



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:40 pm BST

PDB ID : 5E84
Title : ATP-bound state of BiP
Authors : Liu, Q.; Yang, J.; Nune, M.; Zong, Y.; Zhou, L.
Deposited on : 2015-10-13
Resolution : 2.99 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

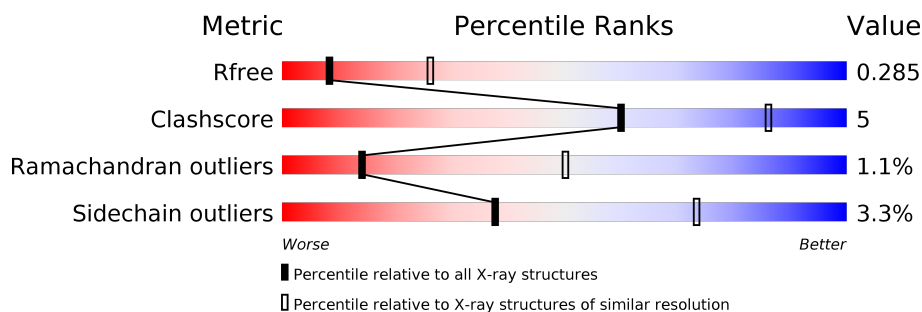
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	606	84% 14% .
1	B	606	89% 9% .
1	C	606	88% 11% .
1	D	606	86% 13% .
1	E	606	85% 14% .
1	F	606	85% 13% .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	D	804	-	-	X	-
5	SO4	A	808	-	-	X	-
5	SO4	C	806	-	-	X	-
5	SO4	D	808	-	-	X	-
5	SO4	E	806	-	-	X	-
5	SO4	F	806	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28484 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 78 kDa glucose-regulated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	606	Total	C	N	O	S	8	0	0
			4710	2955	806	938	11			
1	B	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	C	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	D	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			
1	E	606	Total	C	N	O	S	8	0	0
			4696	2945	805	935	11			
1	F	606	Total	C	N	O	S	8	0	0
			4700	2948	806	935	11			

There are 54 discrepancies between the modelled and reference sequences:

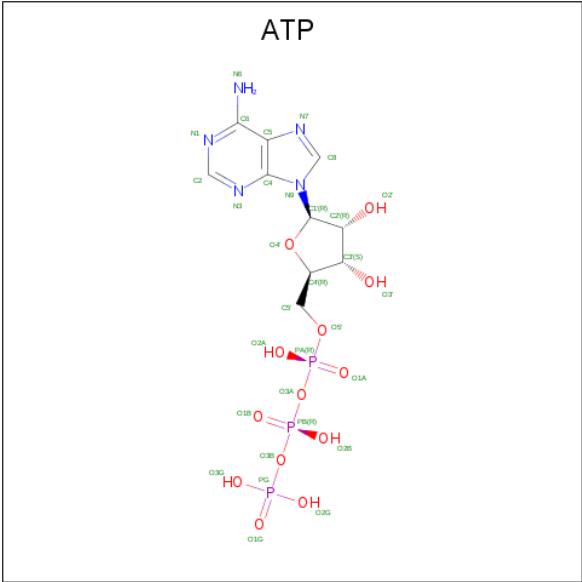
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P11021
A	229	ALA	THR	conflict	UNP P11021
A	?	-	THR	deletion	UNP P11021
A	?	-	ALA	deletion	UNP P11021
A	?	-	SER	deletion	UNP P11021
A	?	-	ASP	deletion	UNP P11021
A	453	VAL	ASN	conflict	UNP P11021
A	454	GLY	GLN	conflict	UNP P11021
A	455	GLY	PRO	conflict	UNP P11021
B	24	SER	-	expression tag	UNP P11021
B	229	ALA	THR	conflict	UNP P11021
B	?	-	THR	deletion	UNP P11021
B	?	-	ALA	deletion	UNP P11021
B	?	-	SER	deletion	UNP P11021
B	?	-	ASP	deletion	UNP P11021
B	453	VAL	ASN	conflict	UNP P11021
B	454	GLY	GLN	conflict	UNP P11021

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Chain	Residue	Modelled	Actual	Comment	Reference
B	455	GLY	PRO	conflict	UNP P11021
C	24	SER	-	expression tag	UNP P11021
C	229	ALA	THR	conflict	UNP P11021
C	?	-	THR	deletion	UNP P11021
C	?	-	ALA	deletion	UNP P11021
C	?	-	SER	deletion	UNP P11021
C	?	-	ASP	deletion	UNP P11021
C	453	VAL	ASN	conflict	UNP P11021
C	454	GLY	GLN	conflict	UNP P11021
C	455	GLY	PRO	conflict	UNP P11021
D	24	SER	-	expression tag	UNP P11021
D	229	ALA	THR	conflict	UNP P11021
D	?	-	THR	deletion	UNP P11021
D	?	-	ALA	deletion	UNP P11021
D	?	-	SER	deletion	UNP P11021
D	?	-	ASP	deletion	UNP P11021
D	453	VAL	ASN	conflict	UNP P11021
D	454	GLY	GLN	conflict	UNP P11021
D	455	GLY	PRO	conflict	UNP P11021
E	24	SER	-	expression tag	UNP P11021
E	229	ALA	THR	conflict	UNP P11021
E	?	-	THR	deletion	UNP P11021
E	?	-	ALA	deletion	UNP P11021
E	?	-	SER	deletion	UNP P11021
E	?	-	ASP	deletion	UNP P11021
E	453	VAL	ASN	conflict	UNP P11021
E	454	GLY	GLN	conflict	UNP P11021
E	455	GLY	PRO	conflict	UNP P11021
F	24	SER	-	expression tag	UNP P11021
F	229	ALA	THR	conflict	UNP P11021
F	?	-	THR	deletion	UNP P11021
F	?	-	ALA	deletion	UNP P11021
F	?	-	SER	deletion	UNP P11021
F	?	-	ASP	deletion	UNP P11021
F	453	VAL	ASN	conflict	UNP P11021
F	454	GLY	GLN	conflict	UNP P11021
F	455	GLY	PRO	conflict	UNP P11021

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

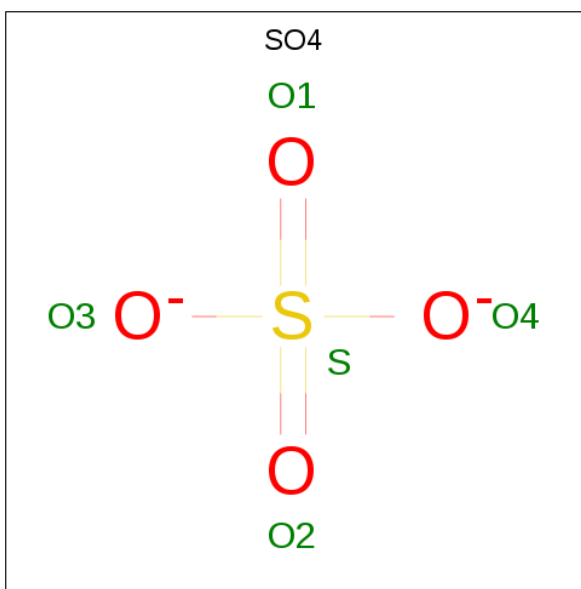
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total	Zn	0	0
			3	3		
3	E	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		
3	C	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		
3	F	3	Total	Zn	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total	Mg	0	0
			3	3		
4	E	1	Total	Mg	0	0
			1	1		
4	B	3	Total	Mg	0	0
			3	3		
4	C	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

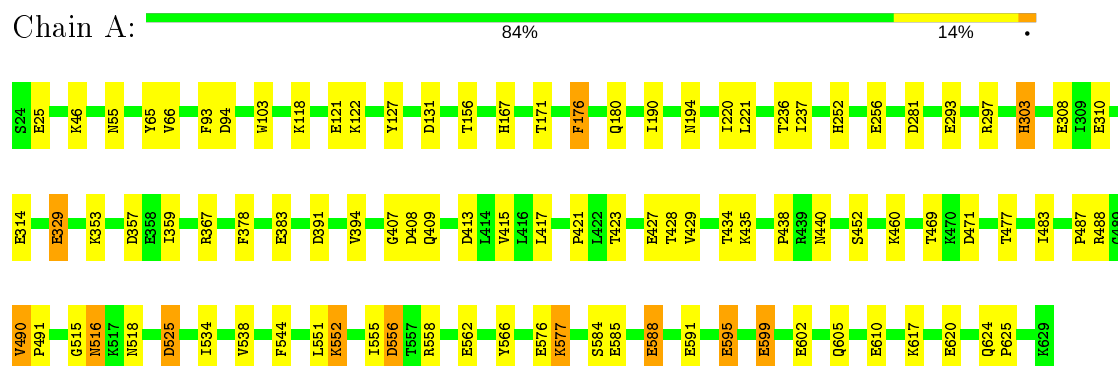
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	5	Total	O	0	0
			5	5		
6	C	4	Total	O	0	0
			4	4		
6	D	4	Total	O	0	0
			4	4		
6	E	9	Total	O	0	0
			9	9		
6	F	3	Total	O	0	0
			3	3		

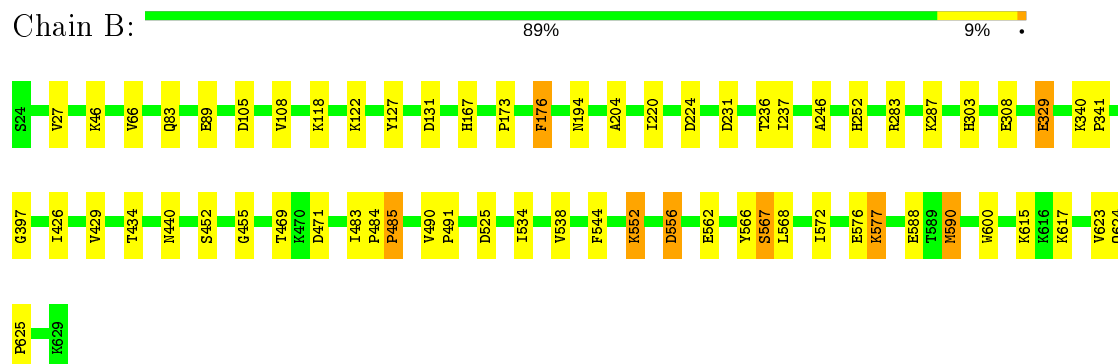
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

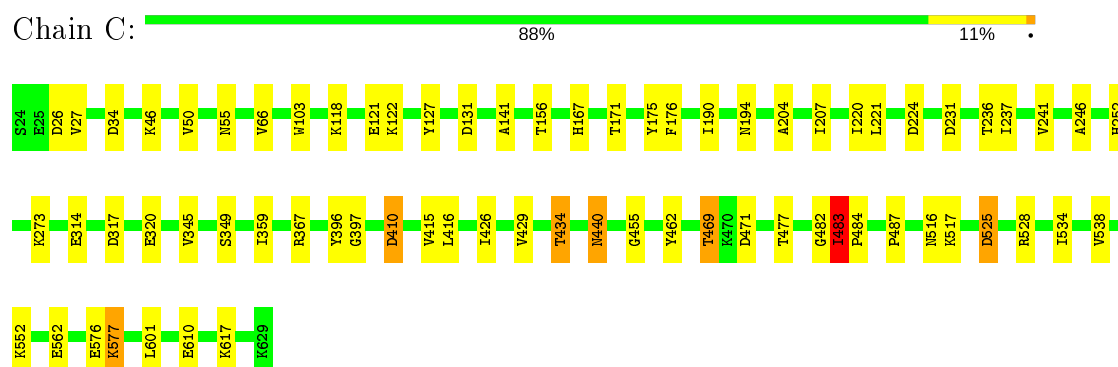
- Molecule 1: 78 kDa glucose-regulated protein



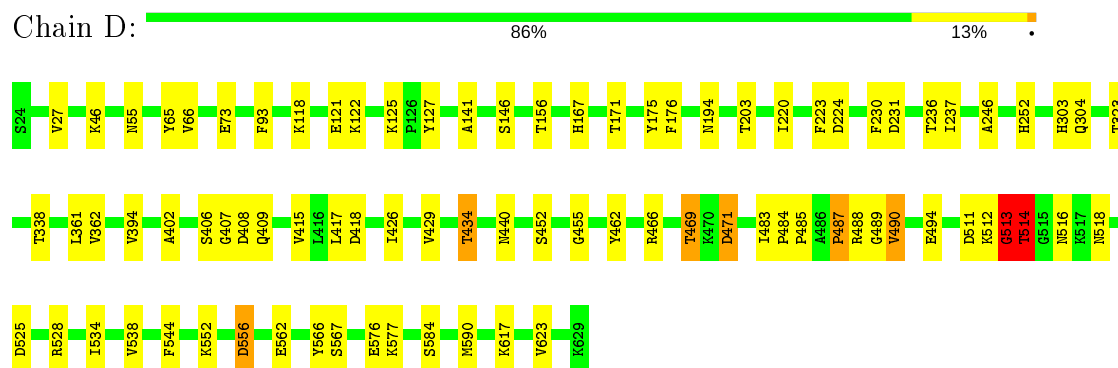
- Molecule 1: 78 kDa glucose-regulated protein



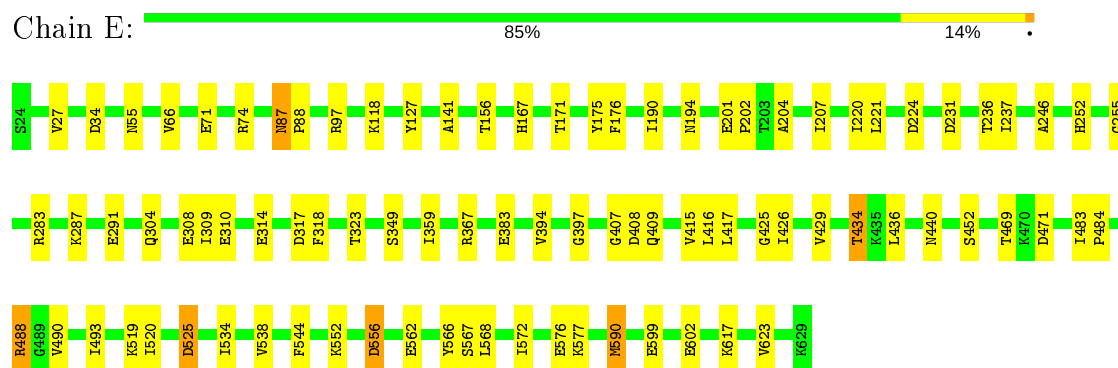
- Molecule 1: 78 kDa glucose-regulated protein



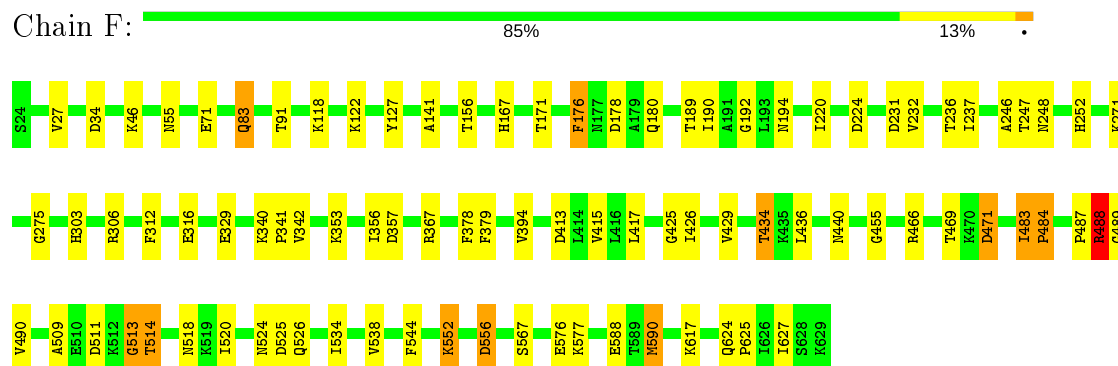
- Molecule 1: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein



- Molecule 1: 78 kDa glucose-regulated protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.47Å 222.47Å 209.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.76 – 2.99 39.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.76-2.99) 97.6 (39.65-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.287 0.241 , 0.285	Depositor DCC
R_{free} test set	5907 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28484	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: MG, ZN, ATP, SO4

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	0.75	9/4777 (0.2%)	0.86	7/6446 (0.1%)
1	B	0.60	4/4767 (0.1%)	0.73	5/6432 (0.1%)
1	C	0.56	1/4767 (0.0%)	0.71	2/6432 (0.0%)
1	D	0.67	3/4767 (0.1%)	0.78	8/6432 (0.1%)
1	E	0.66	1/4763 (0.0%)	0.73	4/6428 (0.1%)
1	F	0.61	3/4767 (0.1%)	0.75	6/6432 (0.1%)
All	All	0.65	21/28608 (0.1%)	0.76	32/38602 (0.1%)

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	A	0	1
1	C	0	3
1	D	2	2
1	F	0	3
All	All	2	9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	576	GLU	CB-CG	25.85	2.01	1.52
1	D	577	LYS	CB-CG	-17.80	1.04	1.52
1	F	577	LYS	CB-CG	-13.61	1.15	1.52
1	B	577	LYS	CB-CG	-13.20	1.17	1.52
1	D	576	GLU	CB-CG	-12.78	1.27	1.52
1	B	576	GLU	CB-CG	10.76	1.72	1.52
1	C	577	LYS	CB-CG	-9.90	1.25	1.52
1	A	599	GLU	CG-CD	9.70	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	595	GLU	CD-OE2	9.02	1.35	1.25
1	A	588	GLU	CD-OE2	8.54	1.35	1.25
1	A	329	GLU	CD-OE2	7.81	1.34	1.25
1	F	556	ASP	CB-CG	7.76	1.68	1.51
1	F	576	GLU	CB-CG	6.94	1.65	1.52
1	A	576	GLU	CB-CG	-6.90	1.39	1.52
1	A	329	GLU	CB-CG	6.21	1.64	1.52
1	B	556	ASP	CB-CG	6.13	1.64	1.51
1	D	556	ASP	CB-CG	5.99	1.64	1.51
1	A	577	LYS	CB-CG	-5.94	1.36	1.52
1	B	329	GLU	CD-OE2	5.40	1.31	1.25
1	A	588	GLU	CG-CD	5.37	1.60	1.51
1	A	595	GLU	CG-CD	5.08	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	556	ASP	CB-CG-OD1	11.50	128.65	118.30
1	A	556	ASP	CB-CG-OD1	11.41	128.57	118.30
1	D	577	LYS	CA-CB-CG	9.73	134.82	113.40
1	A	599	GLU	OE1-CD-OE2	-9.65	111.72	123.30
1	E	576	GLU	CA-CB-CG	-9.10	93.39	113.40
1	E	556	ASP	CB-CG-OD1	9.06	126.45	118.30
1	B	556	ASP	CB-CG-OD1	8.62	126.06	118.30
1	D	576	GLU	CA-CB-CG	-8.18	95.39	113.40
1	B	576	GLU	CA-CB-CG	-8.12	95.53	113.40
1	A	599	GLU	CG-CD-OE1	7.38	133.06	118.30
1	C	576	GLU	CA-CB-CG	7.31	129.48	113.40
1	D	556	ASP	CB-CG-OD1	7.15	124.74	118.30
1	D	513	GLY	N-CA-C	6.84	130.21	113.10
1	A	329	GLU	CG-CD-OE2	6.59	131.48	118.30
1	F	556	ASP	OD1-CG-OD2	-6.15	111.62	123.30
1	B	577	LYS	CA-CB-CG	5.80	126.17	113.40
1	A	329	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	D	576	GLU	CB-CG-CD	-5.63	98.99	114.20
1	B	556	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	B	576	GLU	CB-CG-CD	-5.53	99.28	114.20
1	F	489	GLY	N-CA-C	5.51	126.89	113.10
1	A	357	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	488	ARG	N-CA-C	-5.25	96.82	111.00
1	F	178	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	487	PRO	N-CA-C	5.22	125.66	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	367	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	F	367	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	314	GLU	CB-CA-C	5.04	120.47	110.40
1	D	556	ASP	OD1-CG-OD2	-5.03	113.74	123.30
1	E	97	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	514	THR	N-CA-C	5.02	124.56	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	488	ARG	CA
1	D	514	THR	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	ARG	Peptide
1	C	482	GLY	Peptide
1	C	483	ILE	Peptide
1	C	484	PRO	Peptide
1	D	487	PRO	Peptide
1	D	513	GLY	Peptide
1	F	488	ARG	Peptide
1	F	513	GLY	Peptide
1	F	518	ASN	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	4710	0	4736	47	4
1	B	4700	0	4713	33	2
1	C	4700	0	4713	37	1
1	D	4700	0	4713	52	0
1	E	4696	0	4702	51	4
1	F	4700	0	4713	58	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	1	2
4	B	3	0	0	0	0
4	C	1	0	0	0	1
4	D	3	0	0	0	2
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	6	0
5	B	5	0	0	1	0
5	C	5	0	0	6	0
5	D	5	0	0	5	0
5	E	5	0	0	7	0
5	F	5	0	0	5	0
6	A	7	0	0	2	0
6	B	5	0	0	4	1
6	C	4	0	0	0	0
6	D	4	0	0	1	0
6	E	9	0	0	3	0
6	F	3	0	0	1	0
All	All	28484	0	28362	262	12

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 5.

All (262) 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:303:HIS:ND1	1:F:556:ASP:OD1	1.97	0.95
1:D:556:ASP:OD2	1:F:303:HIS:CE1	2.26	0.89
1:B:552:LYS:HE2	1:B:556:ASP:OD2	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:ASP:OD2	1:F:303:HIS:ND1	2.12	0.82
1:A:415:VAL:HG11	1:D:417:LEU:HD21	1.63	0.81
1:D:303:HIS:ND1	1:F:556:ASP:CG	2.35	0.80
1:D:167:HIS:CE1	5:D:808:SO4:S	2.76	0.79
1:D:167:HIS:CE1	5:D:808:SO4:O4	2.36	0.78
1:C:167:HIS:CE1	5:C:806:SO4:O2	2.37	0.77
1:A:167:HIS:CE1	5:A:808:SO4:O4	2.38	0.76
1:D:73:GLU:OE1	1:F:306:ARG:NH2	2.17	0.76
1:A:308:GLU:OE2	6:A:901:HOH:O	2.03	0.75
1:A:167:HIS:HE1	5:A:808:SO4:S	2.12	0.73
1:B:308:GLU:OE2	6:B:901:HOH:O	2.06	0.73
1:F:466:ARG:NH1	1:F:471:ASP:OD2	2.22	0.73
1:C:194:ASN:ND2	5:C:806:SO4:O1	2.22	0.72
1:B:89:GLU:OE1	6:B:902:HOH:O	2.07	0.72
1:D:534:ILE:O	1:D:538:VAL:HG23	1.89	0.72
1:C:167:HIS:CE1	5:C:806:SO4:S	2.82	0.72
1:E:194:ASN:ND2	5:E:806:SO4:S	2.63	0.71
1:D:484:PRO:HG3	1:D:511:ASP:OD2	1.90	0.71
1:E:167:HIS:CE1	5:E:806:SO4:S	2.83	0.71
1:B:483:ILE:O	1:B:485:PRO:HD3	1.90	0.71
1:F:167:HIS:CE1	5:F:806:SO4:S	2.85	0.70
1:A:194:ASN:ND2	5:A:808:SO4:O3	2.25	0.69
1:E:417:LEU:HD21	1:F:415:VAL:HG11	1.74	0.69
1:D:556:ASP:CG	1:F:303:HIS:ND1	2.46	0.69
1:E:415:VAL:HG11	1:F:417:LEU:HD21	1.73	0.69
1:E:167:HIS:HE1	5:E:806:SO4:O3	1.76	0.69
1:F:534:ILE:O	1:F:538:VAL:HG23	1.93	0.68
1:E:308:GLU:OE2	6:E:902:HOH:O	2.13	0.68
1:E:525:ASP:OD2	6:E:901:HOH:O	2.12	0.68
1:D:194:ASN:ND2	5:D:808:SO4:O1	2.28	0.67
1:E:426:ILE:HG13	1:E:434:THR:HG23	1.75	0.67
1:A:167:HIS:CE1	5:A:808:SO4:S	2.89	0.66
1:E:167:HIS:HE1	5:E:806:SO4:S	2.18	0.66
1:F:167:HIS:CE1	5:F:806:SO4:O3	2.49	0.65
1:D:303:HIS:CE1	1:F:556:ASP:OD2	2.50	0.65
1:B:89:GLU:OE2	6:B:902:HOH:O	2.15	0.65
1:E:194:ASN:ND2	5:E:806:SO4:O3	2.29	0.65
1:A:310:GLU:OE2	4:A:805:MG:MG	1.39	0.64
1:D:246:ALA:HA	1:D:440:ASN:OD1	1.97	0.64
2:F:801:ATP:O3G	6:F:901:HOH:O	2.14	0.64
1:A:585:GLU:OE2	6:A:902:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:GLU:OE2	1:E:602:GLU:OE1	2.18	0.60
1:F:167:HIS:HE1	5:F:806:SO4:S	2.23	0.60
1:C:455:GLY:O	1:C:483:ILE:HG12	2.01	0.59
1:E:194:ASN:ND2	5:E:806:SO4:O1	2.35	0.59
2:D:801:ATP:O3G	6:D:901:HOH:O	2.17	0.59
1:C:127:TYR:CE2	1:C:141:ALA:HB2	2.37	0.59
1:D:466:ARG:NH1	1:D:471:ASP:OD2	2.35	0.59
1:C:534:ILE:O	1:C:538:VAL:HG23	2.02	0.59
1:F:624:GLN:HB3	1:F:625:PRO:HD3	1.85	0.58
1:A:427:GLU:OE1	1:A:460:LYS:HD2	2.04	0.58
1:A:558:ARG:NH1	1:A:605:GLN:O	2.36	0.58
1:B:590:MET:CE	1:B:623:VAL:HG13	2.34	0.58
1:E:562:GLU:HG2	1:E:566:TYR:CE2	2.38	0.58
1:B:252:HIS:ND1	1:B:252:HIS:O	2.37	0.58
1:D:167:HIS:ND1	1:D:194:ASN:HB3	2.19	0.58
1:D:407:GLY:O	1:D:409:GLN:N	2.37	0.58
1:E:599:GLU:HG3	6:E:909:HOH:O	2.04	0.58
1:D:303:HIS:CE1	1:F:556:ASP:CG	2.77	0.58
1:C:167:HIS:HE1	5:C:806:SO4:S	2.26	0.57
1:D:167:HIS:CE1	5:D:808:SO4:O2	2.57	0.57
1:E:55:ASN:HA	1:E:156:THR:HG23	1.86	0.57
1:C:55:ASN:HA	1:C:156:THR:HG23	1.85	0.56
1:E:246:ALA:HA	1:E:440:ASN:OD1	2.05	0.56
1:D:455:GLY:O	1:D:483:ILE:HD12	2.06	0.56
1:A:281:ASP:OD1	1:C:314:GLU:HG2	2.06	0.56
1:F:455:GLY:O	1:F:483:ILE:HD12	2.06	0.56
1:C:221:LEU:HD23	1:C:359:ILE:HG23	1.86	0.56
1:C:190:ILE:HA	1:C:538:VAL:HG22	1.88	0.56
1:B:194:ASN:ND2	5:B:808:SO4:O4	2.40	0.55
1:B:590:MET:HE3	1:B:623:VAL:HG13	1.87	0.55
1:F:55:ASN:HA	1:F:156:THR:HG23	1.89	0.54
1:E:252:HIS:O	1:E:252:HIS:ND1	2.40	0.54
1:A:407:GLY:O	1:A:409:GLN:N	2.40	0.54
1:C:167:HIS:ND1	1:C:194:ASN:HB3	2.23	0.54
1:F:246:ALA:HA	1:F:440:ASN:OD1	2.08	0.54
1:F:27:VAL:HA	1:F:167:HIS:CD2	2.42	0.54
1:A:452:SER:O	1:A:490:VAL:HG13	2.08	0.53
1:A:417:LEU:HD21	1:D:415:VAL:HG11	1.91	0.53
1:A:167:HIS:HE1	5:A:808:SO4:O1	1.92	0.53
1:A:190:ILE:HA	1:A:538:VAL:HG22	1.89	0.53
1:E:291:GLU:HG3	1:E:309:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:HIS:CE1	5:F:806:SO4:O1	2.62	0.53
1:A:176:PHE:CD2	1:A:180:GLN:HB3	2.45	0.52
1:E:283:ARG:O	1:E:287:LYS:HG3	2.09	0.52
1:D:167:HIS:HE1	5:D:808:SO4:S	2.29	0.52
1:D:426:ILE:HG13	1:D:434:THR:HG23	1.90	0.52
1:F:378:PHE:HD1	1:F:379:PHE:CE1	2.27	0.52
1:C:207:ILE:HD11	1:C:416:LEU:HD21	1.90	0.52
1:C:426:ILE:HG13	1:C:434:THR:HG23	1.91	0.52
1:D:304:GLN:HG3	1:D:323:THR:HG22	1.90	0.52
1:A:599:GLU:CD	1:A:602:GLU:OE1	2.48	0.52
1:A:534:ILE:O	1:A:538:VAL:HG23	2.09	0.52
1:E:304:GLN:HG3	1:E:323:THR:HG22	1.91	0.52
1:F:426:ILE:HG13	1:F:434:THR:HG23	1.92	0.52
1:B:534:ILE:O	1:B:538:VAL:HG23	2.09	0.52
1:F:340:LYS:HB2	1:F:341:PRO:HD3	1.92	0.51
1:C:483:ILE:CG2	1:C:483:ILE:O	2.58	0.51
1:E:27:VAL:HA	1:E:167:HIS:CD2	2.46	0.51
1:F:312:PHE:N	1:F:316:GLU:O	2.42	0.51
1:D:65:TYR:CD2	1:D:93:PHE:HB3	2.46	0.51
1:B:590:MET:SD	1:B:623:VAL:HG22	2.50	0.51
1:D:511:ASP:OD2	1:D:514:THR:HG23	2.11	0.50
1:E:534:ILE:O	1:E:538:VAL:HG23	2.11	0.50
1:E:167:HIS:ND1	1:E:194:ASN:HB3	2.26	0.50
1:C:483:ILE:O	1:C:483:ILE:HG23	2.09	0.50
1:E:220:ILE:HG13	1:E:237:ILE:HD12	1.92	0.50
1:E:407:GLY:O	1:E:409:GLN:N	2.44	0.50
1:E:204:ALA:O	1:E:397:GLY:HA3	2.11	0.50
1:A:624:GLN:HB3	1:A:625:PRO:HD3	1.94	0.50
1:C:27:VAL:HG12	5:C:806:SO4:O2	2.12	0.50
1:A:551:LEU:O	1:A:555:ILE:HG12	2.11	0.50
1:C:224:ASP:HB3	1:C:231:ASP:HB2	1.93	0.50
1:A:252:HIS:ND1	1:A:252:HIS:O	2.45	0.50
1:C:34:ASP:HA	1:C:171:THR:OG1	2.12	0.50
1:A:353:LYS:HD3	1:A:378:PHE:O	2.12	0.50
1:C:410:ASP:OD1	1:C:410:ASP:N	2.45	0.50
1:D:203:THR:OG1	1:D:418:ASP:OD2	2.23	0.49
1:B:483:ILE:HG23	1:B:484:PRO:HD2	1.94	0.49
1:C:204:ALA:O	1:C:397:GLY:HA3	2.12	0.49
1:F:487:PRO:O	1:F:488:ARG:HG3	2.12	0.49
1:D:127:TYR:CE2	1:D:141:ALA:HB2	2.47	0.49
1:F:194:ASN:ND2	5:F:806:SO4:O4	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:HA	1:D:156:THR:HG23	1.95	0.49
1:A:435:LYS:O	1:E:488:ARG:HA	2.12	0.49
1:B:220:ILE:HG13	1:B:237:ILE:HD12	1.94	0.49
1:C:462:TYR:CZ	1:C:469:THR:HG23	2.48	0.49
1:B:167:HIS:ND1	1:B:194:ASN:HB3	2.28	0.48
1:F:167:HIS:ND1	1:F:194:ASN:HB3	2.28	0.48
1:C:122:LYS:HG3	1:C:127:TYR:CD1	2.49	0.48
1:C:220:ILE:HG13	1:C:237:ILE:HD12	1.95	0.48
1:A:25:GLU:HG3	5:A:808:SO4:O2	2.14	0.48
1:C:246:ALA:HA	1:C:440:ASN:OD1	2.14	0.48
1:D:224:ASP:HA	1:D:362:VAL:O	2.14	0.48
1:E:519:LYS:O	1:E:520:ILE:HG12	2.14	0.48
1:E:452:SER:O	1:E:490:VAL:CG1	2.62	0.47
1:E:167:HIS:CE1	5:E:806:SO4:O1	2.66	0.47
1:F:220:ILE:HG13	1:F:237:ILE:HD12	1.96	0.47
1:B:455:GLY:O	1:B:483:ILE:HD12	2.15	0.47
1:B:567:SER:OG	1:B:568:LEU:N	2.47	0.47
1:A:591:GLU:OE1	1:A:595:GLU:OE2	2.32	0.47
1:F:552:LYS:HE2	1:F:556:ASP:OD2	2.15	0.47
1:D:484:PRO:CG	1:D:511:ASP:OD2	2.61	0.47
1:A:483:ILE:HG21	1:A:491:PRO:HG2	1.97	0.47
1:D:224:ASP:HB3	1:D:231:ASP:HB2	1.97	0.47
1:B:452:SER:O	1:B:490:VAL:CG1	2.63	0.47
1:E:425:GLY:HA2	1:E:436:LEU:HB2	1.97	0.47
1:D:224:ASP:OD1	1:D:362:VAL:HG23	2.16	0.46
1:E:74:ARG:HD3	1:E:544:PHE:CE2	2.49	0.46
1:B:426:ILE:HG13	1:B:434:THR:HG23	1.97	0.46
1:B:246:ALA:HA	1:B:440:ASN:OD1	2.16	0.46
1:A:620:GLU:O	1:A:624:GLN:HB2	2.16	0.46
1:C:252:HIS:ND1	1:C:252:HIS:O	2.49	0.46
1:F:122:LYS:HG3	1:F:127:TYR:CD1	2.51	0.46
1:D:303:HIS:CG	1:F:556:ASP:OD1	2.66	0.46
1:E:201:GLU:N	1:E:202:PRO:CD	2.79	0.46
1:E:493:ILE:HD11	1:E:520:ILE:HG13	1.97	0.46
1:A:552:LYS:HE2	1:A:556:ASP:OD2	2.16	0.46
1:D:556:ASP:OD1	1:F:303:HIS:ND1	2.48	0.46
1:A:562:GLU:HG2	1:A:566:TYR:CE2	2.51	0.46
1:B:173:PRO:O	1:B:176:PHE:HB2	2.16	0.46
1:D:402:ALA:O	1:D:406:SER:N	2.47	0.46
1:A:221:LEU:HD23	1:A:359:ILE:HG23	1.98	0.45
1:C:27:VAL:HA	1:C:167:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:THR:HG21	1:D:394:VAL:HG12	1.98	0.45
1:A:438:PRO:HG3	1:E:488:ARG:NH2	2.31	0.45
1:E:34:ASP:HA	1:E:171:THR:OG1	2.16	0.45
1:A:103:TRP:CD2	1:A:121:GLU:HB2	2.50	0.45
1:B:89:GLU:CD	6:B:902:HOH:O	2.43	0.45
1:B:122:LYS:HG3	1:B:127:TYR:CD1	2.52	0.45
1:F:378:PHE:HD1	1:F:379:PHE:CD1	2.33	0.45
1:C:103:TRP:CD1	1:C:121:GLU:OE1	2.69	0.45
1:C:525:ASP:OD1	1:C:525:ASP:N	2.49	0.45
1:F:171:THR:HG21	1:F:394:VAL:HG12	1.98	0.45
1:E:255:GLY:HA3	2:E:801:ATP:O3'	2.17	0.45
1:F:252:HIS:O	1:F:252:HIS:ND1	2.49	0.45
1:B:224:ASP:HB3	1:B:231:ASP:HB2	1.98	0.45
1:D:27:VAL:HA	1:D:167:HIS:CD2	2.52	0.45
1:F:232:VAL:HG11	1:F:342:VAL:HG22	1.99	0.44
1:F:176:PHE:CD2	1:F:180:GLN:HB3	2.52	0.44
1:F:552:LYS:CE	1:F:556:ASP:OD2	2.64	0.44
1:B:27:VAL:HA	1:B:167:HIS:CD2	2.52	0.44
1:D:121:GLU:HA	1:D:125:LYS:O	2.17	0.44
1:D:494:GLU:HB2	1:D:512:LYS:HE3	1.98	0.44
1:F:378:PHE:CD1	1:F:379:PHE:CE1	3.05	0.44
1:A:515:GLY:O	1:A:516:ASN:HB2	2.18	0.44
1:D:590:MET:SD	1:D:623:VAL:HG22	2.58	0.44
1:F:484:PRO:HG3	1:F:511:ASP:CG	2.38	0.44
1:A:55:ASN:HA	1:A:156:THR:HG23	2.00	0.44
1:F:483:ILE:HA	1:F:484:PRO:HD3	1.80	0.43
1:F:513:GLY:C	1:F:514:THR:HG23	2.38	0.43
1:C:477:THR:HB	1:C:525:ASP:HB2	2.01	0.43
1:E:127:TYR:CE2	1:E:141:ALA:HB2	2.53	0.43
1:F:34:ASP:HA	1:F:171:THR:OG1	2.18	0.43
1:D:484:PRO:HA	1:D:485:PRO:HD3	1.71	0.43
1:F:189:THR:O	1:F:192:GLY:N	2.50	0.43
1:F:425:GLY:HA2	1:F:436:LEU:HB2	2.00	0.43
1:A:220:ILE:HG13	1:A:237:ILE:HD12	2.01	0.43
1:C:241:VAL:HG22	1:C:415:VAL:CG2	2.49	0.43
1:D:452:SER:O	1:D:490:VAL:CG1	2.67	0.43
1:E:483:ILE:HG23	1:E:484:PRO:HD2	2.01	0.43
1:D:220:ILE:HG13	1:D:237:ILE:HD12	1.99	0.43
1:B:562:GLU:HG2	1:B:566:TYR:CE2	2.55	0.42
1:D:230:PHE:CZ	1:D:338:THR:HB	2.54	0.42
1:E:207:ILE:HD11	1:E:416:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:THR:HG21	1:A:394:VAL:HG12	1.99	0.42
1:D:122:LYS:HG3	1:D:127:TYR:CD1	2.54	0.42
1:D:562:GLU:HG2	1:D:566:TYR:CE2	2.54	0.42
1:B:105:ASP:HB3	1:B:108:VAL:HG23	2.01	0.42
1:B:340:LYS:HB2	1:B:341:PRO:HD3	2.01	0.42
1:A:122:LYS:HG3	1:A:127:TYR:CD1	2.55	0.42
1:D:223:PHE:HB3	1:D:361:LEU:HD23	2.01	0.42
1:A:293:GLU:O	1:A:297:ARG:HG3	2.20	0.42
1:A:599:GLU:OE1	1:A:602:GLU:OE1	2.38	0.42
1:D:483:ILE:HG23	1:D:484:PRO:HD2	2.00	0.42
1:B:572:ILE:HD11	1:B:590:MET:HG3	2.01	0.42
1:E:221:LEU:HD23	1:E:359:ILE:HG23	2.02	0.42
1:E:252:HIS:O	1:E:252:HIS:CG	2.72	0.42
1:F:524:ASN:O	1:F:526:GLN:N	2.53	0.42
1:D:252:HIS:O	1:D:252:HIS:ND1	2.53	0.41
1:B:283:ARG:O	1:B:287:LYS:HG3	2.20	0.41
1:C:320:GLU:OE1	1:C:320:GLU:HA	2.20	0.41
1:F:83:GLN:OE1	1:F:91:THR:OG1	2.38	0.41
1:A:367:ARG:NH2	1:A:391:ASP:OD2	2.41	0.41
1:E:318:PHE:C	1:E:318:PHE:CD1	2.93	0.41
1:F:224:ASP:HB3	1:F:231:ASP:HB2	2.01	0.41
1:F:271:LYS:O	1:F:275:GLY:N	2.46	0.41
1:E:520:ILE:HA	1:E:520:ILE:HD13	1.97	0.41
1:B:204:ALA:O	1:B:397:GLY:HA3	2.21	0.41
1:C:562:GLU:CG	1:C:601:LEU:HD13	2.50	0.41
1:E:572:ILE:HD11	1:E:590:MET:HG3	2.02	0.41
1:F:127:TYR:CE2	1:F:141:ALA:HB2	2.56	0.41
1:F:248:ASN:OD1	1:F:341:PRO:HB3	2.20	0.41
1:B:600:TRP:CE2	1:B:615:LYS:HE3	2.56	0.41
1:A:423:THR:CG2	1:A:435:LYS:HG3	2.50	0.41
1:E:87:ASN:N	1:E:88:PRO:CD	2.84	0.41
1:F:356:ILE:HG13	1:F:379:PHE:HE2	1.85	0.41
1:A:65:TYR:CE2	1:A:93:PHE:HB3	2.56	0.40
1:C:562:GLU:HG3	1:C:601:LEU:HD13	2.03	0.40
1:D:462:TYR:CZ	1:D:469:THR:HG23	2.55	0.40
1:D:556:ASP:CG	1:F:303:HIS:HD1	2.24	0.40
1:F:190:ILE:HA	1:F:538:VAL:HG22	2.03	0.40
1:F:509:ALA:O	1:F:520:ILE:HG12	2.21	0.40
1:A:167:HIS:ND1	1:A:194:ASN:HB3	2.36	0.40
1:A:94:ASP:OD2	1:A:256:GLU:OE1	2.39	0.40
1:A:477:THR:HB	1:A:525:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LYS:HB2	1:C:273:LYS:HE3	1.97	0.40
1:E:171:THR:HG21	1:E:394:VAL:HG12	2.03	0.40
1:F:353:LYS:HD3	1:F:378:PHE:O	2.20	0.40
1:A:428:THR:CG2	1:A:434:THR:HG21	2.51	0.40
1:B:252:HIS:O	1:B:252:HIS:CG	2.74	0.40
1:C:50:VAL:HB	1:C:396:TYR:CE2	2.57	0.40
1:F:590:MET:CE	1:F:627:ILE:HG23	2.52	0.40
1:B:624:GLN:HB3	1:B:625:PRO:HD3	2.03	0.40
1:C:167:HIS:HE1	5:C:806:SO4:O4	2.04	0.40
1:E:224:ASP:HB3	1:E:231:ASP:HB2	2.02	0.40
1:E:190:ILE:HA	1:E:538:VAL:HG22	2.04	0.40
1:E:590:MET:CE	1:E:623:VAL:HG13	2.51	0.40
1:E:568:LEU:HD13	1:E:623:VAL:HG21	2.04	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ASP:OD2	4:D:804:MG:MG[6_654]	1.44	0.76
4:A:803:MG:MG	4:C:803:MG:MG[2_554]	1.48	0.72
1:C:317:ASP:OD2	4:A:804:MG:MG[6_554]	1.50	0.70
1:A:303:HIS:ND1	1:A:556:ASP:OD1[6_554]	1.54	0.66
1:A:595:GLU:OE2	1:A:595:GLU:OE2[5_554]	1.62	0.58
1:E:310:GLU:OE2	4:D:804:MG:MG[6_654]	1.68	0.52
1:A:329:GLU:OE2	1:A:588:GLU:OE2[3_555]	1.73	0.47
1:A:303:HIS:CE1	1:A:556:ASP:OD1[6_554]	1.75	0.45
1:B:303:HIS:ND1	1:E:556:ASP:OD1[2_654]	1.83	0.37
1:F:329:GLU:OE2	1:F:588:GLU:OE2[2_664]	2.01	0.19
1:E:71:GLU:OE2	6:B:901:HOH:O[3_665]	2.07	0.13
1:B:329:GLU:OE2	1:B:588:GLU:OE2[3_665]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	604/606 (100%)	566 (94%)	29 (5%)	9 (2%)	10	42
1	B	604/606 (100%)	569 (94%)	32 (5%)	3 (0%)	29	68
1	C	604/606 (100%)	562 (93%)	36 (6%)	6 (1%)	15	53
1	D	604/606 (100%)	561 (93%)	34 (6%)	9 (2%)	10	42
1	E	604/606 (100%)	560 (93%)	38 (6%)	6 (1%)	15	53
1	F	604/606 (100%)	564 (93%)	32 (5%)	8 (1%)	12	45
All	All	3624/3636 (100%)	3382 (93%)	201 (6%)	41 (1%)	14	50

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	ASP
1	A	516	ASN
1	C	483	ILE
1	C	517	LYS
1	D	408	ASP
1	D	488	ARG
1	E	488	ARG
1	F	488	ARG
1	A	429	VAL
1	B	429	VAL
1	D	516	ASN
1	E	408	ASP
1	F	429	VAL
1	F	514	THR
1	F	525	ASP
1	A	440	ASN
1	A	487	PRO
1	A	518	ASN
1	A	525	ASP
1	B	485	PRO
1	B	525	ASP
1	C	440	ASN
1	C	516	ASN
1	D	429	VAL
1	D	518	ASN
1	E	429	VAL
1	E	525	ASP
1	F	71	GLU

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Mol	Chain	Res	Type
1	F	490	VAL
1	A	490	VAL
1	C	429	VAL
1	D	490	VAL
1	D	525	ASP
1	C	487	PRO
1	F	483	ILE
1	E	314	GLU
1	E	87	ASN
1	F	484	PRO
1	D	489	GLY
1	A	421	PRO
1	D	513	GLY

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	515/518 (99%)	498 (97%)	17 (3%)	38	73
1	B	511/518 (99%)	495 (97%)	16 (3%)	40	75
1	C	511/518 (99%)	490 (96%)	21 (4%)	30	67
1	D	511/518 (99%)	494 (97%)	17 (3%)	38	73
1	E	510/518 (98%)	495 (97%)	15 (3%)	42	76
1	F	511/518 (99%)	495 (97%)	16 (3%)	40	75
All	All	3069/3108 (99%)	2967 (97%)	102 (3%)	38	73

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	66	VAL
1	A	118	LYS
1	A	131	ASP
1	A	176	PHE

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Mol	Chain	Res	Type
1	A	236	THR
1	A	303	HIS
1	A	383	GLU
1	A	413	ASP
1	A	469	THR
1	A	471	ASP
1	A	544	PHE
1	A	552	LYS
1	A	577	LYS
1	A	584	SER
1	A	610	GLU
1	A	617	LYS
1	B	46	LYS
1	B	66	VAL
1	B	83	GLN
1	B	118	LYS
1	B	131	ASP
1	B	176	PHE
1	B	236	THR
1	B	469	THR
1	B	471	ASP
1	B	491	PRO
1	B	544	PHE
1	B	552	LYS
1	B	567	SER
1	B	577	LYS
1	B	590	MET
1	B	617	LYS
1	C	26	ASP
1	C	46	LYS
1	C	66	VAL
1	C	118	LYS
1	C	131	ASP
1	C	175	TYR
1	C	176	PHE
1	C	236	THR
1	C	345	VAL
1	C	349	SER
1	C	410	ASP
1	C	434	THR
1	C	469	THR
1	C	471	ASP

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Mol	Chain	Res	Type
1	C	483	ILE
1	C	525	ASP
1	C	528	ARG
1	C	552	LYS
1	C	577	LYS
1	C	610	GLU
1	C	617	LYS
1	D	46	LYS
1	D	66	VAL
1	D	118	LYS
1	D	146	SER
1	D	175	TYR
1	D	176	PHE
1	D	236	THR
1	D	434	THR
1	D	469	THR
1	D	471	ASP
1	D	514	THR
1	D	528	ARG
1	D	544	PHE
1	D	552	LYS
1	D	567	SER
1	D	584	SER
1	D	617	LYS
1	E	66	VAL
1	E	118	LYS
1	E	175	TYR
1	E	176	PHE
1	E	236	THR
1	E	349	SER
1	E	383	GLU
1	E	434	THR
1	E	469	THR
1	E	471	ASP
1	E	552	LYS
1	E	567	SER
1	E	577	LYS
1	E	590	MET
1	E	617	LYS
1	F	46	LYS
1	F	83	GLN
1	F	118	LYS

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Mol	Chain	Res	Type
1	F	176	PHE
1	F	236	THR
1	F	247	THR
1	F	357	ASP
1	F	413	ASP
1	F	434	THR
1	F	469	THR
1	F	471	ASP
1	F	544	PHE
1	F	552	LYS
1	F	567	SER
1	F	590	MET
1	F	617	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	194	ASN
1	B	167	HIS
1	B	194	ASN
1	C	167	HIS
1	C	194	ASN
1	D	167	HIS
1	E	167	HIS
1	E	492	GLN
1	F	167	HIS
1	F	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 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$
5	SO4	A	808	-	4,4,4	0.41	0	6,6,6	0.39	0
5	SO4	C	806	-	4,4,4	0.30	0	6,6,6	0.37	0
5	SO4	B	808	-	4,4,4	0.41	0	6,6,6	0.44	0
5	SO4	D	808	-	4,4,4	0.37	0	6,6,6	0.25	0
2	ATP	E	801	3	26,33,33	1.00	1 (3%)	31,52,52	1.42	5 (16%)
2	ATP	F	801	3	26,33,33	1.10	2 (7%)	31,52,52	1.67	7 (22%)
2	ATP	C	801	3	26,33,33	0.87	0	31,52,52	1.64	7 (22%)
2	ATP	D	801	3	26,33,33	0.81	0	31,52,52	1.66	7 (22%)
2	ATP	A	801	3	26,33,33	0.92	0	31,52,52	1.60	7 (22%)
2	ATP	B	801	3	26,33,33	0.88	0	31,52,52	1.62	6 (19%)
5	SO4	E	806	-	4,4,4	0.37	0	6,6,6	0.55	0
5	SO4	F	806	-	4,4,4	0.33	0	6,6,6	0.34	0

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
2	ATP	E	801	3	-	5/18/38/38	0/3/3/3
2	ATP	F	801	3	-	1/18/38/38	0/3/3/3
2	ATP	C	801	3	-	1/18/38/38	0/3/3/3
2	ATP	D	801	3	-	1/18/38/38	0/3/3/3
2	ATP	A	801	3	-	1/18/38/38	0/3/3/3
2	ATP	B	801	3	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	ATP	C5-C4	2.76	1.48	1.40
2	E	801	ATP	C5-C4	2.25	1.46	1.40
2	F	801	ATP	C2-N3	2.03	1.35	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	ATP	PA-O3A-PB	-5.17	115.09	132.83
2	C	801	ATP	N3-C2-N1	-4.57	121.54	128.68
2	B	801	ATP	PA-O3A-PB	-4.49	117.41	132.83
2	D	801	ATP	PA-O3A-PB	-4.08	118.83	132.83
2	B	801	ATP	N3-C2-N1	-3.78	122.77	128.68
2	A	801	ATP	O3G-PG-O2G	3.69	121.74	107.64
2	F	801	ATP	N3-C2-N1	-3.57	123.09	128.68
2	D	801	ATP	N3-C2-N1	-3.50	123.20	128.68
2	C	801	ATP	PB-O3B-PG	-3.48	120.88	132.83
2	A	801	ATP	N3-C2-N1	-3.46	123.27	128.68
2	D	801	ATP	N6-C6-N1	3.24	125.30	118.57
2	C	801	ATP	C1'-N9-C4	-3.08	121.23	126.64
2	E	801	ATP	O4'-C1'-C2'	-2.95	102.61	106.93
2	A	801	ATP	C4-C5-N7	-2.90	106.38	109.40
2	E	801	ATP	C1'-N9-C4	-2.89	121.56	126.64
2	E	801	ATP	N3-C2-N1	-2.85	124.22	128.68
2	B	801	ATP	C1'-N9-C4	-2.85	121.63	126.64
2	A	801	ATP	C1'-N9-C4	-2.78	121.76	126.64
2	E	801	ATP	PB-O3B-PG	-2.69	123.59	132.83
2	D	801	ATP	C2-N1-C6	2.54	123.09	118.75
2	C	801	ATP	C2-N1-C6	2.53	123.08	118.75
2	C	801	ATP	C3'-C2'-C1'	2.40	104.59	100.98
2	C	801	ATP	O3G-PG-O2G	2.36	116.66	107.64
2	A	801	ATP	C2'-C3'-C4'	2.33	107.17	102.64
2	A	801	ATP	PA-O3A-PB	-2.30	124.93	132.83
2	D	801	ATP	O4'-C4'-C5'	-2.30	101.81	109.37
2	B	801	ATP	O3G-PG-O2G	2.23	116.18	107.64
2	F	801	ATP	C2-N1-C6	2.22	122.56	118.75
2	B	801	ATP	O3G-PG-O3B	2.21	112.04	104.64
2	E	801	ATP	C2-N1-C6	2.21	122.53	118.75
2	C	801	ATP	C4-C5-N7	-2.20	107.11	109.40
2	F	801	ATP	C1'-N9-C4	-2.17	122.83	126.64
2	F	801	ATP	N6-C6-N1	2.17	123.07	118.57
2	F	801	ATP	O3G-PG-O2G	2.14	115.83	107.64
2	D	801	ATP	O2A-PA-O1A	2.10	122.62	112.24
2	D	801	ATP	PB-O3B-PG	-2.09	125.66	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ATP	N6-C6-N1	2.08	122.90	118.57
2	F	801	ATP	O4'-C1'-C2'	-2.05	103.93	106.93
2	A	801	ATP	O3B-PG-O1G	-2.03	99.94	111.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	801	ATP	PB-O3B-PG-O2G
2	B	801	ATP	PB-O3B-PG-O3G
2	E	801	ATP	PB-O3B-PG-O3G
2	E	801	ATP	C5'-O5'-PA-O3A
2	E	801	ATP	PB-O3A-PA-O1A
2	C	801	ATP	C3'-C4'-C5'-O5'
2	D	801	ATP	PB-O3B-PG-O1G
2	A	801	ATP	PB-O3B-PG-O1G
2	B	801	ATP	PB-O3B-PG-O2G
2	E	801	ATP	PB-O3A-PA-O2A
2	F	801	ATP	PB-O3A-PA-O1A
2	B	801	ATP	C5'-O5'-PA-O1A

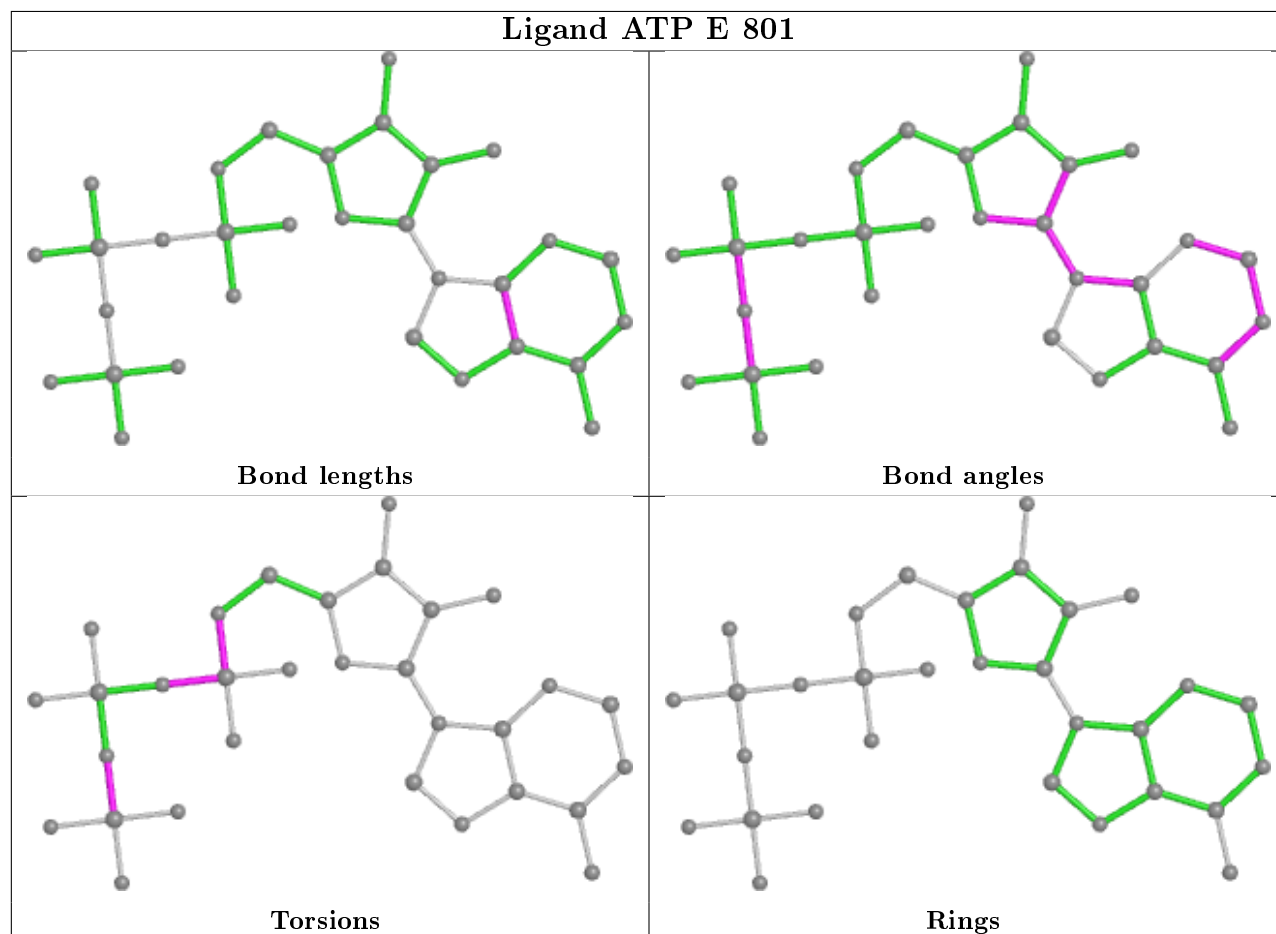
There are no ring outliers.

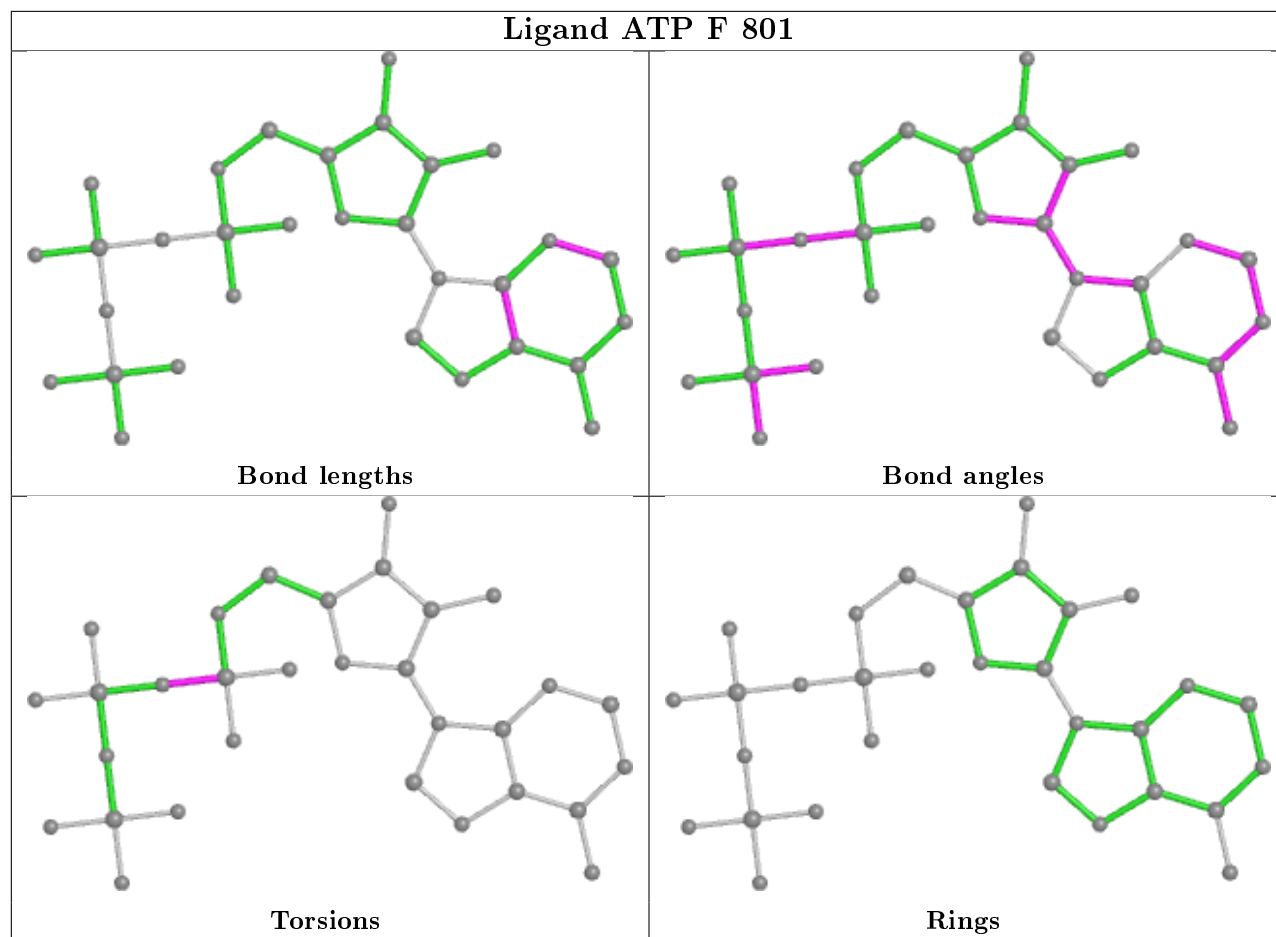
9 monomers are involved in 33 short contacts:

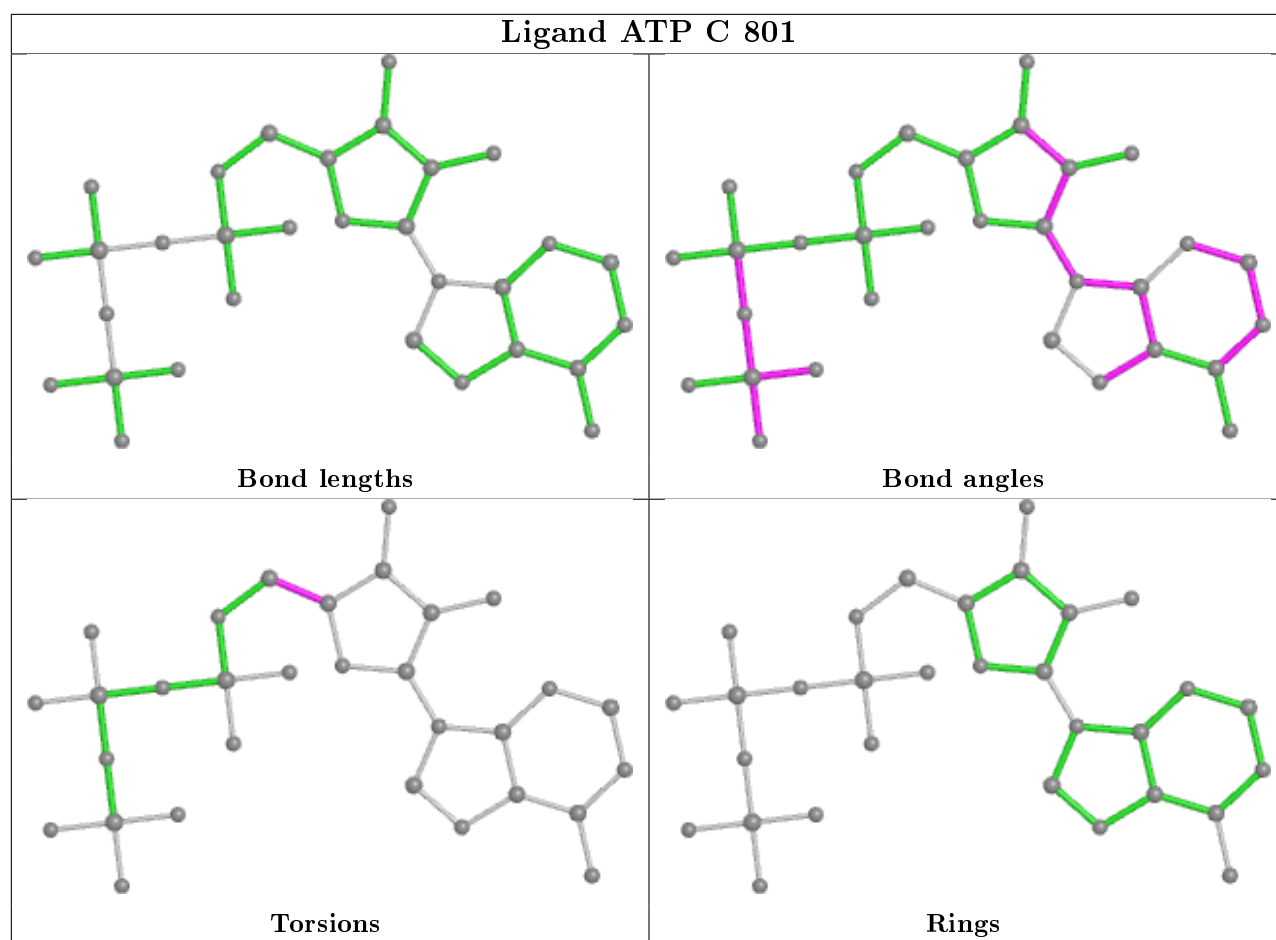
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	SO4	6	0
5	C	806	SO4	6	0
5	B	808	SO4	1	0
5	D	808	SO4	5	0
2	E	801	ATP	1	0
2	F	801	ATP	1	0
2	D	801	ATP	1	0
5	E	806	SO4	7	0
5	F	806	SO4	5	0

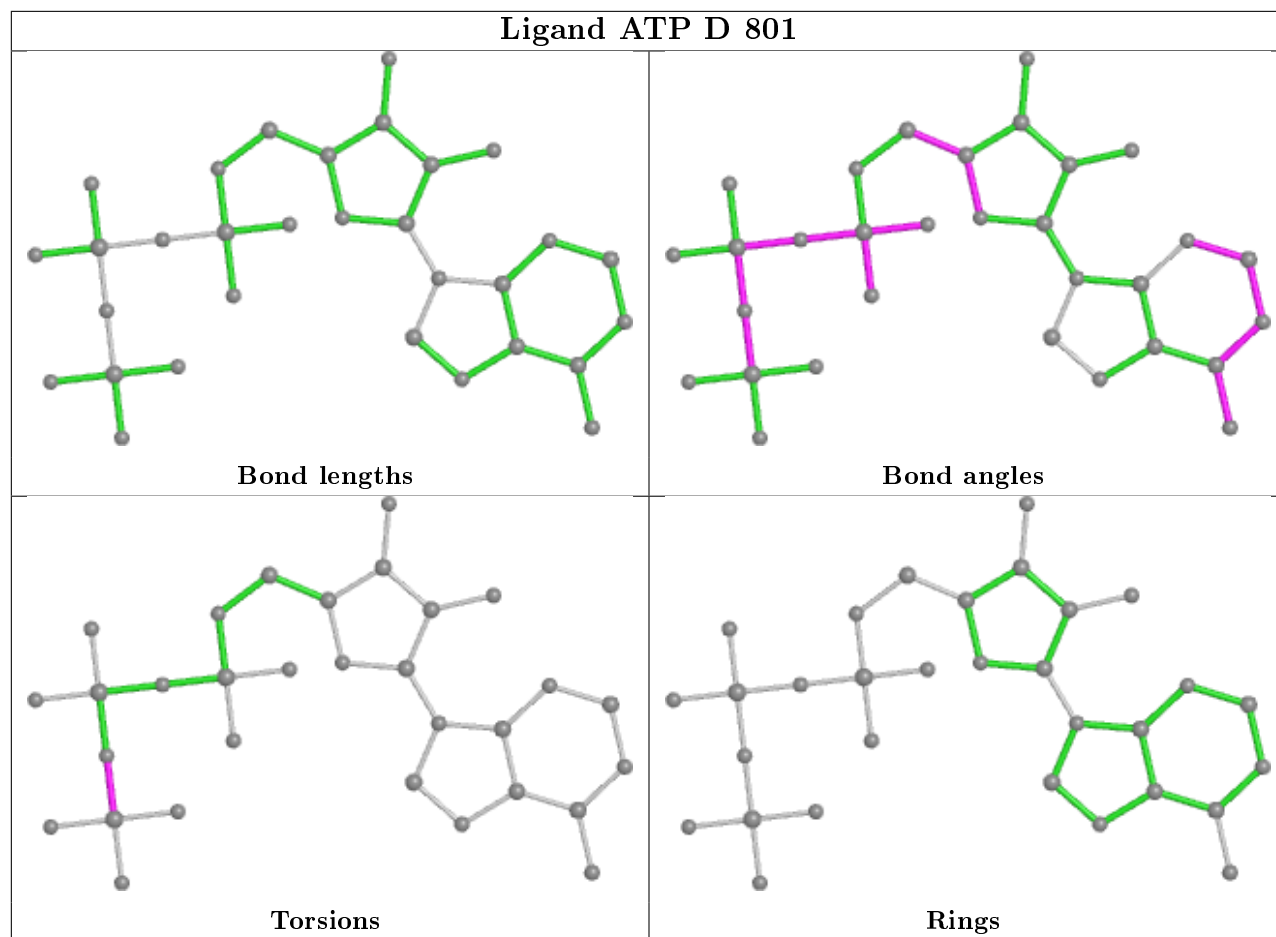
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

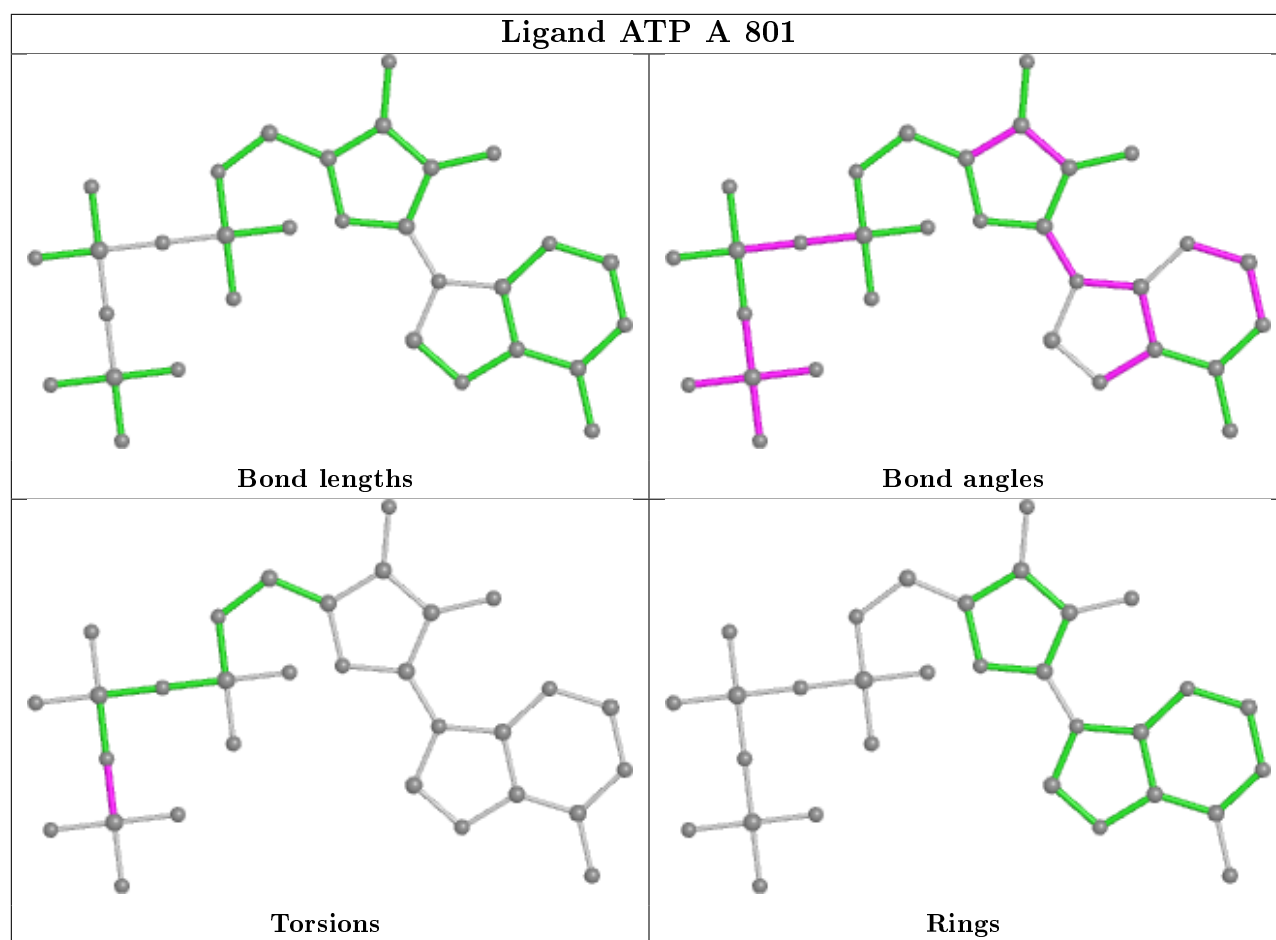
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

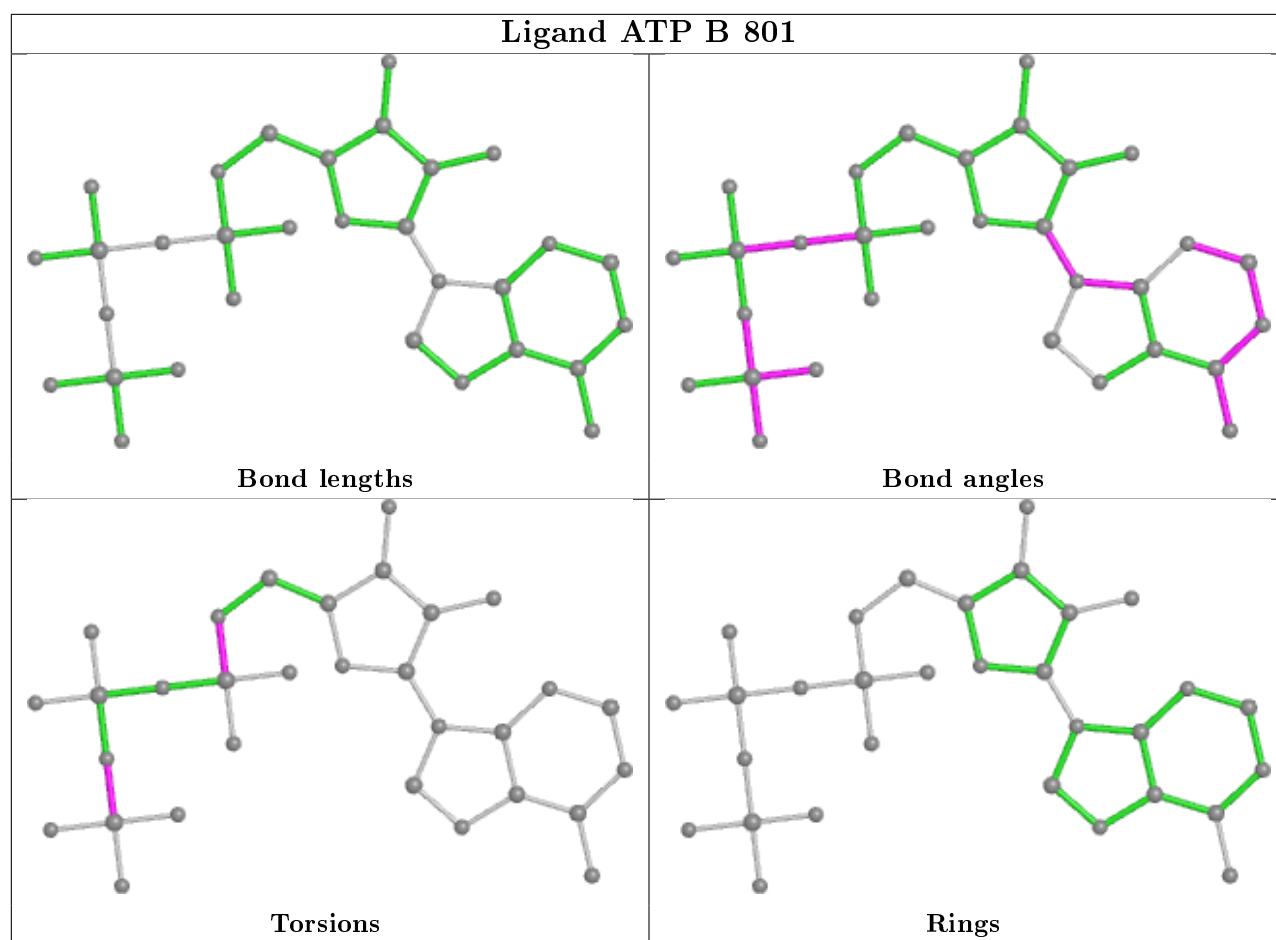












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

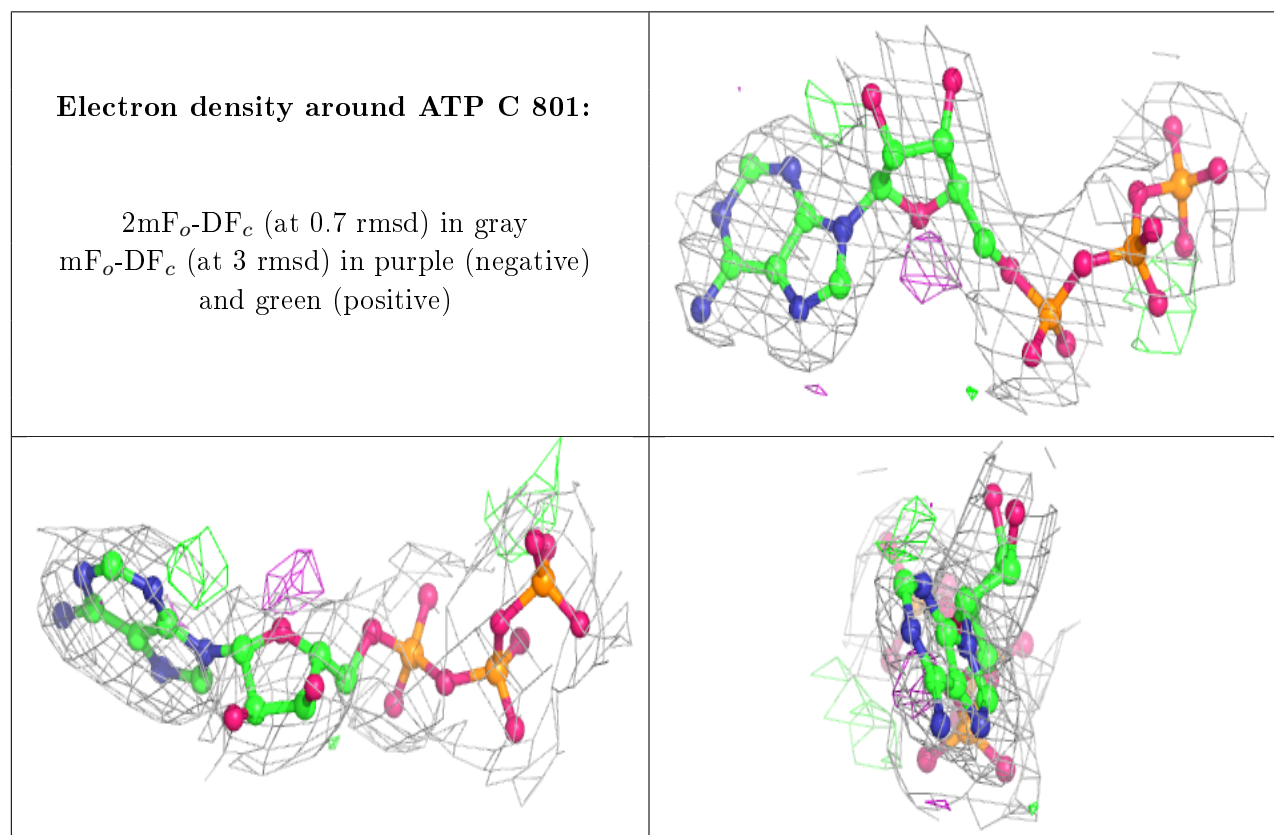
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

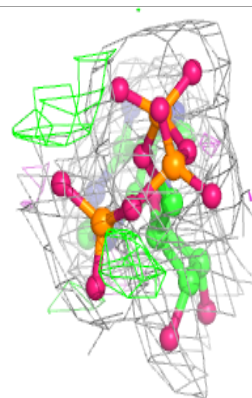
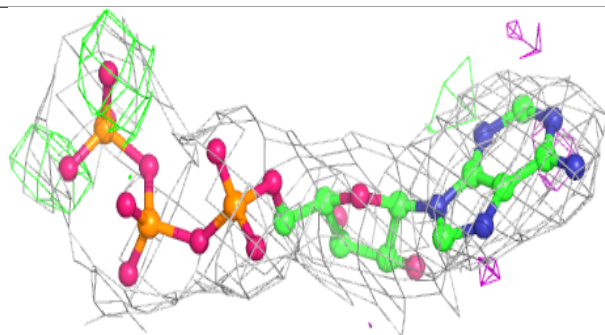
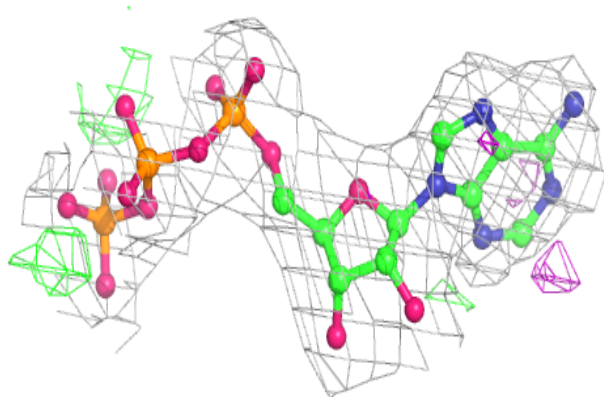
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

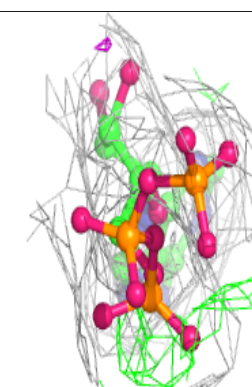
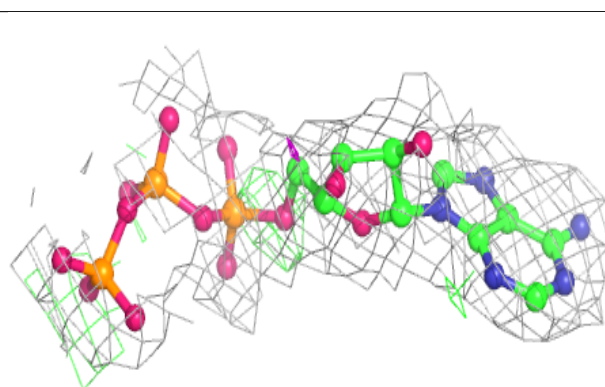
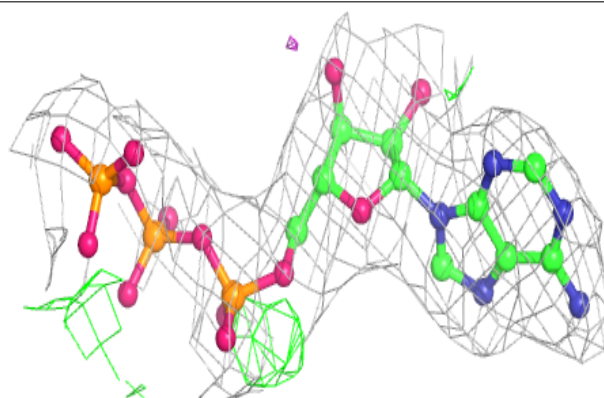


Electron density around ATP E 801:

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

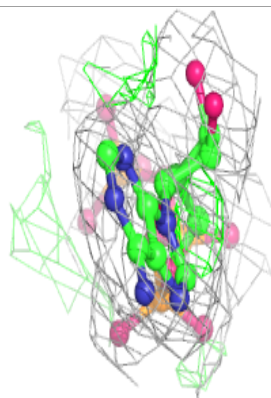
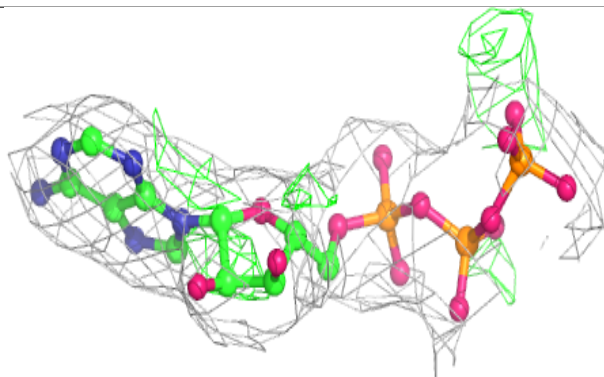
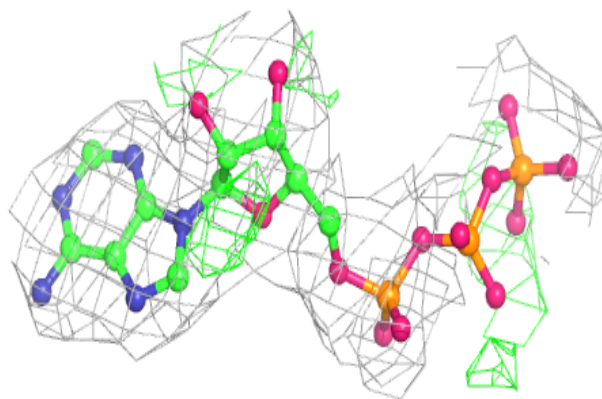
**Electron density around ATP D 801:**

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

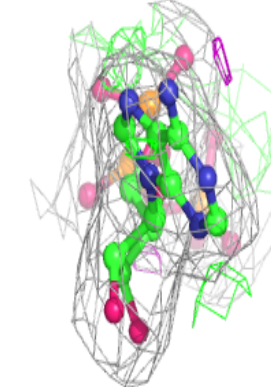
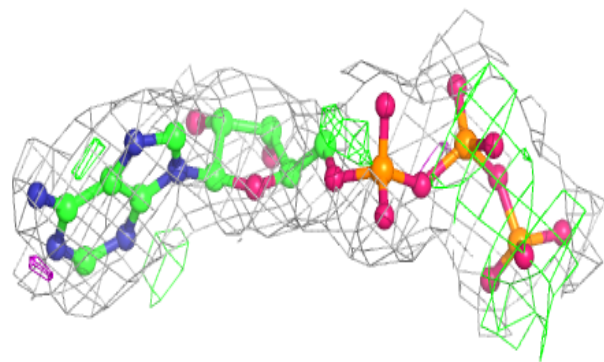
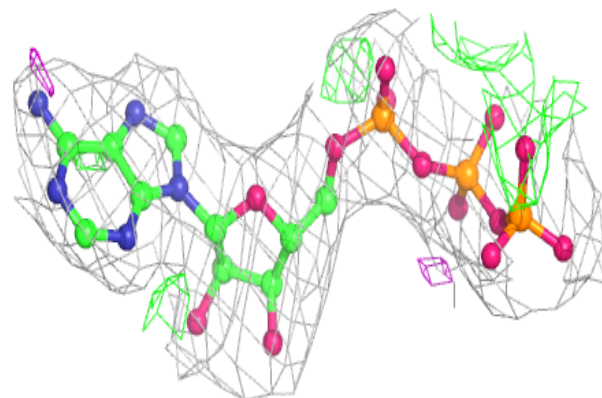


Electron density around ATP B 801:

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

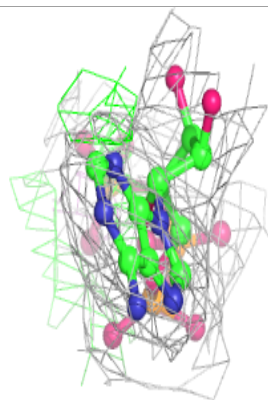
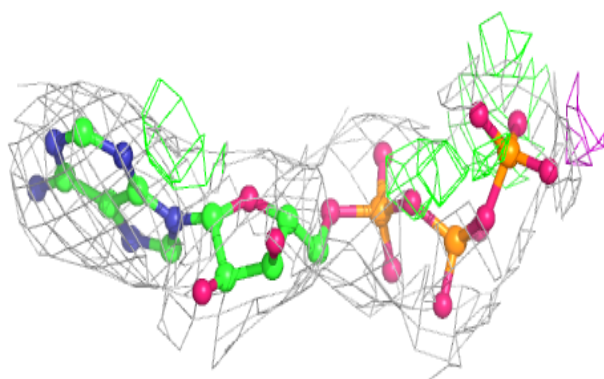
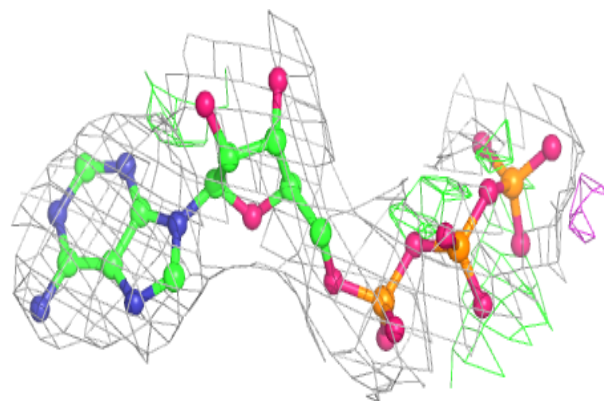
**Electron density around ATP A 801:**

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



Electron density around ATP F 801:

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.