



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 11:45 PM UTC

PDB ID : 3WV9 / pdb_00003wv9
Title : Guanylylpyridinol (GP)- and ATP-bound HcgE from Methanothermobacter marburgensis
Authors : Fujishiro, T.; Ermler, U.; Shima, S.
Deposited on : 2014-05-16
Resolution : 2.75 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

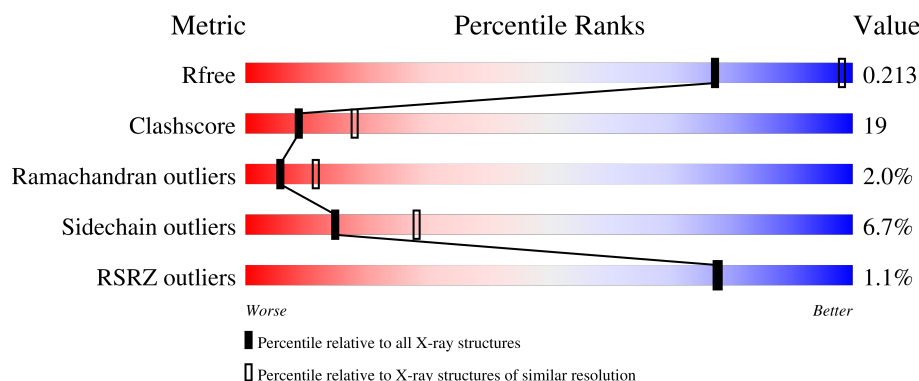
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	218	71% 21% 6%
1	B	218	70% 21% 6%
1	C	218	3% 54% 30% 7% 6%
1	D	218	52% 30% 8% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6515 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 Hmd co-occurring protein HcgE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1555	981	270	298	6			
1	B	205	Total	C	N	O	S	0	0	0
			1555	981	270	298	6			
1	C	205	Total	C	N	O	S	0	0	0
			1555	981	270	298	6			
1	D	205	Total	C	N	O	S	0	0	0
			1555	981	270	298	6			

There are 24 discrepancies between the modelled and reference sequences:

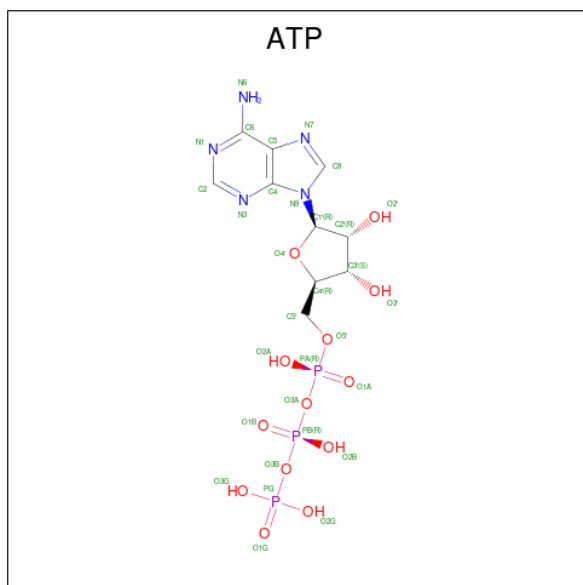
Chain	Residue	Modelled	Actual	Comment	Reference
A	213	LEU	-	expression tag	UNP D9PY12
A	214	GLU	-	expression tag	UNP D9PY12
A	215	LEU	-	expression tag	UNP D9PY12
A	216	VAL	-	expression tag	UNP D9PY12
A	217	PRO	-	expression tag	UNP D9PY12
A	218	ARG	-	expression tag	UNP D9PY12
B	213	LEU	-	expression tag	UNP D9PY12
B	214	GLU	-	expression tag	UNP D9PY12
B	215	LEU	-	expression tag	UNP D9PY12
B	216	VAL	-	expression tag	UNP D9PY12
B	217	PRO	-	expression tag	UNP D9PY12
B	218	ARG	-	expression tag	UNP D9PY12
C	213	LEU	-	expression tag	UNP D9PY12
C	214	GLU	-	expression tag	UNP D9PY12
C	215	LEU	-	expression tag	UNP D9PY12
C	216	VAL	-	expression tag	UNP D9PY12
C	217	PRO	-	expression tag	UNP D9PY12
C	218	ARG	-	expression tag	UNP D9PY12
D	213	LEU	-	expression tag	UNP D9PY12
D	214	GLU	-	expression tag	UNP D9PY12
D	215	LEU	-	expression tag	UNP D9PY12

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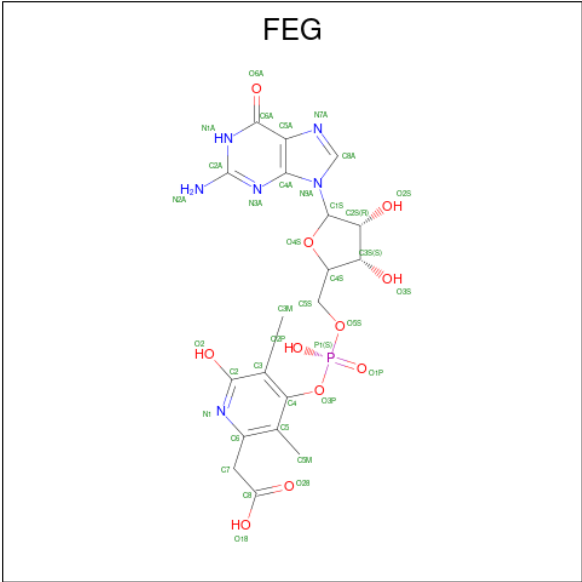
Chain	Residue	Modelled	Actual	Comment	Reference
D	216	VAL	-	expression tag	UNP D9PY12
D	217	PRO	-	expression tag	UNP D9PY12
D	218	ARG	-	expression tag	UNP D9PY12

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



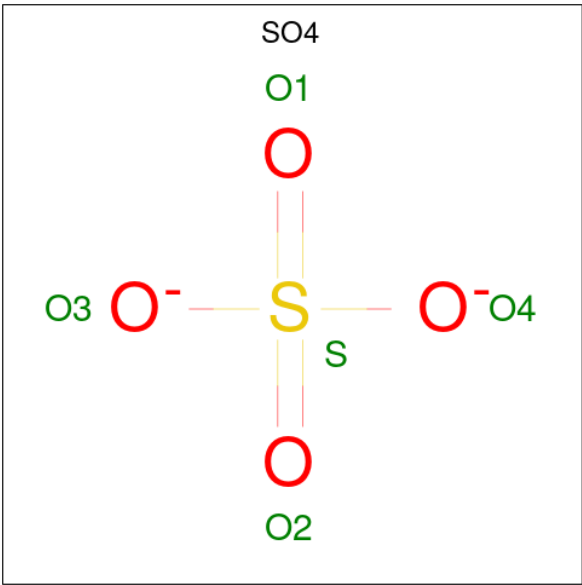
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 5'-O-[(S)-{[2-(carboxymethyl)-6-hydroxy-3,5-dimethylpyridin-4-yl]oxy}(hydroxy)phosphoryl]guanosine (CCD ID: FEG) (formula: $C_{19}H_{23}N_6O_{11}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	19	6	11	1		
3	B	1	Total	C	N	O	P	0	0
			37	19	6	11	1		
3	C	1	Total	C	N	O	P	0	0
			37	19	6	11	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

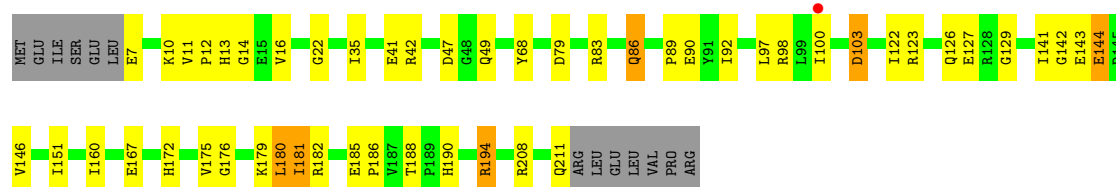
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	5	Total	O	0	0
			5	5		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		

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.

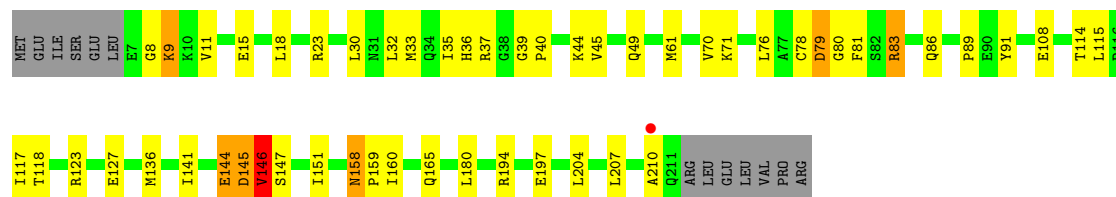
- Molecule 1: Hmd co-occurring protein HcgE

Chain A: 



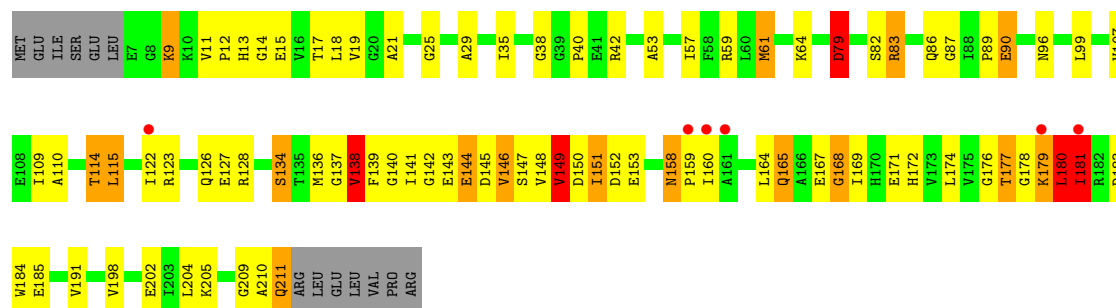
- Molecule 1: Hmd co-occurring protein HcgE

Chain B: 



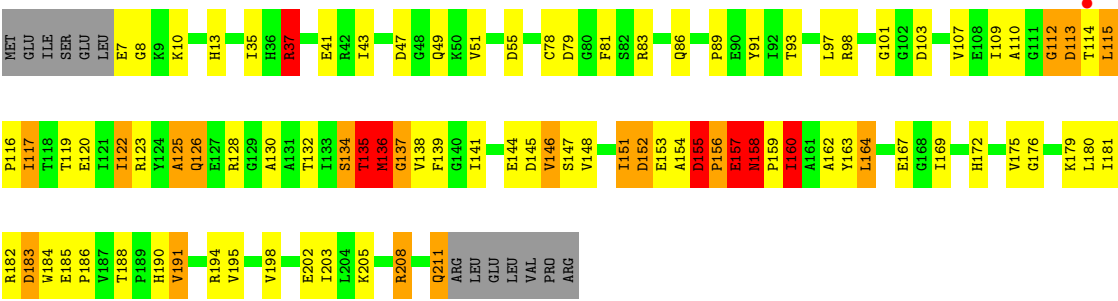
- Molecule 1: Hmd co-occurring protein HcgE

Chain C: 



- Molecule 1: Hmd co-occurring protein HcgE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	85.00Å 85.00Å 120.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.69 – 2.75 46.69 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.69-2.75) 100.0 (46.69-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	70.94 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.165 , 0.214 0.166 , 0.213	Depositor DCC
R_{free} test set	1173 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.108 for -h,-k,l 0.034 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6515	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.94% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FEG, SO4, 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	1.44	5/1578 (0.3%)	1.43	14/2135 (0.7%)
1	B	1.45	4/1578 (0.3%)	1.46	17/2135 (0.8%)
1	C	1.36	6/1578 (0.4%)	1.60	28/2135 (1.3%)
1	D	1.42	5/1578 (0.3%)	1.58	29/2135 (1.4%)
All	All	1.42	20/6312 (0.3%)	1.52	88/8540 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	2
All	All	0	4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	ARG	NE-CZ	10.29	1.44	1.33
1	D	208	ARG	CZ-NH2	9.67	1.46	1.33
1	C	153	GLU	CG-CD	7.08	1.69	1.52
1	C	87	GLY	C-O	-6.88	1.14	1.23
1	C	149	VAL	C-O	-6.70	1.16	1.24
1	C	29	ALA	C-O	6.21	1.31	1.24
1	B	44	LYS	N-CA	-6.13	1.39	1.46
1	B	11	VAL	CA-C	6.04	1.58	1.52
1	B	40	PRO	C-O	-5.99	1.17	1.23
1	B	108	GLU	CA-C	-5.90	1.46	1.53
1	D	208	ARG	CD-NE	5.89	1.54	1.46
1	C	90	GLU	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	VAL	CA-C	-5.78	1.45	1.52
1	C	17	THR	C-O	-5.65	1.17	1.23
1	A	16	VAL	C-O	-5.40	1.18	1.24
1	A	146	VAL	CA-CB	5.31	1.60	1.53
1	A	143	GLU	CD-OE2	5.28	1.35	1.25
1	D	152	ASP	CA-C	5.21	1.60	1.53
1	A	129	GLY	CA-C	5.17	1.58	1.51
1	D	101	GLY	C-O	-5.04	1.17	1.23

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	LEU	N-CA-C	15.57	131.68	113.15
1	D	112	GLY	N-CA-C	-9.54	99.03	111.52
1	B	9	LYS	N-CA-C	9.12	121.71	108.86
1	B	11	VAL	N-CA-C	9.05	116.61	109.19
1	D	208	ARG	NE-CZ-NH2	9.05	127.34	119.20
1	C	153	GLU	CB-CG-CD	8.41	126.90	112.60
1	C	164	LEU	N-CA-C	8.38	120.04	111.07
1	D	137	GLY	N-CA-C	-8.01	94.21	113.18
1	C	142	GLY	N-CA-C	7.59	131.17	113.18
1	B	8	GLY	N-CA-C	-7.55	95.29	113.18
1	D	185	GLU	C-N-CD	-7.51	104.09	120.60
1	B	146	VAL	N-CA-C	7.10	124.11	109.34
1	B	146	VAL	CA-C-N	-7.09	110.59	122.64
1	B	146	VAL	C-N-CA	-7.09	110.59	122.64
1	B	118	THR	N-CA-C	-6.99	103.66	111.28
1	B	144	GLU	CA-C-N	-6.98	112.47	122.94
1	B	144	GLU	C-N-CA	-6.98	112.47	122.94
1	B	158	ASN	CA-C-N	6.70	126.96	119.32
1	B	158	ASN	C-N-CA	6.70	126.96	119.32
1	D	146	VAL	N-CA-C	6.70	118.48	108.23
1	D	183	ASP	N-CA-C	-6.66	100.72	111.04
1	D	79	ASP	N-CA-C	6.65	120.26	111.75
1	C	176	GLY	N-CA-C	6.62	120.28	110.42
1	D	163	TYR	N-CA-C	-6.57	104.90	113.12
1	A	208	ARG	N-CA-C	-6.56	103.62	111.69
1	D	147	SER	N-CA-C	6.53	120.17	109.72
1	C	79	ASP	N-CA-C	6.52	124.68	110.80
1	A	7	GLU	CB-CG-CD	6.43	123.53	112.60
1	D	160	ILE	N-CA-C	-6.38	102.90	111.44
1	A	103	ASP	N-CA-C	-6.37	105.64	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ILE	CA-C-N	-6.36	112.63	122.05
1	C	151	ILE	C-N-CA	-6.36	112.63	122.05
1	B	145	ASP	N-CA-C	6.33	119.71	109.40
1	D	125	ALA	N-CA-C	6.25	117.90	111.14
1	C	153	GLU	N-CA-C	-6.25	104.92	113.30
1	D	157	GLU	N-CA-C	6.14	123.88	110.80
1	C	138	VAL	N-CA-C	6.13	118.00	112.17
1	C	14	GLY	CA-C-O	-6.10	118.26	122.22
1	A	79	ASP	N-CA-C	6.09	119.55	111.75
1	A	180	LEU	N-CA-C	6.06	117.78	109.18
1	D	208	ARG	N-CA-C	-6.02	104.29	111.69
1	A	49	GLN	N-CA-C	6.01	119.45	110.14
1	D	126	GLN	N-CA-CB	5.96	120.12	110.40
1	D	208	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	C	18	LEU	CA-C-N	-5.94	115.30	122.90
1	C	18	LEU	C-N-CA	-5.94	115.30	122.90
1	B	15	GLU	N-CA-C	5.92	118.59	109.07
1	C	165	GLN	N-CA-CB	5.88	119.39	110.28
1	D	195	VAL	CB-CA-C	-5.88	104.34	112.04
1	D	113	ASP	CA-C-N	-5.85	112.08	123.13
1	D	113	ASP	C-N-CA	-5.85	112.08	123.13
1	D	155	ASP	CA-C-N	-5.84	112.54	119.84
1	D	155	ASP	C-N-CA	-5.84	112.54	119.84
1	D	135	THR	N-CA-C	5.78	118.67	109.65
1	D	155	ASP	N-CA-C	5.70	122.41	109.81
1	C	96	ASN	N-CA-C	5.65	119.36	111.56
1	C	145	ASP	N-CA-C	5.64	118.17	110.55
1	D	107	VAL	N-CA-C	5.62	116.19	107.99
1	C	140	GLY	N-CA-C	5.53	119.19	111.00
1	D	103	ASP	N-CA-C	-5.53	106.66	113.41
1	B	71	LYS	CD-CE-NZ	-5.49	94.34	111.90
1	B	78	CYS	CA-C-O	-5.47	116.27	122.01
1	C	38	GLY	N-CA-C	5.41	117.22	110.29
1	D	138	VAL	N-CA-C	-5.38	107.48	112.43
1	A	194	ARG	CG-CD-NE	5.37	123.82	112.00
1	A	181	ILE	CA-C-N	5.37	127.73	120.38
1	A	181	ILE	C-N-CA	5.37	127.73	120.38
1	C	83	ARG	CB-CG-CD	-5.36	98.97	111.30
1	C	184	TRP	CA-C-N	5.35	127.92	120.65
1	C	184	TRP	C-N-CA	5.35	127.92	120.65
1	B	147	SER	N-CA-C	5.32	118.73	110.17
1	A	188	THR	CA-C-N	-5.27	113.60	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	THR	C-N-CA	-5.27	113.60	119.19
1	D	117	ILE	N-CA-C	5.25	115.98	110.62
1	A	190	HIS	CA-C-O	5.23	125.97	120.42
1	D	8	GLY	N-CA-C	-5.22	103.51	111.14
1	C	114	THR	N-CA-C	5.19	119.77	113.38
1	C	168	GLY	N-CA-C	5.19	125.48	113.18
1	D	37	ARG	CB-CG-CD	5.13	123.10	111.30
1	C	158	ASN	O-C-N	5.13	126.41	121.28
1	A	22	GLY	N-CA-C	-5.12	103.87	112.77
1	C	115	LEU	N-CA-C	5.12	121.12	109.81
1	C	169	ILE	N-CA-C	5.09	116.61	108.87
1	C	181	ILE	CG1-CB-CG2	-5.07	95.48	110.70
1	C	185	GLU	CB-CA-C	5.07	117.58	109.62
1	A	68	TYR	N-CA-C	-5.05	102.39	109.96
1	D	122	ILE	N-CA-C	-5.02	105.50	110.62
1	B	197	GLU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	152	ASP	Peptide
1	C	179	LYS	Peptide
1	D	135	THR	Peptide
1	D	136	MET	Peptide

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	1555	0	1577	35	0
1	B	1555	0	1577	35	0
1	C	1555	0	1577	97	0
1	D	1555	0	1577	87	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
2	C	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	12	2	0
3	A	37	0	21	7	0
3	B	37	0	21	1	0
3	C	37	0	21	10	0
4	A	15	0	0	1	0
4	B	5	0	0	0	0
4	C	20	0	0	0	0
4	D	5	0	0	0	0
5	A	3	0	0	0	0
5	B	5	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	6515	0	6419	241	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 19.

All (241) 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:D:158:ASN:CB	1:D:159:PRO:HA	1.66	1.20
1:D:158:ASN:HB2	1:D:159:PRO:CA	1.75	1.16
1:A:86:GLN:HG2	1:C:86:GLN:HG2	1.34	1.02
1:C:139:PHE:HB2	1:C:180:LEU:HB2	1.43	0.97
1:A:92:ILE:HD12	1:A:100:ILE:HD11	1.48	0.95
1:C:178:GLY:HA2	1:C:180:LEU:HD11	1.49	0.95
1:C:178:GLY:CA	1:C:180:LEU:HD11	1.99	0.92
1:C:158:ASN:HB2	1:C:179:LYS:HD2	1.50	0.92
1:D:141:ILE:HD12	1:D:184:TRP:HH2	1.35	0.92
1:C:180:LEU:HD12	1:C:180:LEU:H	1.34	0.91
1:C:159:PRO:HG2	3:C:303:FEG:C6A	2.00	0.91
1:A:98:ARG:NH2	1:C:90:GLU:HG2	1.86	0.90
1:D:158:ASN:HB3	1:D:162:ALA:HB2	1.52	0.89
1:A:180:LEU:HD22	3:A:302:FEG:C8A	2.05	0.87
1:C:165:GLN:HG3	1:C:168:GLY:HA2	1.57	0.87
1:D:151:ILE:HG21	1:D:164:LEU:HD22	1.58	0.86
1:D:151:ILE:HD13	1:D:164:LEU:CD2	2.05	0.84
1:D:141:ILE:HD12	1:D:184:TRP:CH2	2.12	0.84
1:B:123:ARG:O	1:B:127:GLU:HG3	1.77	0.83
1:C:158:ASN:HD22	1:C:179:LYS:CD	1.92	0.82
1:D:122:ILE:HG22	1:D:126:GLN:HE22	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:OG1	1:C:178:GLY:HA3	1.81	0.81
1:C:15:GLU:HB2	1:C:42:ARG:HH11	1.45	0.79
1:A:86:GLN:CG	1:C:86:GLN:HG2	2.12	0.79
1:C:158:ASN:ND2	1:C:179:LYS:CD	2.46	0.78
1:D:136:MET:HB3	1:D:160:ILE:CD1	2.14	0.78
1:A:41:GLU:HG2	1:C:79:ASP:OD1	1.84	0.78
1:C:158:ASN:ND2	1:C:179:LYS:HD3	2.00	0.77
1:D:139:PHE:HB2	1:D:179:LYS:HB2	1.65	0.77
1:D:158:ASN:HB2	1:D:159:PRO:HA	0.81	0.76
1:C:180:LEU:HD12	1:C:180:LEU:N	2.01	0.75
1:D:159:PRO:HD2	1:D:180:LEU:HD21	1.67	0.74
1:C:177:THR:CB	1:C:178:GLY:HA3	2.18	0.74
1:C:123:ARG:HH22	1:C:167:GLU:HB3	1.54	0.73
1:A:180:LEU:HD22	3:A:302:FEG:N7A	2.04	0.73
1:D:154:ALA:O	1:D:156:PRO:HD3	1.88	0.73
1:D:134:SER:HB3	1:D:172:HIS:HE2	1.53	0.73
1:D:122:ILE:HG23	1:D:132:THR:HG21	1.71	0.72
1:A:180:LEU:HD22	3:A:302:FEG:H8A	1.71	0.71
1:D:115:LEU:HG	1:D:160:ILE:HG23	1.72	0.70
1:B:45:VAL:HG23	1:B:70:VAL:HB	1.74	0.70
1:C:139:PHE:HB2	1:C:180:LEU:CB	2.21	0.69
1:D:180:LEU:HG	1:D:181:ILE:HD12	1.75	0.69
1:D:158:ASN:CB	1:D:162:ALA:HB2	2.24	0.68
1:D:148:VAL:HG22	1:D:175:VAL:HG22	1.76	0.68
1:C:158:ASN:CB	1:C:179:LYS:HD2	2.21	0.68
1:D:151:ILE:HD11	1:D:172:HIS:HB3	1.75	0.68
1:C:11:VAL:HG13	1:C:12:PRO:HD2	1.76	0.67
1:D:202:GLU:HA	1:D:205:LYS:HE3	1.76	0.67
1:A:11:VAL:HG12	1:A:12:PRO:O	1.94	0.66
1:B:35:ILE:HB	1:B:83:ARG:HH22	1.59	0.66
1:C:160:ILE:HD11	3:C:303:FEG:H8A	1.76	0.66
1:C:158:ASN:ND2	1:C:179:LYS:HD2	2.10	0.66
1:C:139:PHE:CE1	1:C:181:ILE:HG13	2.30	0.66
1:D:132:THR:HG22	1:D:172:HIS:ND1	2.11	0.66
1:D:109:ILE:HD12	1:D:114:THR:HB	1.78	0.65
1:B:146:VAL:HG23	1:B:146:VAL:O	1.96	0.65
1:A:35:ILE:O	1:A:83:ARG:NH2	2.29	0.65
1:D:155:ASP:OD1	1:D:155:ASP:N	2.24	0.65
1:C:15:GLU:HG3	1:C:42:ARG:HB2	1.79	0.64
1:C:137:GLY:HA3	1:C:178:GLY:O	1.97	0.64
1:D:167:GLU:O	1:D:167:GLU:HG3	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:SER:OG	1:D:135:THR:N	2.29	0.64
1:B:145:ASP:OD1	1:B:146:VAL:HG13	1.98	0.64
1:D:157:GLU:C	1:D:158:ASN:HD22	2.06	0.64
1:A:86:GLN:HG2	1:C:86:GLN:CG	2.19	0.64
1:C:141:ILE:N	1:C:144:GLU:OE2	2.30	0.64
1:D:180:LEU:H	1:D:183:ASP:HB2	1.63	0.63
1:D:141:ILE:HB	1:D:184:TRP:CZ3	2.32	0.63
1:C:146:VAL:HG11	1:C:198:VAL:HG21	1.81	0.62
1:A:160:ILE:HD11	3:A:302:FEG:H8A	1.81	0.62
1:A:97:LEU:HA	1:A:100:ILE:HD13	1.80	0.61
1:B:89:PRO:O	1:D:98:ARG:HD2	1.99	0.61
1:D:208:ARG:O	1:D:211:GLN:HG3	2.00	0.61
1:B:86:GLN:HG2	1:D:86:GLN:HG2	1.82	0.61
1:D:159:PRO:HD2	1:D:180:LEU:CD2	2.31	0.61
1:A:92:ILE:HD12	1:A:100:ILE:CD1	2.26	0.61
1:C:35:ILE:O	1:C:83:ARG:NH2	2.34	0.61
1:D:134:SER:HB3	1:D:172:HIS:NE2	2.16	0.61
1:C:158:ASN:HD22	1:C:179:LYS:HD2	1.64	0.60
1:C:128:ARG:HG3	1:C:128:ARG:HH11	1.66	0.60
1:C:149:VAL:CG2	1:C:174:LEU:HB2	2.32	0.60
1:D:151:ILE:HD13	1:D:164:LEU:HD23	1.82	0.59
1:A:180:LEU:HB3	3:A:302:FEG:N7A	2.18	0.59
1:C:158:ASN:HD22	1:C:179:LYS:HD3	1.62	0.59
1:C:179:LYS:N	1:C:180:LEU:HD12	2.17	0.59
1:D:156:PRO:O	1:D:157:GLU:HB2	2.03	0.59
1:A:144:GLU:CD	1:A:144:GLU:H	2.11	0.58
1:D:78:CYS:O	1:D:81:PHE:HB2	2.03	0.58
1:C:149:VAL:HG22	1:C:174:LEU:HB2	1.84	0.58
1:C:177:THR:CB	1:C:178:GLY:CA	2.81	0.58
1:D:135:THR:OG1	1:D:136:MET:N	2.35	0.58
1:C:57:ILE:O	1:C:61:MET:HG2	2.03	0.58
1:C:109:ILE:HD12	1:C:114:THR:HB	1.86	0.58
1:C:148:VAL:HG11	1:C:202:GLU:OE2	2.05	0.57
1:D:132:THR:HG22	1:D:172:HIS:CE1	2.40	0.57
1:D:49:GLN:HG3	1:D:91:TYR:OH	2.05	0.56
1:D:110:ALA:HB3	2:D:301:ATP:H5'1	1.87	0.56
1:C:144:GLU:CD	1:C:144:GLU:H	2.13	0.56
1:D:35:ILE:O	1:D:83:ARG:NH2	2.30	0.56
1:B:32:LEU:O	1:B:83:ARG:NH2	2.38	0.56
1:D:151:ILE:HD13	1:D:164:LEU:HD21	1.87	0.56
1:A:90:GLU:OE2	1:C:99:LEU:HD21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:HA2	1:A:103:ASP:OD2	2.06	0.55
1:D:158:ASN:CB	1:D:162:ALA:CB	2.84	0.55
1:C:165:GLN:C	1:C:168:GLY:H	2.15	0.55
1:B:141:ILE:N	1:B:144:GLU:OE2	2.30	0.55
1:D:153:GLU:H	1:D:154:ALA:HA	1.72	0.55
1:A:42:ARG:HH22	1:C:79:ASP:CG	2.15	0.55
1:B:79:ASP:OD2	1:D:13:HIS:HD2	1.89	0.54
1:C:11:VAL:CG1	1:C:12:PRO:HD2	2.37	0.54
1:B:146:VAL:HG13	1:B:194:ARG:HH21	1.73	0.54
1:C:141:ILE:O	1:C:191:VAL:CG2	2.56	0.54
1:B:151:ILE:HD11	1:B:165:GLN:HG3	1.90	0.53
1:C:179:LYS:N	1:C:180:LEU:CD1	2.72	0.53
1:D:198:VAL:O	1:D:202:GLU:HG2	2.08	0.53
1:D:109:ILE:CD1	1:D:114:THR:HB	2.38	0.53
1:D:93:THR:HA	1:D:117:ILE:HD11	1.90	0.53
1:D:153:GLU:N	1:D:154:ALA:HA	2.24	0.53
1:C:115:LEU:HD11	3:C:303:FEG:H23	1.91	0.52
1:D:179:LYS:HD2	1:D:184:TRP:HB3	1.91	0.52
1:D:159:PRO:CD	1:D:180:LEU:HD21	2.38	0.52
1:D:112:GLY:O	1:D:114:THR:N	2.43	0.52
1:C:61:MET:HA	1:C:61:MET:HE2	1.92	0.52
1:D:91:TYR:HB3	2:D:301:ATP:N6	2.25	0.51
1:C:21:ALA:HA	1:C:25:GLY:HA3	1.91	0.51
1:C:160:ILE:CD1	3:C:303:FEG:H8A	2.39	0.51
1:D:188:THR:OG1	1:D:191:VAL:HG13	2.10	0.51
1:D:119:THR:HG23	1:D:169:ILE:CG1	2.40	0.51
1:A:98:ARG:HH22	1:C:90:GLU:HG2	1.73	0.51
1:D:158:ASN:HB3	1:D:162:ALA:CB	2.32	0.51
3:B:302:FEG:H3S	3:B:302:FEG:H3MB	1.93	0.51
1:C:137:GLY:O	1:C:177:THR:N	2.39	0.51
1:B:49:GLN:HG3	1:B:91:TYR:OH	2.10	0.51
1:D:135:THR:HG23	1:D:136:MET:HB2	1.92	0.50
1:C:109:ILE:CD1	1:C:114:THR:HB	2.41	0.50
2:C:302:ATP:H3'	2:C:302:ATP:O2B	2.11	0.50
1:C:19:VAL:HG12	2:C:302:ATP:C2	2.47	0.50
1:C:123:ARG:NH2	1:C:167:GLU:HB3	2.23	0.50
1:B:33:MET:HE1	1:B:76:LEU:HB2	1.94	0.50
1:D:139:PHE:CD1	1:D:179:LYS:O	2.64	0.49
1:B:145:ASP:HA	1:B:194:ARG:HH22	1.78	0.49
1:C:9:LYS:O	1:C:9:LYS:HG2	2.12	0.49
1:C:122:ILE:O	1:C:126:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PHE:HD1	1:D:179:LYS:O	1.96	0.49
1:A:98:ARG:HD2	1:C:89:PRO:O	2.13	0.49
1:C:15:GLU:HB2	1:C:42:ARG:HD2	1.95	0.49
1:D:119:THR:HG21	1:D:167:GLU:HG2	1.95	0.49
1:A:97:LEU:HA	1:A:100:ILE:CD1	2.44	0.48
2:A:301:ATP:H3'	2:A:301:ATP:O3A	2.12	0.48
1:C:138:VAL:HG23	1:C:138:VAL:O	2.14	0.48
1:B:30:LEU:HD11	1:B:61:MET:HE3	1.94	0.48
1:B:145:ASP:OD1	1:B:146:VAL:N	2.46	0.48
1:A:122:ILE:O	1:A:126:GLN:HG3	2.14	0.48
1:B:115:LEU:HD21	1:B:160:ILE:HG12	1.96	0.48
1:D:158:ASN:HB2	1:D:162:ALA:HB3	1.95	0.48
1:C:158:ASN:CG	1:C:179:LYS:HD2	2.38	0.48
1:D:152:ASP:O	1:D:153:GLU:HG3	2.14	0.48
1:A:175:VAL:HG12	1:A:176:GLY:N	2.29	0.48
1:C:136:MET:CG	1:C:136:MET:O	2.62	0.48
1:A:42:ARG:NH2	1:C:79:ASP:OD1	2.47	0.48
1:C:110:ALA:CB	3:C:303:FEG:C5	2.92	0.48
1:C:110:ALA:HB3	2:C:302:ATP:H5'1	1.95	0.47
1:D:115:LEU:HB2	1:D:116:PRO:HD3	1.95	0.47
1:C:159:PRO:HG2	3:C:303:FEG:C5A	2.43	0.47
1:A:181:ILE:HD11	3:A:302:FEG:H2S	1.97	0.47
1:C:40:PRO:O	1:C:83:ARG:HD3	2.15	0.47
1:D:151:ILE:O	1:D:152:ASP:HB2	2.14	0.47
1:C:178:GLY:CA	1:C:180:LEU:CD1	2.82	0.47
1:D:151:ILE:CG2	1:D:164:LEU:HD22	2.39	0.47
1:C:180:LEU:H	1:C:180:LEU:CD1	2.17	0.47
1:C:35:ILE:HB	1:C:83:ARG:HH22	1.80	0.47
1:C:136:MET:HE3	1:C:147:SER:HB2	1.97	0.47
1:B:30:LEU:CD1	1:B:61:MET:HE3	2.46	0.46
1:C:53:ALA:O	1:C:59:ARG:NH1	2.45	0.46
1:C:134:SER:OG	1:C:172:HIS:NE2	2.47	0.46
1:B:79:ASP:OD2	1:D:13:HIS:CD2	2.68	0.46
1:C:178:GLY:C	1:C:180:LEU:CD1	2.89	0.46
1:D:137:GLY:O	1:D:176:GLY:HA3	2.15	0.46
1:D:182:ARG:HG3	1:D:182:ARG:O	2.16	0.46
1:C:110:ALA:HB1	3:C:303:FEG:C5	2.45	0.46
1:D:51:VAL:HG13	1:D:55:ASP:HB2	1.98	0.45
1:D:151:ILE:CD1	1:D:164:LEU:CD2	2.87	0.45
1:D:158:ASN:HB2	1:D:162:ALA:CB	2.47	0.45
1:C:136:MET:O	1:C:136:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:OD1	1:D:41:GLU:HG2	2.17	0.45
1:B:114:THR:O	1:B:117:ILE:HG22	2.16	0.45
1:B:79:ASP:C	1:B:81:PHE:H	2.25	0.45
1:D:47:ASP:O	1:D:89:PRO:HA	2.17	0.45
1:A:47:ASP:O	1:A:89:PRO:HA	2.17	0.45
1:A:142:GLY:N	1:A:144:GLU:OE2	2.40	0.45
1:C:110:ALA:HB1	3:C:303:FEG:C6	2.47	0.44
1:B:36:HIS:ND1	1:B:37:ARG:N	2.66	0.44
1:C:110:ALA:HB2	3:C:303:FEG:C4	2.48	0.44
1:C:11:VAL:HG12	1:C:12:PRO:O	2.18	0.44
1:C:149:VAL:HG23	1:C:150:ASP:N	2.33	0.44
1:D:119:THR:HG23	1:D:169:ILE:HG13	1.99	0.44
1:D:10:LYS:HE3	1:D:37:ARG:O	2.17	0.44
1:A:123:ARG:NH2	1:A:167:GLU:O	2.50	0.44
1:C:19:VAL:HB	1:C:107:VAL:HG22	1.98	0.44
1:C:138:VAL:HG21	3:C:303:FEG:H3M	1.99	0.44
1:B:136:MET:HA	1:B:160:ILE:HD13	2.00	0.43
1:D:115:LEU:H	1:D:116:PRO:CD	2.30	0.43
1:D:190:HIS:CE1	1:D:194:ARG:HD2	2.53	0.43
1:C:143:GLU:O	1:C:144:GLU:C	2.60	0.43
1:D:157:GLU:O	1:D:158:ASN:ND2	2.40	0.43
1:A:13:HIS:HB3	4:A:305:SO4:O4	2.18	0.43
1:A:141:ILE:HG22	1:A:186:PRO:HD2	1.99	0.43
1:B:146:VAL:O	1:B:146:VAL:CG2	2.63	0.43
1:A:182:ARG:HG2	3:A:302:FEG:O6A	2.18	0.43
1:D:180:LEU:HG	1:D:181:ILE:H	1.82	0.43
1:C:136:MET:O	1:C:178:GLY:O	2.37	0.43
1:C:178:GLY:HA3	1:C:180:LEU:HD11	1.95	0.43
1:D:136:MET:HB3	1:D:160:ILE:HD12	2.00	0.43
1:D:125:ALA:HB1	1:D:130:ALA:HB3	2.00	0.43
1:B:79:ASP:O	1:B:81:PHE:N	2.52	0.42
1:D:151:ILE:CD1	1:D:164:LEU:HD21	2.48	0.42
1:C:13:HIS:O	1:C:40:PRO:HA	2.20	0.42
1:A:151:ILE:HB	1:A:172:HIS:HB3	2.02	0.42
1:B:35:ILE:HD13	1:B:204:LEU:HD21	2.01	0.42
1:A:179:LYS:HD2	1:A:185:GLU:CD	2.45	0.42
1:C:15:GLU:CB	1:C:42:ARG:HH11	2.24	0.42
1:D:146:VAL:O	1:D:146:VAL:HG13	2.19	0.42
1:B:23:ARG:NH1	2:B:301:ATP:O2B	2.53	0.42
1:B:144:GLU:H	1:B:144:GLU:CD	2.25	0.42
1:C:115:LEU:HA	1:C:115:LEU:HD23	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HG3	1:C:128:ARG:NH1	2.32	0.42
1:D:119:THR:HG23	1:D:169:ILE:HG12	2.02	0.42
1:C:35:ILE:HD13	1:C:204:LEU:HD21	2.02	0.41
1:B:158:ASN:HA	1:B:159:PRO:HD3	1.82	0.41
1:C:178:GLY:C	1:C:180:LEU:HD12	2.45	0.41
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.55	0.41
1:B:39:GLY:HA3	1:B:83:ARG:HH12	1.84	0.41
1:C:177:THR:HB	1:C:178:GLY:CA	2.51	0.41
1:D:135:THR:HG23	1:D:136:MET:CB	2.50	0.41
1:B:207:LEU:O	1:B:210:ALA:HB3	2.21	0.41
1:C:158:ASN:HA	1:C:159:PRO:HD3	2.00	0.41
1:B:18:LEU:HD12	1:B:45:VAL:HG12	2.03	0.41
1:C:209:GLY:C	1:C:211:GLN:H	2.29	0.40
1:D:169:ILE:HD13	1:D:169:ILE:HA	1.94	0.40
1:A:86:GLN:CD	1:C:86:GLN:HG2	2.46	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	203/218 (93%)	191 (94%)	12 (6%)	0	100	100
1	B	203/218 (93%)	189 (93%)	11 (5%)	3 (2%)	8	15
1	C	203/218 (93%)	185 (91%)	14 (7%)	4 (2%)	6	11
1	D	203/218 (93%)	181 (89%)	13 (6%)	9 (4%)	2	2
All	All	812/872 (93%)	746 (92%)	50 (6%)	16 (2%)	6	11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	VAL
1	C	79	ASP
1	D	113	ASP
1	D	136	MET
1	D	155	ASP
1	D	158	ASN
1	D	186	PRO
1	C	149	VAL
1	C	151	ILE
1	D	144	GLU
1	B	79	ASP
1	D	156	PRO
1	C	210	ALA
1	D	157	GLU
1	B	80	GLY
1	D	115	LEU

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	165/178 (93%)	159 (96%)	6 (4%)	31	55
1	B	165/178 (93%)	161 (98%)	4 (2%)	43	65
1	C	165/178 (93%)	149 (90%)	16 (10%)	8	15
1	D	165/178 (93%)	147 (89%)	18 (11%)	6	12
All	All	660/712 (93%)	616 (93%)	44 (7%)	15	28

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	86	GLN
1	A	127	GLU
1	A	144	GLU
1	A	194	ARG
1	A	211	GLN

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Mol	Chain	Res	Type
1	B	9	LYS
1	B	83	ARG
1	B	146	VAL
1	B	180	LEU
1	C	9	LYS
1	C	61	MET
1	C	64	LYS
1	C	82	SER
1	C	127	GLU
1	C	134	SER
1	C	138	VAL
1	C	144	GLU
1	C	146	VAL
1	C	171	GLU
1	C	177	THR
1	C	180	LEU
1	C	181	ILE
1	C	183	ASP
1	C	205	LYS
1	C	211	GLN
1	D	7	GLU
1	D	37	ARG
1	D	43	ILE
1	D	97	LEU
1	D	120	GLU
1	D	123	ARG
1	D	128	ARG
1	D	134	SER
1	D	145	ASP
1	D	151	ILE
1	D	155	ASP
1	D	157	GLU
1	D	158	ASN
1	D	160	ILE
1	D	164	LEU
1	D	191	VAL
1	D	203	ILE
1	D	211	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	31	ASN
1	C	49	GLN
1	C	158	ASN
1	D	13	HIS
1	D	86	GLN
1	D	158	ASN

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](#)

16 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	$\# Z > 2$
4	SO4	A	305	-	4,4,4	0.50	0	6,6,6	0.43	0
3	FEG	A	302	-	38,40,40	1.90	8 (21%)	56,61,61	2.28	17 (30%)
2	ATP	A	301	-	32,33,33	1.67	7 (21%)	48,52,52	1.79	9 (18%)
4	SO4	C	305	-	4,4,4	0.74	0	6,6,6	0.75	0
4	SO4	A	304	-	4,4,4	0.57	0	6,6,6	0.39	0
3	FEG	B	302	-	38,40,40	2.10	7 (18%)	56,61,61	2.19	16 (28%)
4	SO4	C	304	-	4,4,4	0.46	0	6,6,6	0.68	0
2	ATP	B	301	-	32,33,33	1.64	6 (18%)	48,52,52	1.96	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	301	-	4,4,4	0.52	0	6,6,6	0.55	0
4	SO4	A	303	-	4,4,4	0.53	0	6,6,6	0.77	0
3	FEG	C	303	-	38,40,40	2.32	8 (21%)	56,61,61	2.38	16 (28%)
4	SO4	C	306	-	4,4,4	0.62	0	6,6,6	0.88	0
4	SO4	D	302	-	4,4,4	0.46	0	6,6,6	0.66	0
4	SO4	B	303	-	4,4,4	0.65	0	6,6,6	0.22	0
2	ATP	C	302	-	32,33,33	1.36	3 (9%)	48,52,52	1.91	13 (27%)
2	ATP	D	301	-	32,33,33	1.54	6 (18%)	48,52,52	1.80	10 (20%)

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	FEG	A	302	-	-	5/19/35/35	0/4/4/4
2	ATP	A	301	-	-	5/22/38/38	0/3/3/3
3	FEG	B	302	-	-	6/19/35/35	0/4/4/4
2	ATP	B	301	-	-	6/22/38/38	0/3/3/3
3	FEG	C	303	-	-	3/19/35/35	0/4/4/4
2	ATP	C	302	-	-	11/22/38/38	0/3/3/3
2	ATP	D	301	-	-	6/22/38/38	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	FEG	C5-C6	9.61	1.48	1.39
3	B	302	FEG	C5-C6	8.87	1.48	1.39
3	A	302	FEG	C5-C6	7.06	1.46	1.39
2	B	301	ATP	C5-C4	5.00	1.48	1.39
3	C	303	FEG	C4-C3	4.78	1.48	1.39
3	C	303	FEG	C4-C5	4.57	1.47	1.39
2	A	301	ATP	C5-C4	4.54	1.47	1.39
2	B	301	ATP	PB-O3B	4.52	1.64	1.59
2	C	302	ATP	C5-C4	4.31	1.46	1.39
2	D	301	ATP	C5-C4	4.21	1.46	1.39
3	B	302	FEG	C4-C3	4.05	1.46	1.39
2	A	301	ATP	PA-O3A	3.83	1.63	1.59
3	B	302	FEG	C4-C5	3.65	1.46	1.39
3	C	303	FEG	C5A-C4A	3.43	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	FEG	O3P-C4	-3.36	1.35	1.40
3	C	303	FEG	C6A-N1A	-3.29	1.32	1.38
2	A	301	ATP	PB-O3B	3.29	1.63	1.59
3	A	302	FEG	C4-C3	3.27	1.45	1.39
2	D	301	ATP	C5-N7	-3.23	1.33	1.39
2	A	301	ATP	C5-N7	-3.19	1.33	1.39
3	A	302	FEG	C4-C5	3.17	1.45	1.39
3	A	302	FEG	C5A-N7A	-3.16	1.32	1.39
2	D	301	ATP	PB-O3B	3.08	1.62	1.59
3	B	302	FEG	C5A-C4A	2.90	1.46	1.38
3	C	303	FEG	C5A-N7A	-2.89	1.33	1.39
2	B	301	ATP	C5-C6	2.81	1.48	1.41
2	C	302	ATP	C5-N7	-2.78	1.34	1.39
2	B	301	ATP	C5-N7	-2.76	1.34	1.39
3	B	302	FEG	C2A-N3A	2.74	1.39	1.33
2	A	301	ATP	C4-N9	-2.69	1.32	1.37
3	A	302	FEG	C2A-N3A	2.69	1.39	1.33
3	B	302	FEG	O3P-C4	-2.67	1.36	1.40
2	D	301	ATP	C4-N9	-2.63	1.32	1.37
2	B	301	ATP	C8-N7	2.51	1.36	1.31
2	A	301	ATP	PB-O3A	2.49	1.62	1.59
2	C	302	ATP	C8-N7	2.47	1.36	1.31
2	D	301	ATP	C5-C6	2.44	1.47	1.41
3	A	302	FEG	C5A-C4A	2.42	1.45	1.38
2	B	301	ATP	C4-N9	-2.34	1.32	1.37
2	D	301	ATP	PA-O3A	2.33	1.62	1.59
3	C	303	FEG	C2A-N1A	-2.31	1.32	1.37
2	A	301	ATP	C5-C6	2.27	1.47	1.41
3	B	302	FEG	C4A-N9A	-2.22	1.32	1.38
3	C	303	FEG	O3P-C4	-2.13	1.37	1.40
3	A	302	FEG	C4A-N3A	2.11	1.39	1.34

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	FEG	C5A-C4A-N3A	-8.45	114.95	128.39
3	A	302	FEG	C5A-C4A-N3A	-7.17	116.99	128.39
3	A	302	FEG	N9A-C4A-N3A	7.00	139.94	125.95
2	B	301	ATP	O4'-C1'-N9	6.56	120.70	108.09
3	C	303	FEG	C2A-N3A-C4A	6.21	122.99	112.30
3	B	302	FEG	C5A-C4A-N3A	-5.87	119.05	128.39
3	C	303	FEG	N9A-C4A-N3A	5.84	137.63	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	FEG	C2A-N3A-C4A	5.75	122.21	112.30
2	B	301	ATP	C5-C4-N3	-5.62	118.97	126.72
3	B	302	FEG	C2A-N3A-C4A	5.51	121.80	112.30
2	A	301	ATP	C5-C4-N3	-5.46	119.20	126.72
2	C	302	ATP	C5-C4-N3	-5.45	119.22	126.72
2	D	301	ATP	C5-C4-N3	-5.37	119.32	126.72
3	A	302	FEG	O6A-C6A-C5A	-5.04	113.22	126.53
2	A	301	ATP	N3-C4-N9	4.95	135.59	127.17
2	C	302	ATP	N3-C4-N9	4.94	135.57	127.17
3	B	302	FEG	N9A-C4A-N3A	4.64	135.24	125.95
3	B	302	FEG	O3P-C4-C3	4.39	123.77	118.08
2	C	302	ATP	N3-C2-N1	-4.37	121.96	128.58
3	C	303	FEG	C2-N1-C6	4.28	126.26	116.42
2	D	301	ATP	N3-C4-N9	4.28	134.45	127.17
3	C	303	FEG	C5-C6-N1	-4.15	119.50	123.84
2	B	301	ATP	N3-C4-N9	4.05	134.06	127.17
2	C	302	ATP	C2-N3-C4	3.99	121.56	111.83
3	B	302	FEG	O6A-C6A-C5A	-3.97	116.05	126.53
2	D	301	ATP	O4'-C1'-N9	3.96	115.70	108.09
3	A	302	FEG	C3S-C2S-C1S	3.91	108.86	101.46
3	C	303	FEG	C5-C4-C3	-3.77	116.28	122.58
3	C	303	FEG	O3P-C4-C3	3.71	122.89	118.08
2	D	301	ATP	C2-N3-C4	3.66	120.77	111.83
2	B	301	ATP	C2-N3-C4	3.63	120.70	111.83
2	A	301	ATP	C2-N3-C4	3.60	120.62	111.83
3	B	302	FEG	C1S-N9A-C4A	-3.58	115.90	126.49
2	C	302	ATP	C4-N9-C8	3.53	109.44	105.74
2	A	301	ATP	N3-C2-N1	-3.52	123.25	128.58
3	B	302	FEG	C2-N1-C6	3.47	124.39	116.42
2	D	301	ATP	N3-C2-N1	-3.45	123.35	128.58
3	A	302	FEG	C2-N1-C6	3.45	124.35	116.42
2	A	301	ATP	C4-N9-C8	3.40	109.31	105.74
2	B	301	ATP	C4-C5-N7	-3.32	106.79	110.58
3	B	302	FEG	C6A-C5A-N7A	3.31	136.31	130.29
3	B	302	FEG	C5A-C6A-N1A	3.23	121.48	113.25
3	A	302	FEG	O6A-C6A-N1A	3.16	126.06	120.11
3	B	302	FEG	C5-C4-C3	-3.03	117.51	122.58
2	B	301	ATP	N3-C2-N1	-3.00	124.05	128.58
2	A	301	ATP	O4'-C1'-N9	2.94	113.74	108.09
3	A	302	FEG	C5A-C6A-N1A	2.93	120.71	113.25
3	C	303	FEG	C6A-C5A-N7A	2.92	135.60	130.29
3	B	302	FEG	C7-C6-N1	2.90	122.48	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	ATP	C4-C5-N7	-2.85	107.32	110.58
3	C	303	FEG	C2A-N1A-C6A	-2.85	119.94	125.11
3	C	303	FEG	C4-C5-C6	2.84	119.80	116.64
3	B	302	FEG	C5-C6-N1	-2.83	120.89	123.84
2	A	301	ATP	C4-C5-N7	-2.82	107.36	110.58
3	B	302	FEG	C1S-N9A-C8A	2.70	134.40	126.73
3	A	302	FEG	C2A-N1A-C6A	-2.69	120.22	125.11
3	B	302	FEG	C2A-N1A-C6A	-2.68	120.25	125.11
3	C	303	FEG	C5A-C6A-N1A	2.62	119.93	113.25
3	C	303	FEG	C3S-C2S-C1S	2.60	106.39	101.46
2	C	302	ATP	N9-C8-N7	-2.58	110.28	113.94
2	C	302	ATP	C4-C5-N7	-2.50	107.73	110.58
3	C	303	FEG	C4A-C5A-N7A	-2.49	106.72	110.67
2	C	302	ATP	C5-N7-C8	2.48	107.35	103.45
2	D	301	ATP	C4-N9-C8	2.45	108.31	105.74
2	A	301	ATP	C5-N7-C8	2.45	107.30	103.45
3	A	302	FEG	C8A-N9A-C4A	2.43	110.58	106.03
3	A	302	FEG	C7-C6-N1	2.36	121.31	116.23
2	C	302	ATP	O4'-C1'-C2'	-2.34	101.60	106.62
3	A	302	FEG	C5-C4-C3	-2.33	118.68	122.58
2	D	301	ATP	C4'-O4'-C1'	-2.27	104.45	109.47
3	A	302	FEG	C5S-C4S-C3S	-2.27	107.05	115.21
2	B	301	ATP	O3A-PA-O1A	-2.25	103.92	110.70
3	B	302	FEG	O2P-P1-O3P	2.25	112.21	104.94
2	B	301	ATP	C6-C5-N7	2.23	136.40	132.09
3	A	302	FEG	N9A-C8A-N7A	-2.23	109.26	113.40
2	D	301	ATP	O3G-PG-O2G	2.20	116.07	107.80
3	A	302	FEG	O3P-C4-C3	2.20	120.94	118.08
3	B	302	FEG	C6A-C5A-C4A	-2.20	115.52	118.83
2	B	301	ATP	C5-N7-C8	2.18	106.87	103.45
2	D	301	ATP	C5-N7-C8	2.18	106.87	103.45
2	A	301	ATP	N9-C8-N7	-2.18	110.85	113.94
3	A	302	FEG	C8A-N7A-C5A	2.17	108.12	104.26
2	C	302	ATP	O3G-PG-O2G	2.16	115.91	107.80
2	B	301	ATP	O2A-PA-O1A	2.13	122.36	112.44
2	B	301	ATP	O4'-C4'-C5'	2.13	116.15	109.33
2	C	302	ATP	C6-C5-N7	2.12	136.19	132.09
3	C	303	FEG	O3P-C4-C5	2.10	120.80	118.08
2	C	302	ATP	C2'-C3'-C4'	2.07	106.62	102.61
3	A	302	FEG	C5-C6-N1	-2.07	121.67	123.84
3	C	303	FEG	C5M-C5-C6	-2.07	120.92	122.70
2	C	302	ATP	C5-C6-N6	-2.04	118.23	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	FEG	O2P-P1-O3P	2.04	111.53	104.94

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	ATP	PB-O3B-PG-O3G
2	C	302	ATP	C5'-O5'-PA-O2A
2	C	302	ATP	C5'-O5'-PA-O3A
2	D	301	ATP	PB-O3A-PA-O5'
2	D	301	ATP	C5'-O5'-PA-O1A
2	D	301	ATP	C5'-O5'-PA-O2A
2	D	301	ATP	C5'-O5'-PA-O3A
3	A	302	FEG	C5S-O5S-P1-O3P
3	A	302	FEG	C5S-O5S-P1-O1P
3	A	302	FEG	C5S-O5S-P1-O2P
3	A	302	FEG	O4S-C4S-C5S-O5S
3	C	303	FEG	C5S-O5S-P1-O1P
3	A	302	FEG	C3S-C4S-C5S-O5S
2	B	301	ATP	O4'-C4'-C5'-O5'
2	B	301	ATP	C3'-C4'-C5'-O5'
2	D	301	ATP	O4'-C4'-C5'-O5'
2	C	302	ATP	C3'-C4'-C5'-O5'
2	C	302	ATP	O4'-C4'-C5'-O5'
3	B	302	FEG	O4S-C4S-C5S-O5S
2	D	301	ATP	C3'-C4'-C5'-O5'
3	B	302	FEG	C3S-C4S-C5S-O5S
2	A	301	ATP	O4'-C4'-C5'-O5'
2	A	301	ATP	C3'-C4'-C5'-O5'
2	B	301	ATP	PB-O3A-PA-O1A
2	C	302	ATP	PB-O3A-PA-O2A
3	C	303	FEG	N1-C6-C7-C8
2	C	302	ATP	C5'-O5'-PA-O1A
3	B	302	FEG	C5S-O5S-P1-O3P
3	B	302	FEG	C5S-O5S-P1-O1P
3	B	302	FEG	C5S-O5S-P1-O2P
2	B	301	ATP	PB-O3A-PA-O2A
2	C	302	ATP	PB-O3B-PG-O1G
3	B	302	FEG	C3-C4-O3P-P1
3	C	303	FEG	C5-C6-C7-C8
2	C	302	ATP	C2'-C1'-N9-C8
2	C	302	ATP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
2	A	301	ATP	PA-O3A-PB-O2B
2	B	301	ATP	PG-O3B-PB-O1B
2	A	301	ATP	C4'-C5'-O5'-PA
2	A	301	ATP	PB-O3A-PA-O2A
2	B	301	ATP	PG-O3B-PB-O2B
2	C	302	ATP	PB-O3A-PA-O1A

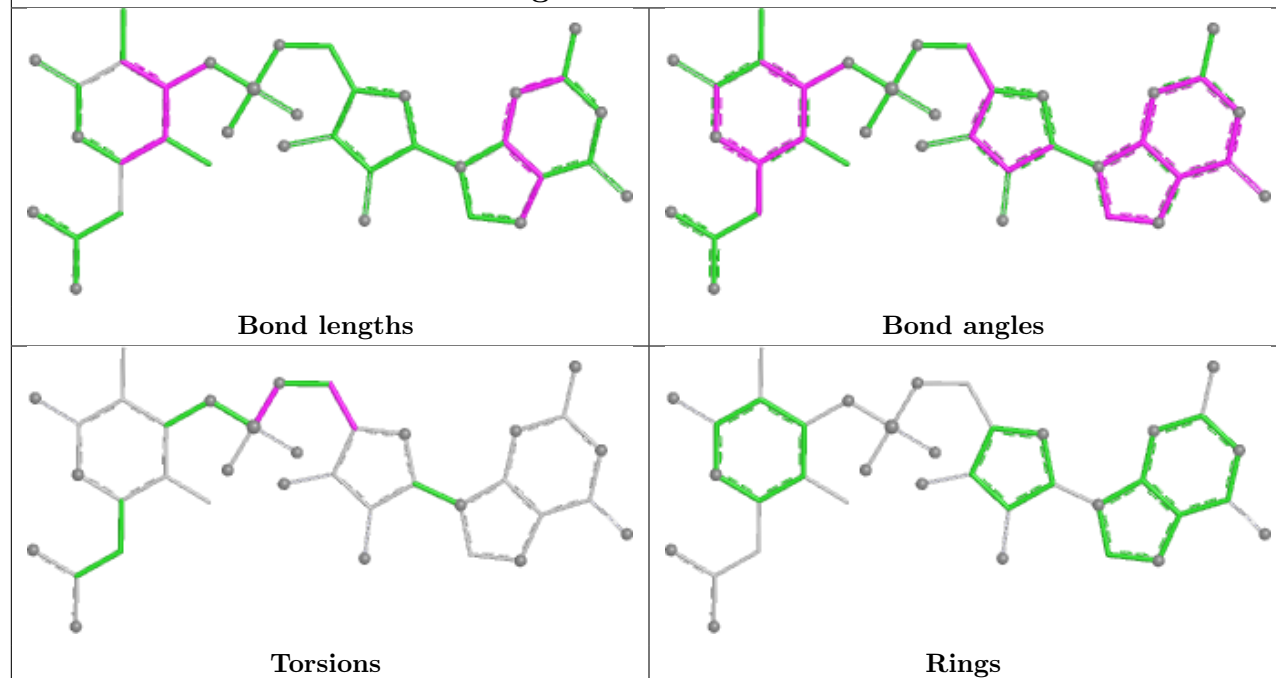
There are no ring outliers.

8 monomers are involved in 26 short contacts:

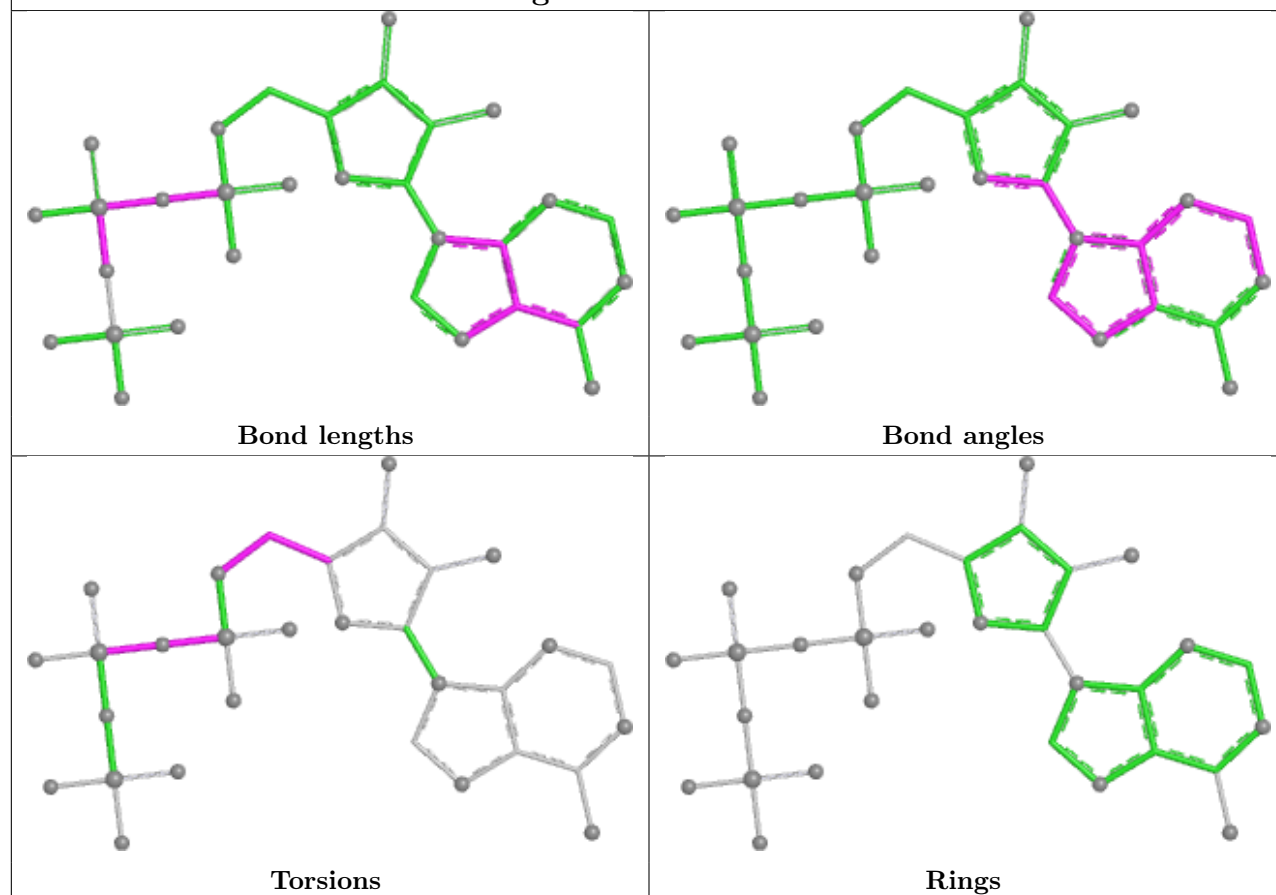
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	SO4	1	0
3	A	302	FEG	7	0
2	A	301	ATP	1	0
3	B	302	FEG	1	0
2	B	301	ATP	1	0
3	C	303	FEG	10	0
2	C	302	ATP	3	0
2	D	301	ATP	2	0

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 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.

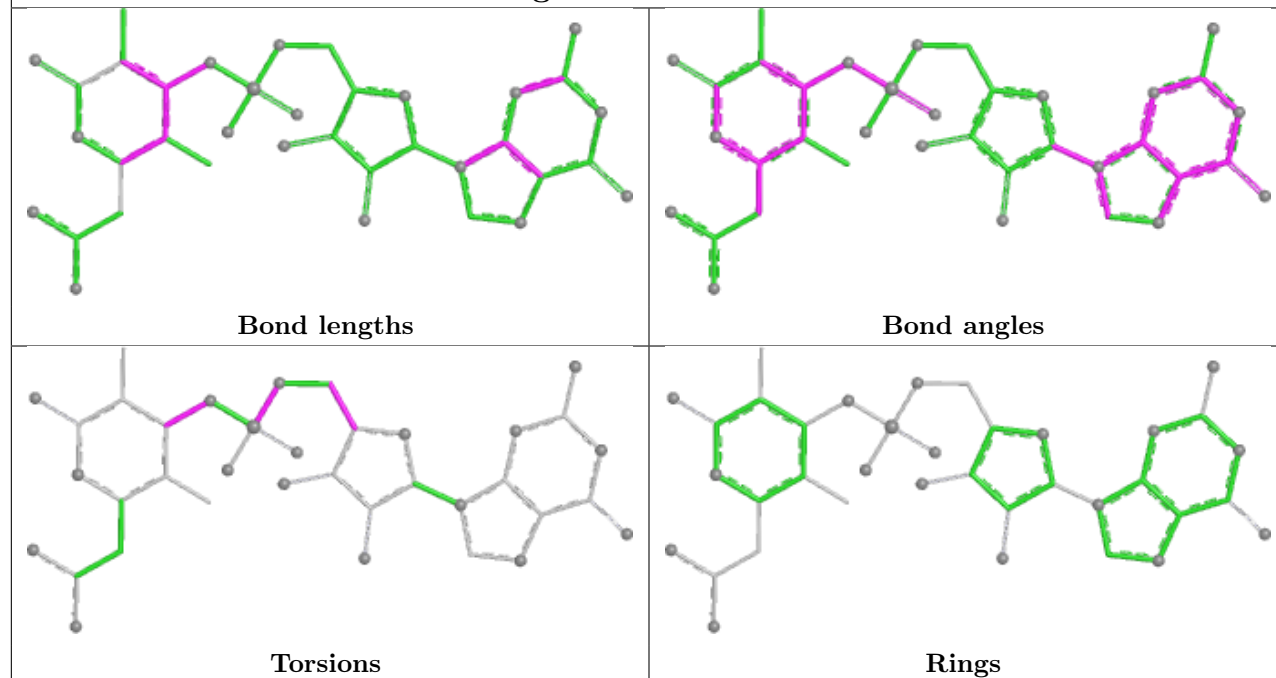
Ligand FEG A 302



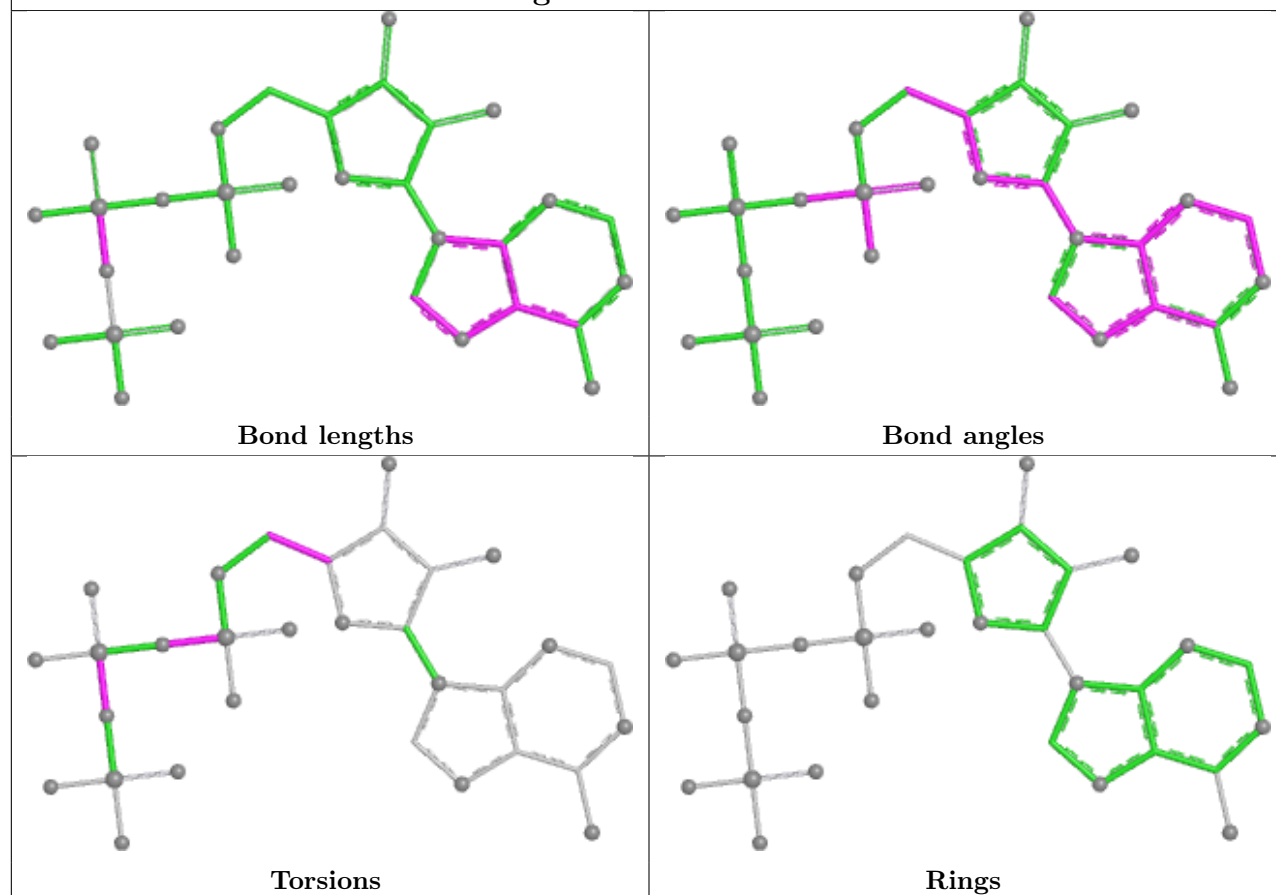
Ligand ATP A 301



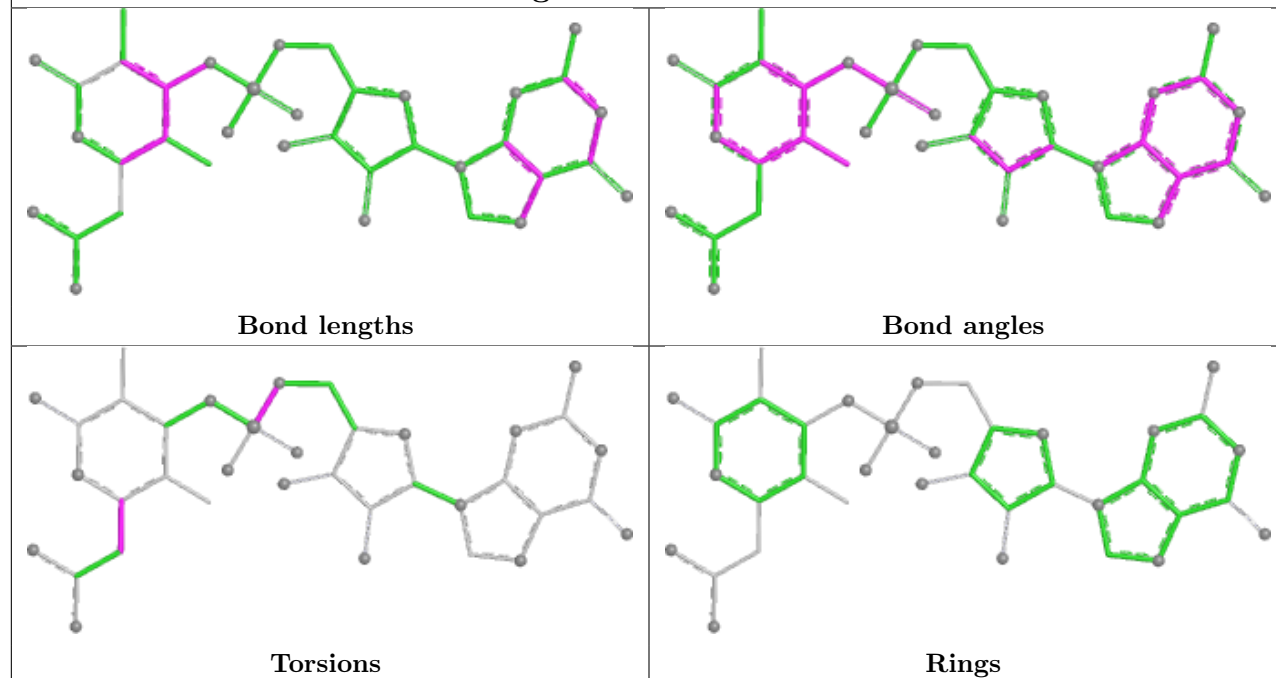
Ligand FEG B 302



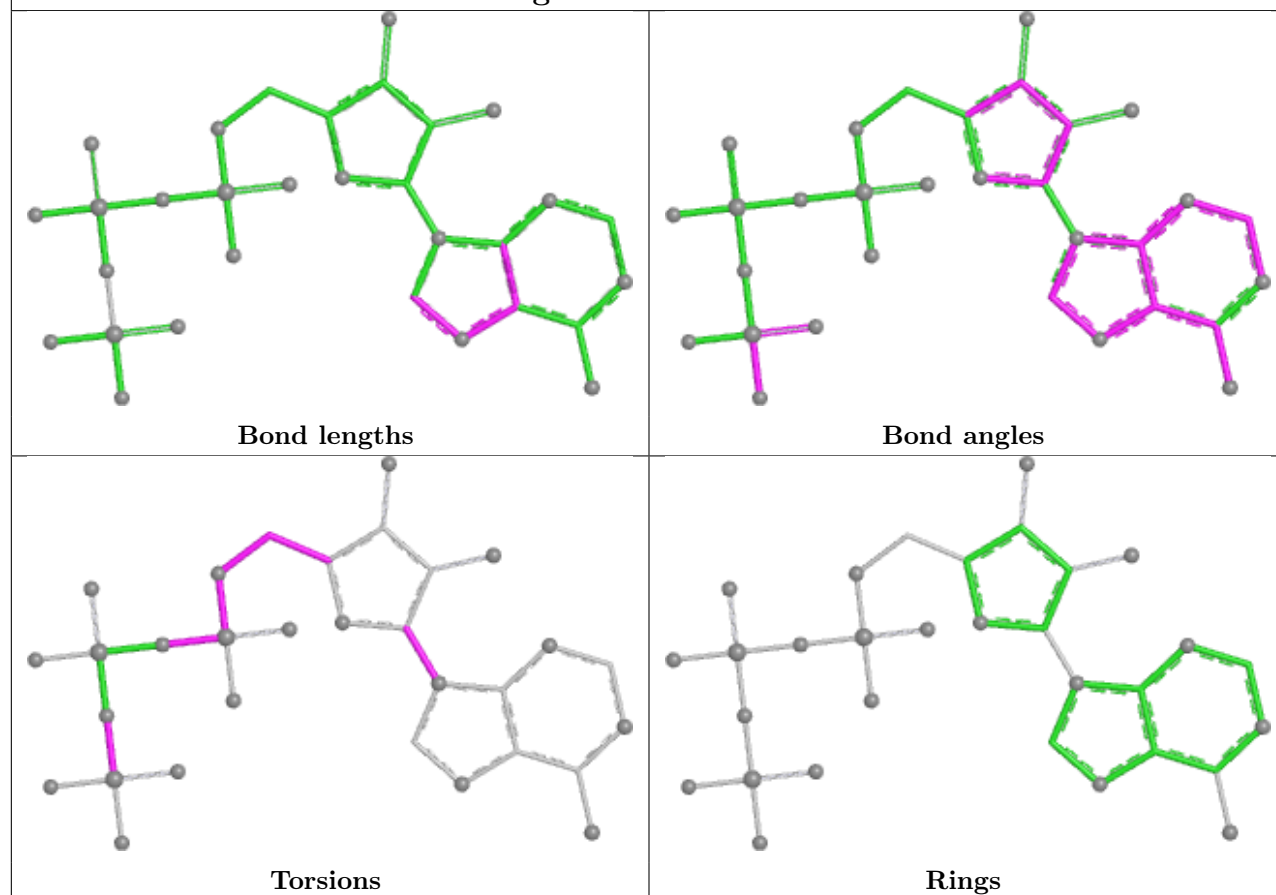
Ligand ATP B 301

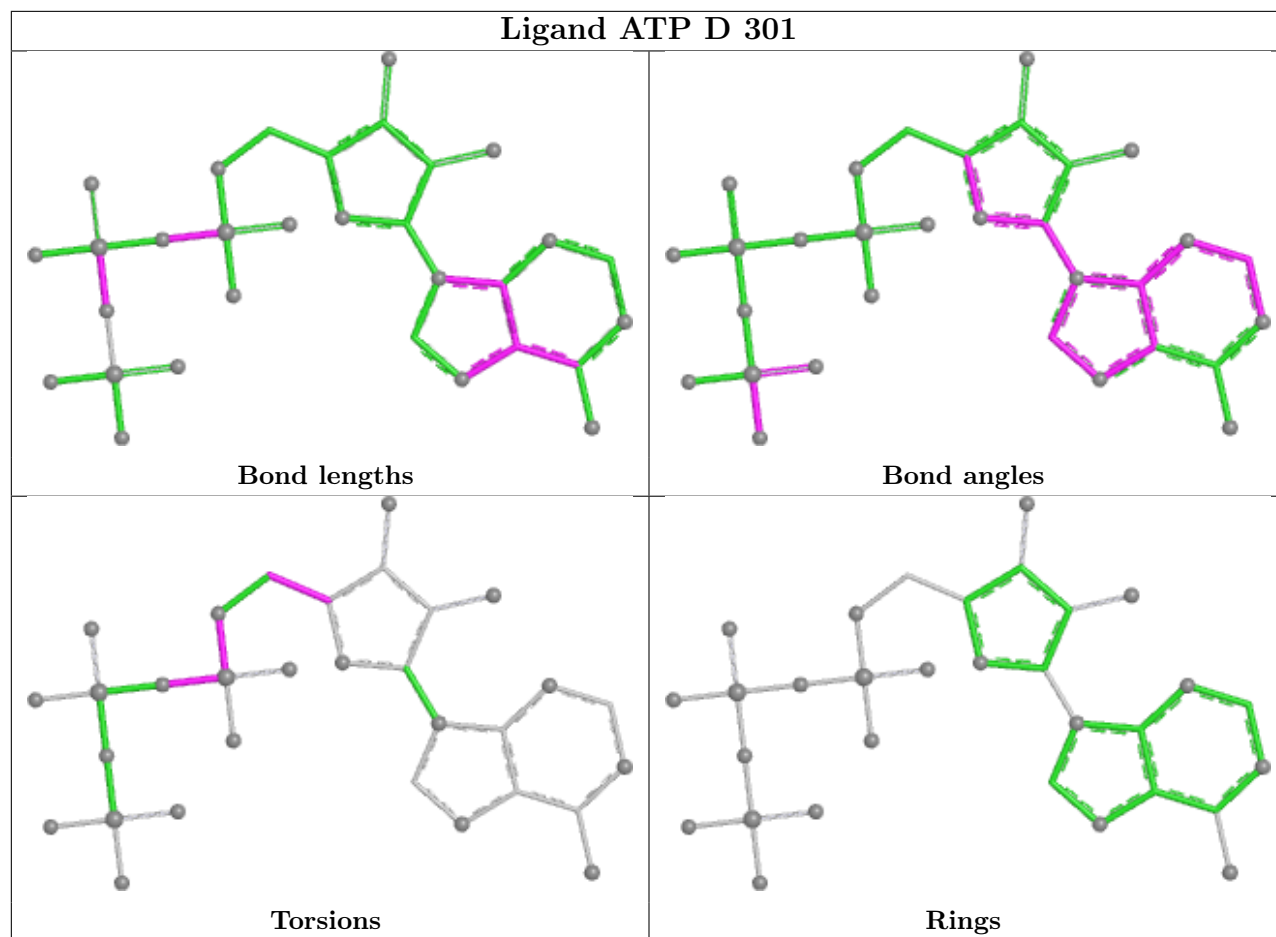


Ligand FEG C 303



Ligand ATP C 302





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	205/218 (94%)	-0.35	1 (0%) 87 87	36, 55, 70, 90	0
1	B	205/218 (94%)	-0.40	1 (0%) 87 87	36, 52, 72, 96	0
1	C	205/218 (94%)	0.07	6 (2%) 53 52	41, 65, 87, 111	0
1	D	205/218 (94%)	0.07	1 (0%) 87 87	37, 66, 89, 108	0
All	All	820/872 (94%)	-0.15	9 (1%) 78 77	36, 59, 84, 111	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	LYS	3.4
1	C	181	ILE	2.8
1	C	122	ILE	2.6
1	C	159	PRO	2.4
1	B	210	ALA	2.3
1	C	160	ILE	2.3
1	C	161	ALA	2.2
1	D	114	THR	2.2
1	A	100	ILE	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 oligosaccharides in this entry.

6.4 Ligands

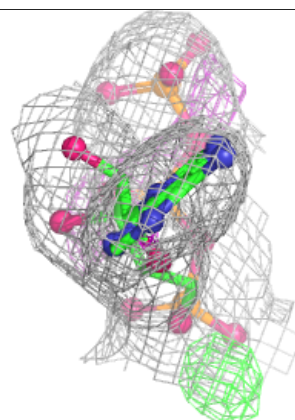
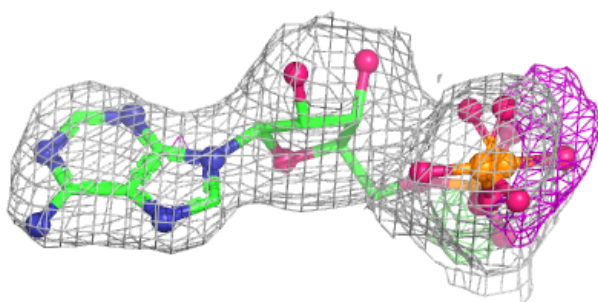
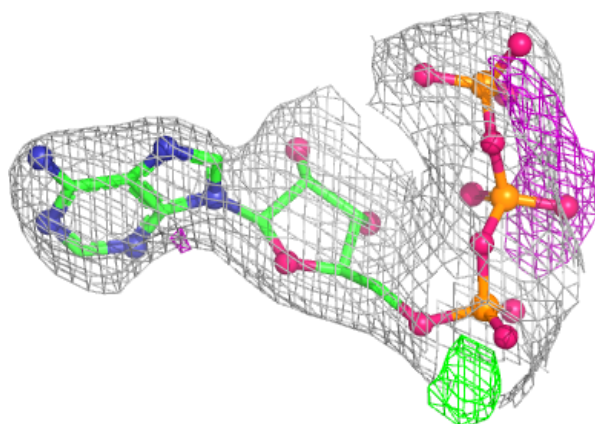
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	C	302	31/31	0.91	0.10	44,67,103,115	0
4	SO4	A	305	5/5	0.91	0.08	75,80,92,102	0
2	ATP	D	301	31/31	0.92	0.09	51,63,106,113	0
2	ATP	B	301	31/31	0.92	0.09	50,60,87,103	0
3	FEG	A	302	37/37	0.93	0.09	47,64,74,79	0
3	FEG	B	302	37/37	0.93	0.08	46,57,66,70	0
3	FEG	C	303	37/37	0.93	0.09	46,64,79,85	0
2	ATP	A	301	31/31	0.93	0.09	44,54,90,97	0
4	SO4	C	301	5/5	0.93	0.07	78,83,85,94	0
4	SO4	C	305	5/5	0.93	0.08	58,58,70,72	0
4	SO4	A	303	5/5	0.94	0.07	51,57,74,76	0
4	SO4	D	302	5/5	0.94	0.06	75,88,90,97	0
4	SO4	C	304	5/5	0.96	0.08	68,69,78,87	0
4	SO4	A	304	5/5	0.96	0.06	60,63,66,76	0
4	SO4	C	306	5/5	0.97	0.08	53,53,64,66	0
4	SO4	B	303	5/5	0.98	0.06	50,57,59,62	0

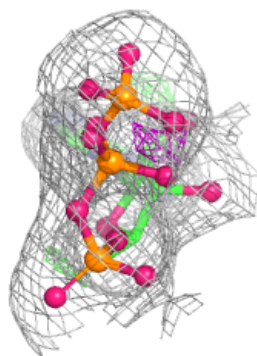
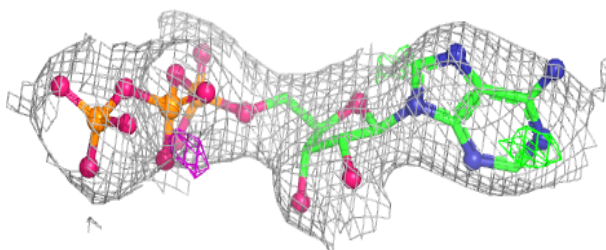
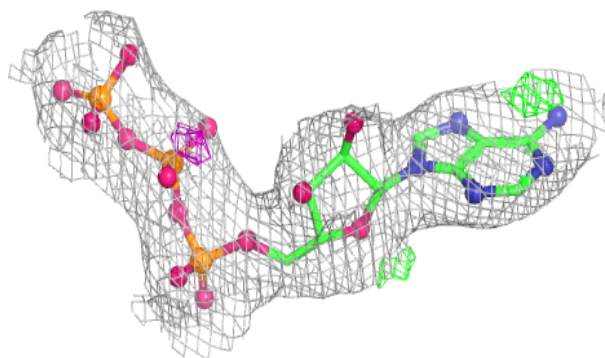
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 302:

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

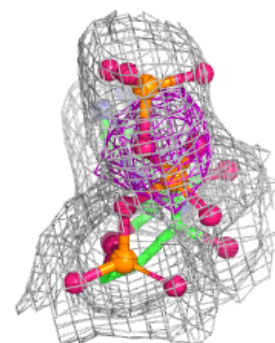
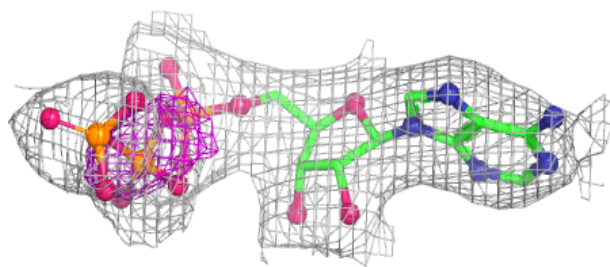
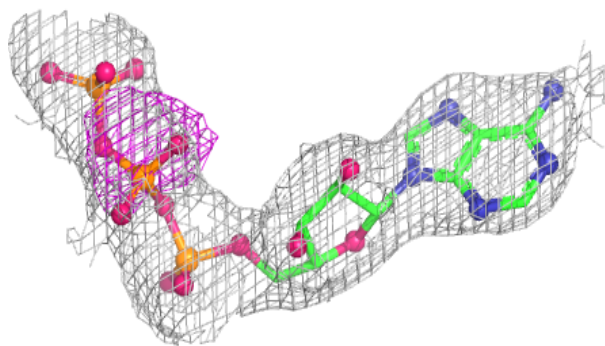
**Electron density around ATP D 301:**

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

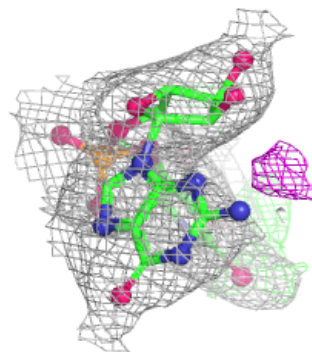
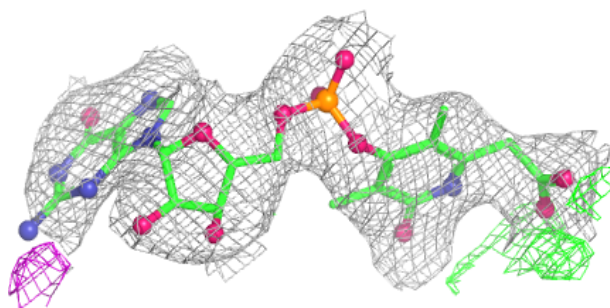
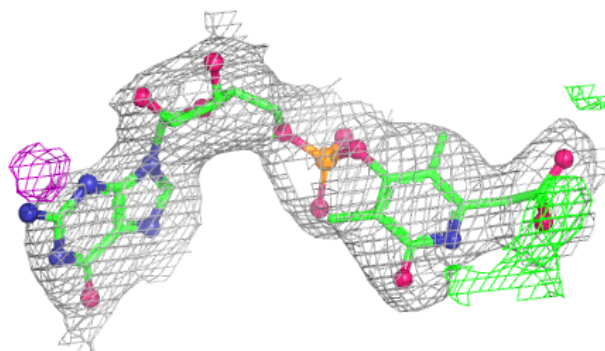


Electron density around ATP B 301:

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

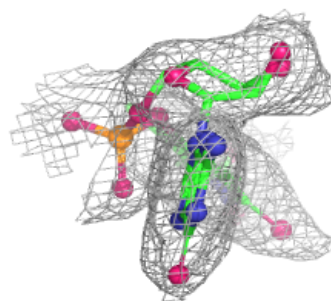
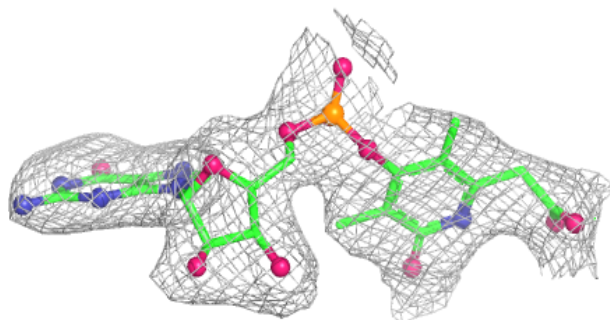
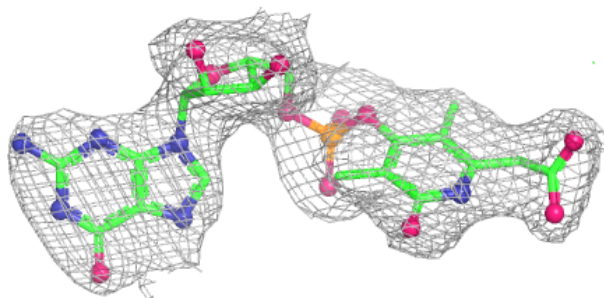
**Electron density around FEG A 302:**

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

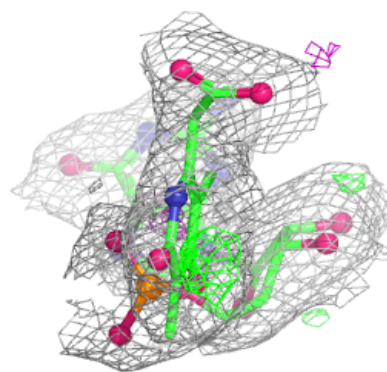
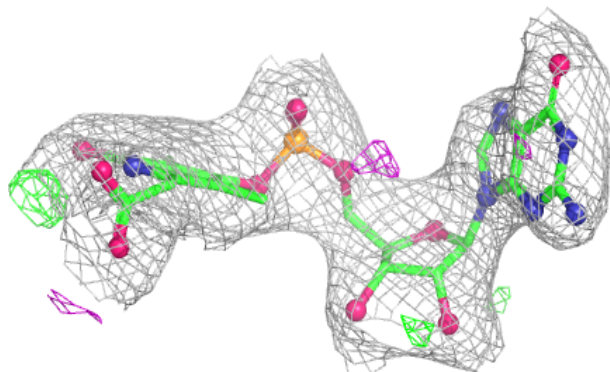
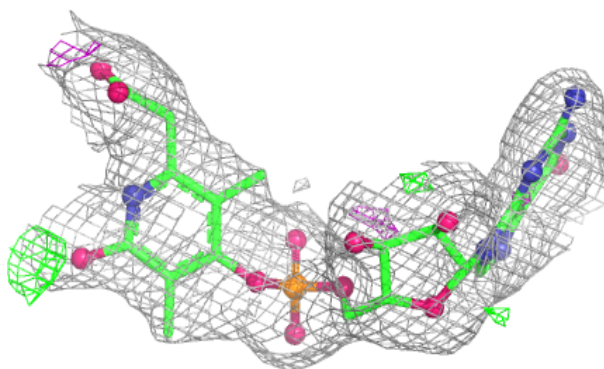


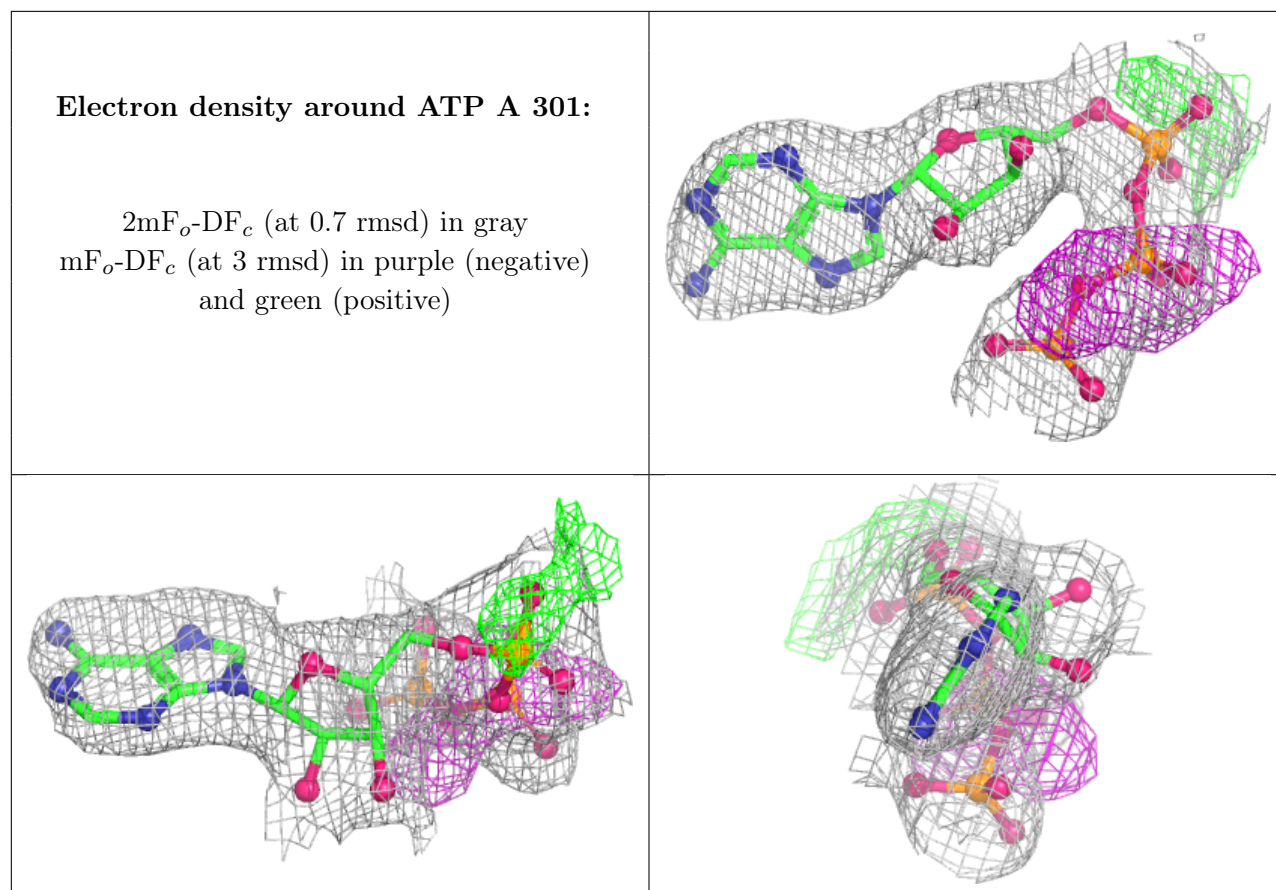
Electron density around FEG B 302:

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

**Electron density around FEG C 303:**

$2mF_o-DF_c$ (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.