E	984	SER	2.1
1	B	1286	VAL	2.1
1	E	788	THR	2.1
1	E	1230	GLU	2.1
1	E	1300	GLU	2.1
1	E	1150	SER	2.1
2	J	102	LEU	2.1
1	E	1044	THR	2.1
1	E	972	VAL	2.0
1	A	780	SER	2.0
1	E	1118	THR	2.0
1	E	1215	TYR	2.0
1	E	1227	PRO	2.0
1	C	1195	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	861	CYS	2.0
1	E	855	GLN	2.0
1	E	936	VAL	2.0
1	E	971	VAL	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

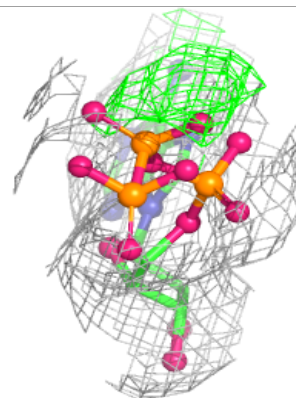
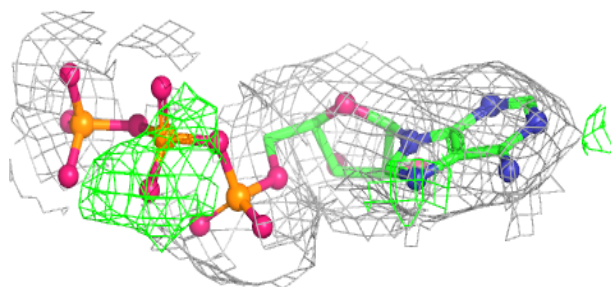
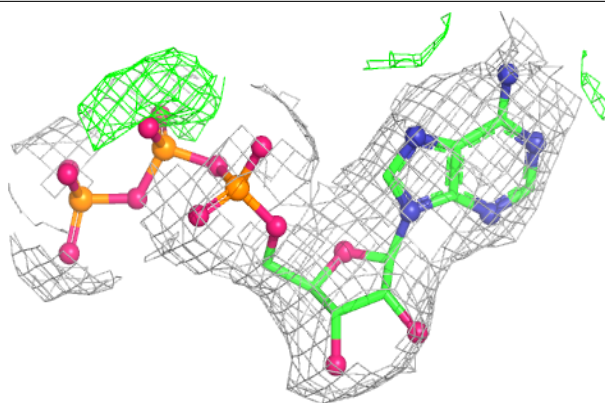
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	E	1401	1/1	0.26	0.44	204,204,204,204	0
4	MG	E	1402	1/1	0.51	0.25	286,286,286,286	0
4	MG	A	1403	1/1	0.84	0.32	43,43,43,43	0
4	MG	B	1403	1/1	0.90	0.17	48,48,48,48	0
4	MG	A	1404	1/1	0.92	0.16	45,45,45,45	0
3	ATP	C	1402	31/31	0.94	0.09	54,68,77,83	0
4	MG	C	1403	1/1	0.94	0.18	55,55,55,55	0
3	ATP	B	1402	31/31	0.94	0.10	43,58,78,120	0
3	ATP	C	1401	31/31	0.94	0.09	35,60,79,88	0
3	ATP	B	1401	31/31	0.95	0.09	28,44,68,79	0
3	ATP	A	1401	31/31	0.96	0.09	38,62,77,82	0
4	MG	B	1404	1/1	0.97	0.13	34,34,34,34	0
3	ATP	A	1402	31/31	0.97	0.06	24,39,57,88	0
4	MG	C	1404	1/1	0.98	0.14	45,45,45,45	0

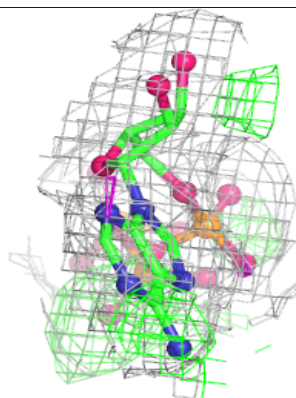
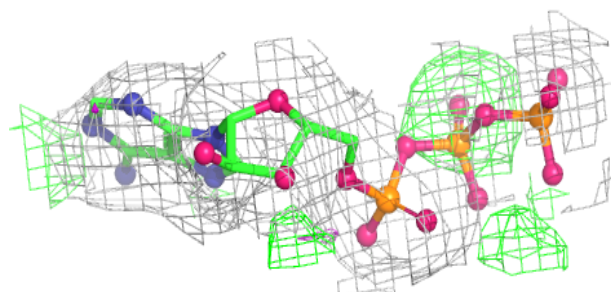
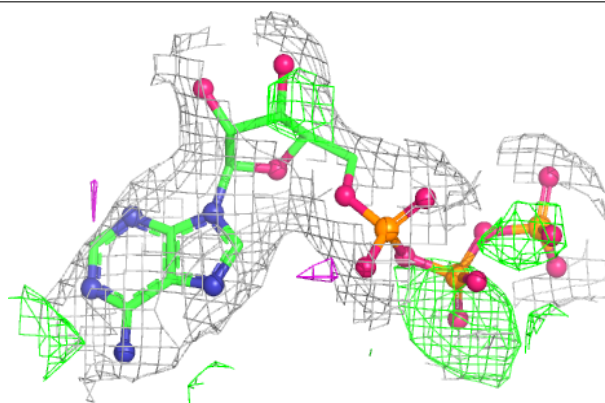
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 1402:

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

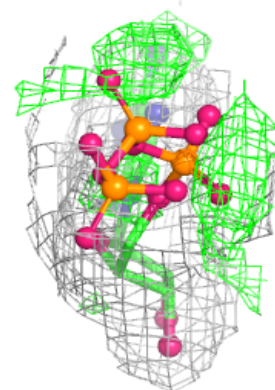
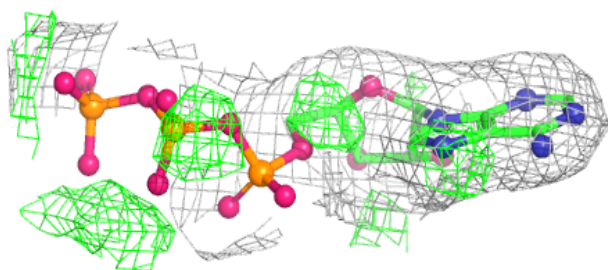
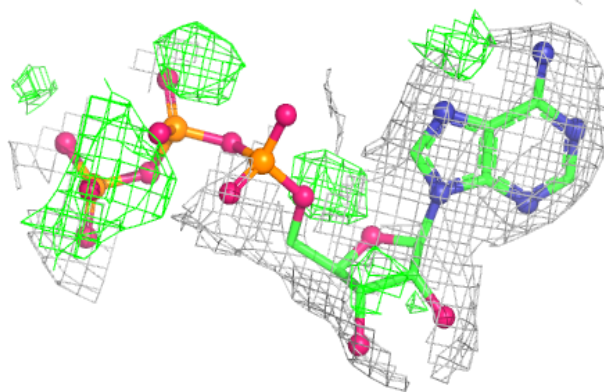
**Electron density around ATP B 1402:**

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

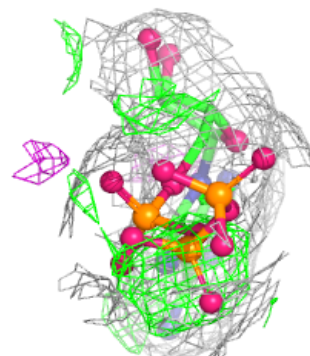
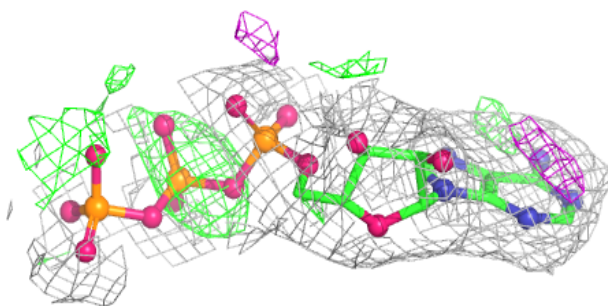
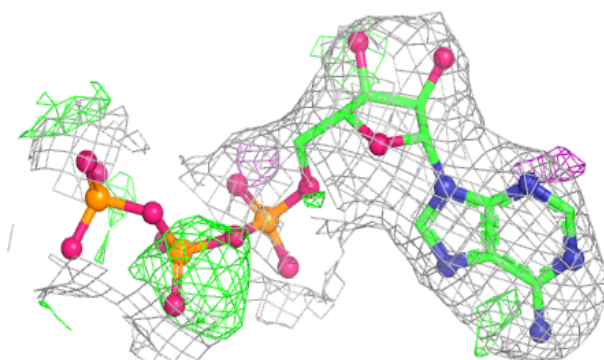


Electron density around ATP C 1401:

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

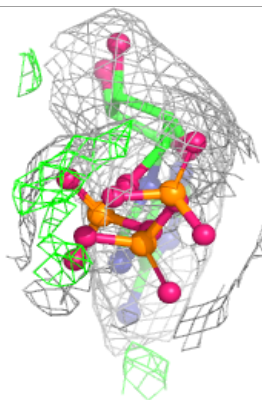
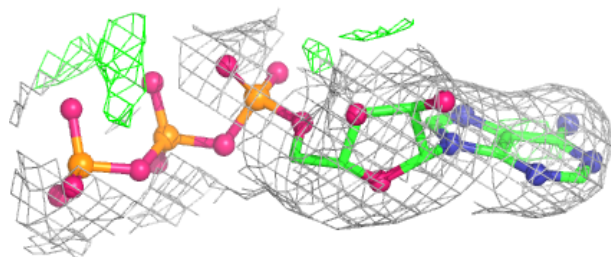
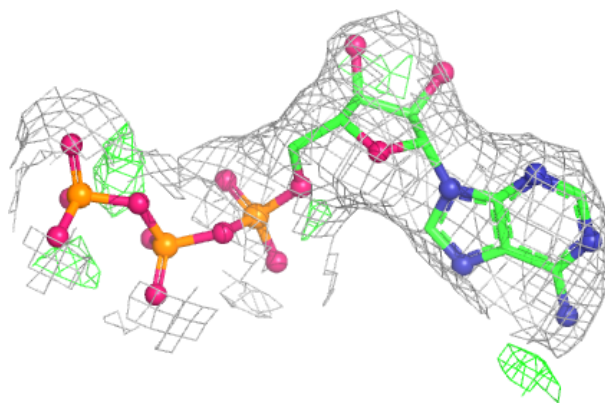
**Electron density around ATP B 1401:**

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

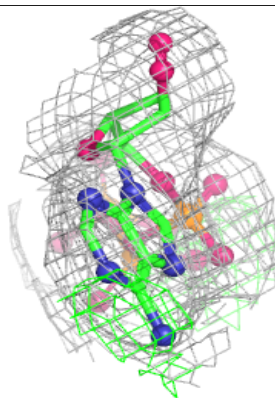
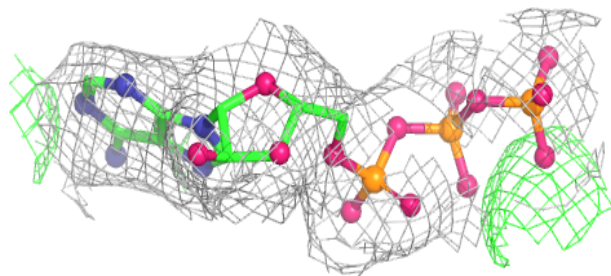
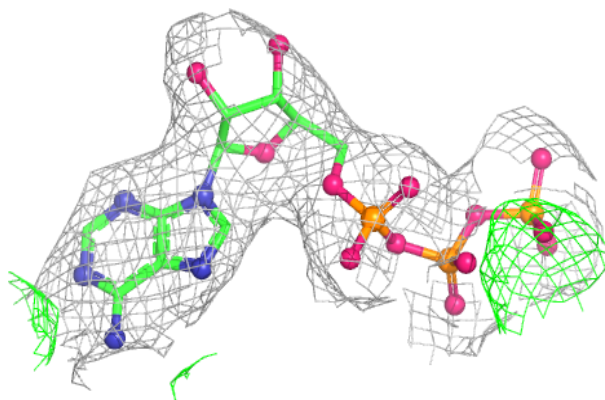


Electron density around ATP A 1401:

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

**Electron density around ATP A 1402:**

$2mF_o-DF_c$ (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.