Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 04:39 AM EDT

PDB ID	:	7TGK
Title	:	Crystal structure of ATP bound DesD, the desferrioxamine synthetase from the Streptomyces griseoflavus ferrimycin biosynthetic pathway
Authors	:	Patel, K.D.; Gulick, A.M.
Deposited on	:	2022-01-07
Resolution	:	2.30 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:

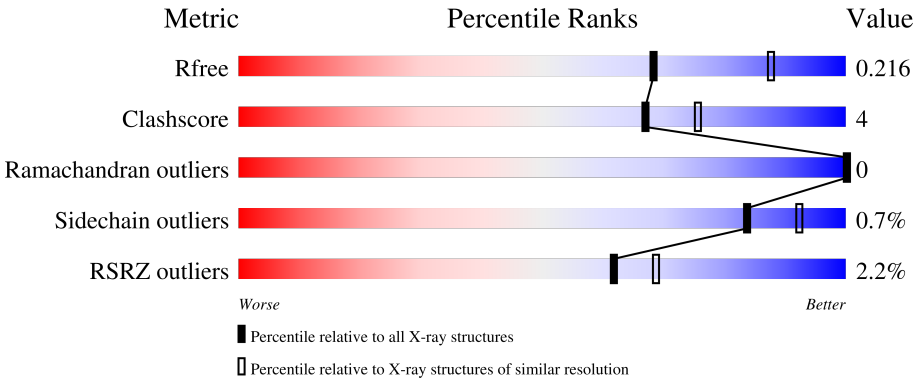
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	612	88% 8%
1	B	612	88% 8%
1	C	612	3% 87% 9%
1	D	612	88% 8%
1	E	612	89% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	611	-	-	-	X
2	SO4	D	608	-	-	-	X
2	SO4	E	602	-	-	X	-
6	MPD	A	616	-	-	-	X

2 Entry composition

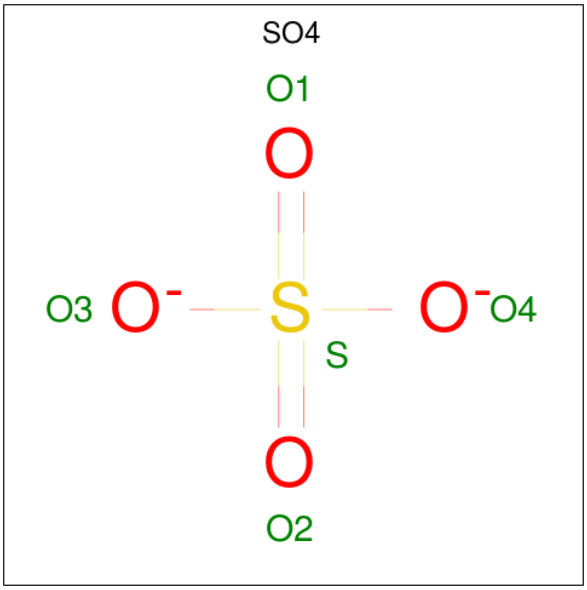
There are 7 unique types of molecules in this entry. The entry contains 47754 atoms, of which 23042 are hydrogens and 0 are deuteriums.

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 Desferrioxamine synthetase DesD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	593	Total	C	H	N	O	S	0	0	0
			9250	2981	4560	817	877	15			
1	B	593	Total	C	H	N	O	S	0	0	0
			9235	2978	4553	819	870	15			
1	E	593	Total	C	H	N	O	S	0	0	0
			9261	2983	4568	820	875	15			
1	A	592	Total	C	H	N	O	S	0	0	0
			9242	2977	4560	819	871	15			
1	C	592	Total	C	H	N	O	S	0	0	0
			9228	2975	4551	816	871	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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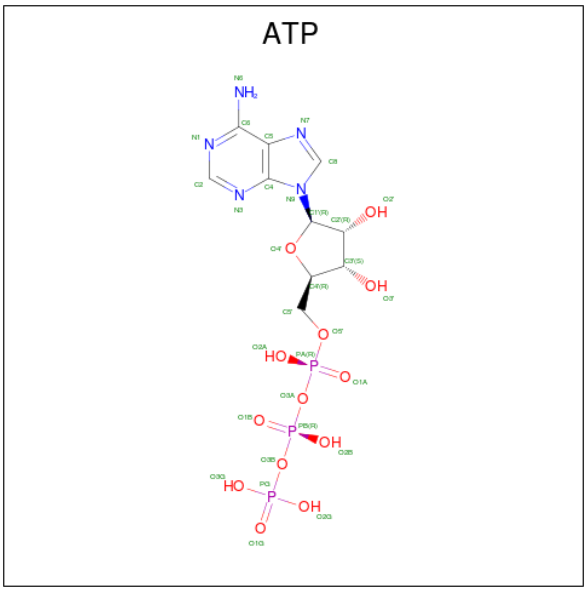
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

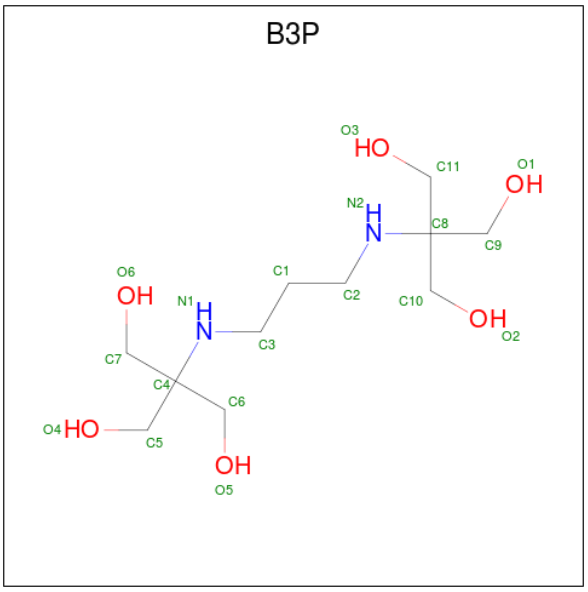


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
3	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
3	E	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
3	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
3	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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

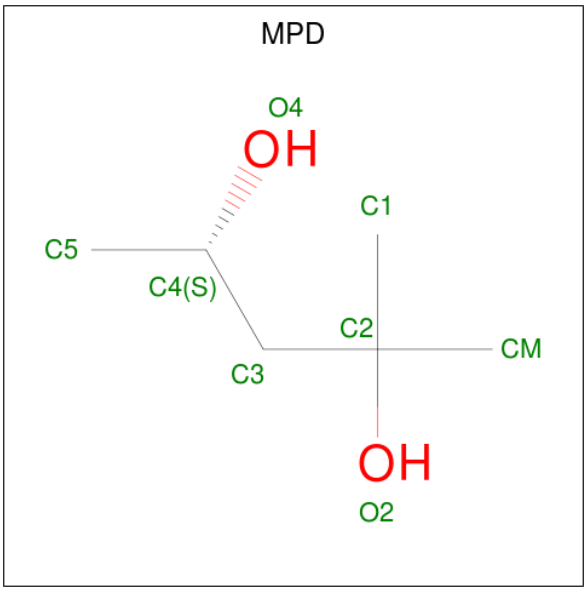
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
5	A	1	Total	C	H	N	O	0	0
			45	11	26	2	6		
5	C	1	Total	C	H	N	O	0	0
			45	11	26	2	6		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	0	0
			22	6	14	2		
6	D	1	Total	C	H	O	0	0
			22	6	14	2		
6	D	1	Total	C	H	O	0	0
			22	6	14	2		
6	B	1	Total	C	H	O	0	0
			22	6	14	2		
6	E	1	Total	C	H	O	0	0
			22	6	14	2		
6	A	1	Total	C	H	O	0	0
			22	6	14	2		
6	C	1	Total	C	H	O	0	0
			22	6	14	2		
6	C	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 7 is water.

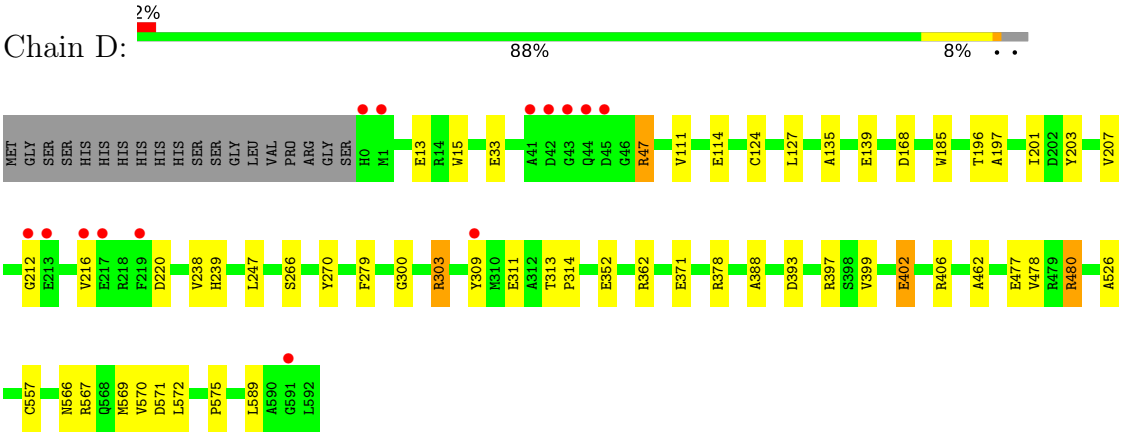
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	174	Total	O	0	0
			174	174		
7	B	202	Total	O	0	0
			202	202		
7	E	132	Total	O	0	0
			132	132		
7	A	183	Total	O	0	0
			183	183		
7	C	116	Total	O	0	0
			116	116		

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.

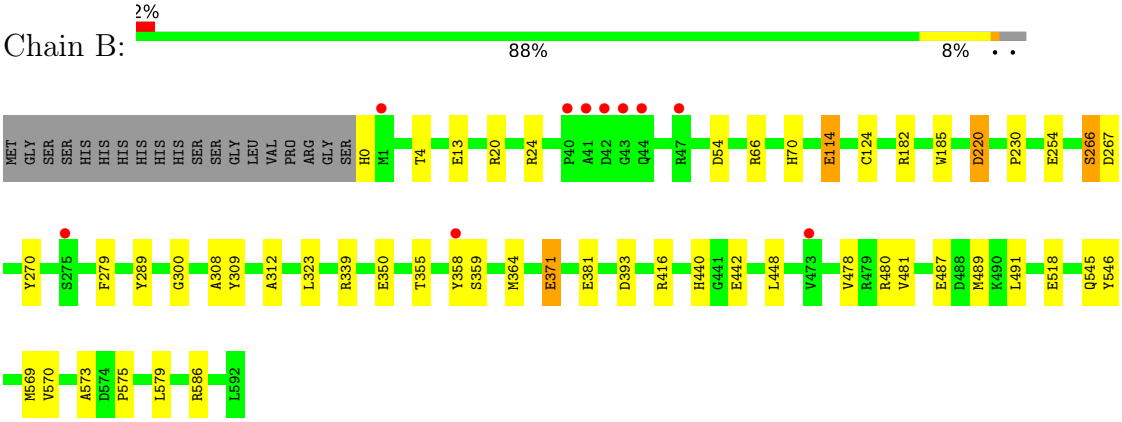
• Molecule 1: Desferrioxamine synthetase DesD

Chain D:



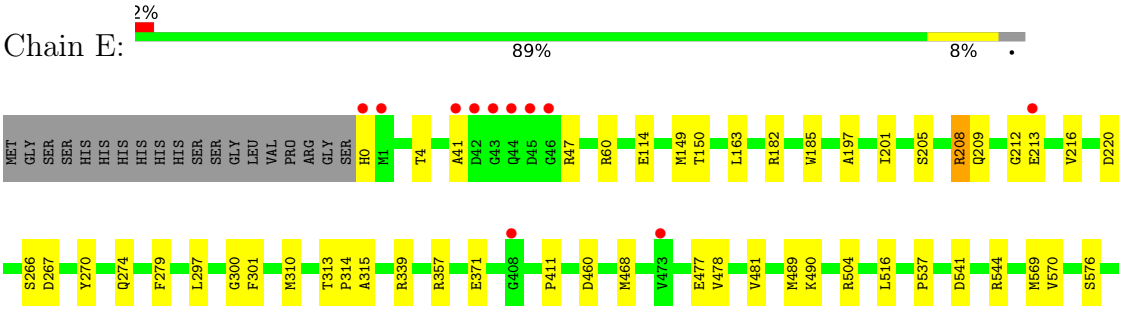
• Molecule 1: Desferrioxamine synthetase DesD

Chain B:



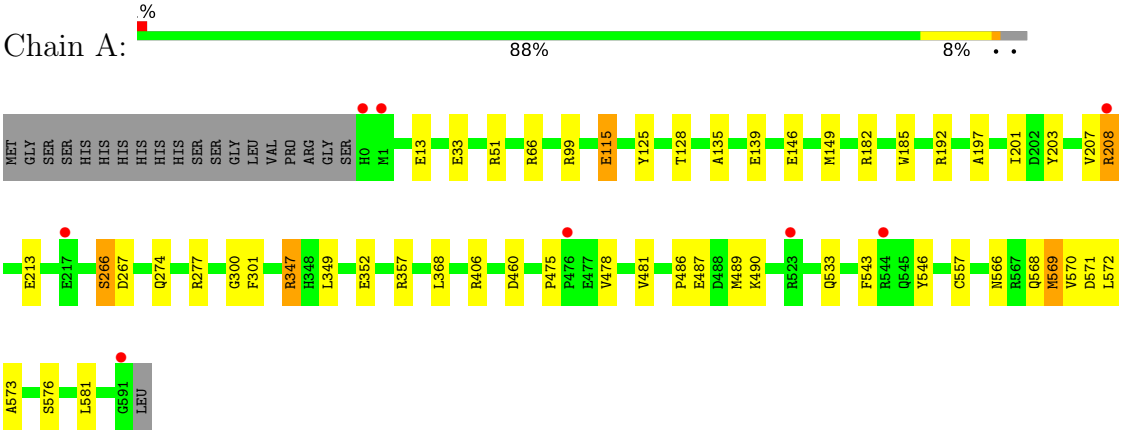
• Molecule 1: Desferrioxamine synthetase DesD

Chain E:



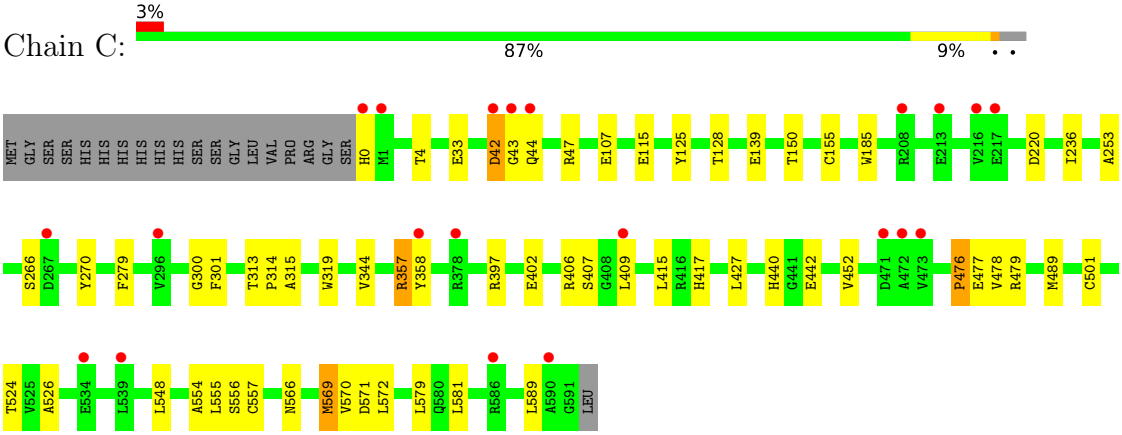
• Molecule 1: Desferrioxamine synthetase DesD

Chain A:



• Molecule 1: Desferrioxamine synthetase DesD

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.41Å 237.53Å 326.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.30 48.95 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-2.30) 92.2 (48.95-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.69 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.216 0.181 , 0.216	Depositor DCC
R_{free} test set	1978 reflections (0.91%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	47754	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, ATP, SO4, MG, B3P

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	0.76	4/4796 (0.1%)	0.77	5/6530 (0.1%)
1	B	0.77	6/4796 (0.1%)	0.80	8/6529 (0.1%)
1	C	0.72	4/4791 (0.1%)	0.71	3/6524 (0.0%)
1	D	0.72	5/4804 (0.1%)	0.77	7/6540 (0.1%)
1	E	0.67	1/4807 (0.0%)	0.71	3/6543 (0.0%)
All	All	0.73	20/23994 (0.1%)	0.75	26/32666 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	476	PRO	N-CD	-16.94	1.24	1.47
1	E	537	PRO	N-CD	-14.30	1.27	1.47
1	A	475	PRO	N-CD	-14.01	1.28	1.47
1	D	124	CYS	CB-SG	-7.20	1.70	1.82
1	B	350	GLU	CG-CD	6.64	1.61	1.51
1	C	107	GLU	CG-CD	6.21	1.61	1.51
1	C	155	CYS	CB-SG	-5.88	1.72	1.81
1	B	124	CYS	CB-SG	-5.79	1.72	1.81
1	B	13	GLU	CG-CD	5.69	1.60	1.51
1	B	266	SER	CB-OG	5.65	1.49	1.42
1	D	402	GLU	CD-OE1	-5.47	1.19	1.25
1	C	501	CYS	CB-SG	-5.41	1.73	1.81
1	B	416	ARG	CG-CD	5.35	1.65	1.51
1	D	13	GLU	CG-CD	5.19	1.59	1.51
1	A	13	GLU	CD-OE1	5.14	1.31	1.25
1	B	371	GLU	CB-CG	-5.13	1.42	1.52
1	A	266	SER	CB-OG	5.07	1.48	1.42
1	A	115	GLU	CD-OE1	-5.04	1.20	1.25
1	D	371	GLU	CB-CG	-5.03	1.42	1.52
1	D	114	GLU	CD-OE2	-5.01	1.20	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	402	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	C	43	GLY	N-CA-C	-6.70	96.35	113.10
1	A	460	ASP	CB-CG-OD1	6.66	124.30	118.30
1	C	42	ASP	N-CA-C	6.59	128.79	111.00
1	D	480	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	569	MET	CG-SD-CE	6.43	110.49	100.20
1	B	24	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	114	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	D	47	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	66	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	569	MET	CG-SD-CE	5.84	109.54	100.20
1	E	504	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	B	20	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	303	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	364	MET	CG-SD-CE	5.51	109.02	100.20
1	B	289	TYR	CA-CB-CG	5.44	123.73	113.40
1	B	254	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	B	393	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	D	362	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	114	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	E	114	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	E	460	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	277	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	B	54	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	393	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4682	4560	4562	31	0
1	B	4682	4553	4558	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4677	4551	4553	47	0
1	D	4690	4560	4561	37	0
1	E	4693	4568	4570	31	0
2	A	55	0	0	0	0
2	B	40	0	0	0	0
2	C	15	0	0	0	0
2	D	55	0	0	0	0
2	E	30	0	0	3	0
3	A	31	12	12	0	0
3	B	31	12	12	0	0
3	C	31	12	12	0	0
3	D	31	12	12	1	0
3	E	31	12	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	19	26	26	0	0
5	C	19	26	26	0	0
5	D	19	26	26	0	0
6	A	8	14	14	0	0
6	B	8	14	14	0	0
6	C	16	28	28	1	0
6	D	24	42	42	1	0
6	E	8	14	14	2	0
7	A	183	0	0	0	0
7	B	202	0	0	1	0
7	C	116	0	0	0	0
7	D	174	0	0	0	0
7	E	132	0	0	0	0
All	All	24712	23042	23054	182	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 4.

All (182) 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:B:309:TYR:CE1	1:B:480:ARG:CZ	1.97	1.47
1:C:357:ARG:HG3	1:C:358:TYR:CE2	1.86	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TYR:CZ	1:B:480:ARG:NH2	2.22	1.07
1:E:205:SER:O	1:E:209:GLN:HG3	1.61	0.99
1:B:309:TYR:CE1	1:B:480:ARG:NH2	2.32	0.96
1:B:309:TYR:CE1	1:B:480:ARG:NE	2.35	0.95
1:C:44:GLN:HG2	1:C:47:ARG:HH21	1.36	0.90
1:B:309:TYR:CD1	1:B:480:ARG:NH1	2.39	0.90
1:D:309:TYR:CZ	1:D:480:ARG:NH2	2.40	0.89
1:C:556:SER:HA	1:C:581:LEU:HD23	1.56	0.85
1:B:309:TYR:CE1	1:B:480:ARG:NH1	2.44	0.84
1:D:309:TYR:CE1	1:D:480:ARG:NH2	2.44	0.84
1:B:309:TYR:CZ	1:B:480:ARG:CZ	2.59	0.83
1:D:309:TYR:CE1	1:D:480:ARG:CZ	2.63	0.82
1:C:44:GLN:CG	1:C:47:ARG:HH21	1.94	0.81
1:B:309:TYR:CD1	1:B:480:ARG:CZ	2.64	0.80
1:B:114:GLU:OE1	7:B:701:HOH:O	1.97	0.80
1:E:60:ARG:NH2	2:E:602:SO4:O1	2.14	0.80
1:A:115:GLU:OE2	1:A:566:ASN:OD1	2.00	0.78
1:B:309:TYR:HE1	1:B:480:ARG:NE	1.77	0.78
1:C:315:ALA:HB1	1:C:477:GLU:HG3	1.65	0.77
1:B:358:TYR:OH	1:B:573:ALA:HB2	1.86	0.75
1:C:556:SER:HB2	1:C:581:LEU:HD21	1.68	0.74
1:C:357:ARG:CG	1:C:358:TYR:CE2	2.70	0.74
1:C:554:ALA:CB	1:C:581:LEU:HD13	2.20	0.72
1:D:571:ASP:O	1:D:572:LEU:HB2	1.91	0.71
1:D:203:TYR:O	1:D:207:VAL:HG22	1.91	0.70
1:C:556:SER:HB2	1:C:581:LEU:CD2	2.22	0.70
1:B:66:ARG:HD2	1:B:518:GLU:OE2	1.94	0.68
1:A:347:ARG:HD2	1:A:352:GLU:OE2	1.96	0.66
1:C:556:SER:CA	1:C:581:LEU:HD23	2.24	0.66
1:D:309:TYR:CD1	1:D:480:ARG:NH2	2.64	0.66
1:C:150:THR:HG21	6:C:609:MPD:H31	1.79	0.65
1:D:300:GLY:HA3	1:D:569:MET:HG3	1.79	0.65
1:B:312:ALA:HB3	1:B:480:ARG:CZ	2.26	0.65
1:D:309:TYR:CE2	1:D:480:ARG:NH2	2.63	0.64
1:C:185:TRP:HE1	1:C:266:SER:HB3	1.63	0.64
1:B:182:ARG:NH1	1:B:267:ASP:O	2.31	0.63
1:A:571:ASP:O	1:A:572:LEU:HB2	1.98	0.63
1:B:487:GLU:OE2	1:B:545:GLN:NE2	2.32	0.63
1:B:220:ASP:OD2	1:B:230:PRO:HG2	1.99	0.62
1:E:208:ARG:HD2	1:E:213:GLU:HG3	1.80	0.62
1:D:185:TRP:HE1	1:D:266:SER:HB3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:ARG:HG3	1:C:358:TYR:CD2	2.35	0.62
1:E:150:THR:HG21	6:E:610:MPD:H31	1.81	0.61
1:B:309:TYR:HE1	1:B:480:ARG:CZ	1.87	0.61
1:A:487:GLU:OE2	1:A:546:TYR:CE1	2.53	0.61
1:B:300:GLY:HA3	1:B:569:MET:HG3	1.81	0.61
1:C:554:ALA:HB1	1:C:581:LEU:HD13	1.82	0.61
1:A:571:ASP:OD2	1:A:573:ALA:HB3	2.00	0.60
1:B:66:ARG:HB2	1:B:70:HIS:HB3	1.84	0.59
1:D:309:TYR:CD1	1:D:480:ARG:CZ	2.85	0.59
1:C:300:GLY:HA3	1:C:569:MET:HG3	1.85	0.59
1:C:44:GLN:CG	1:C:47:ARG:NH2	2.64	0.59
1:D:127:LEU:HD21	6:D:616:MPD:H53	1.84	0.59
1:A:182:ARG:NH1	1:A:267:ASP:O	2.35	0.59
1:D:309:TYR:OH	1:D:462:ALA:O	2.19	0.58
1:A:208:ARG:NH1	1:A:213:GLU:CD	2.56	0.58
1:C:571:ASP:O	1:C:572:LEU:HB2	2.02	0.58
1:E:339:ARG:NH2	1:E:371:GLU:OE2	2.28	0.58
1:E:0:HIS:O	1:E:4:THR:HG23	2.04	0.58
1:E:315:ALA:CB	1:E:477:GLU:HG3	2.33	0.58
1:E:197:ALA:HB1	1:E:201:ILE:HB	1.86	0.57
1:C:556:SER:CB	1:C:581:LEU:CD2	2.82	0.57
1:A:185:TRP:HE1	1:A:266:SER:HB3	1.68	0.57
1:E:489:MET:CE	1:E:576:SER:HB2	2.35	0.57
1:C:555:LEU:O	1:C:581:LEU:HA	2.05	0.57
1:B:570:VAL:HG13	1:B:575:PRO:HA	1.87	0.57
1:A:149:MET:HE2	1:A:149:MET:HA	1.85	0.57
1:A:301:PHE:HZ	1:A:570:VAL:HG22	1.68	0.56
1:B:309:TYR:CE2	1:B:480:ARG:NH2	2.73	0.56
1:C:44:GLN:HG2	1:C:47:ARG:NH2	2.12	0.56
1:C:402:GLU:OE2	1:C:406:ARG:HD2	2.05	0.56
1:E:315:ALA:HB1	1:E:477:GLU:HG3	1.87	0.55
1:E:60:ARG:NH2	2:E:602:SO4:S	2.78	0.55
1:D:402:GLU:HG3	1:D:406:ARG:HD2	1.89	0.54
1:A:135:ALA:HB1	1:A:406:ARG:HH21	1.72	0.54
1:B:489:MET:CE	1:B:579:LEU:HD12	2.36	0.54
1:C:407:SER:HB2	1:C:409:LEU:HD13	1.89	0.54
1:E:300:GLY:HA3	1:E:569:MET:HE2	1.90	0.54
1:D:309:TYR:CE1	1:D:480:ARG:NE	2.75	0.54
1:C:556:SER:CA	1:C:581:LEU:CD2	2.86	0.54
1:D:571:ASP:O	1:D:572:LEU:CB	2.57	0.53
1:B:185:TRP:HE1	1:B:266:SER:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ALA:HB3	1:B:480:ARG:NH1	2.24	0.52
1:E:468:MET:HB3	1:E:490:LYS:HE3	1.92	0.52
1:D:197:ALA:HB1	1:D:201:ILE:HB	1.90	0.51
1:E:310:MET:CE	1:E:310:MET:HA	2.41	0.51
1:C:139:GLU:OE2	1:C:139:GLU:HA	2.09	0.51
1:B:308:ALA:HB1	1:C:42:ASP:CB	2.41	0.51
1:E:185:TRP:HE1	1:E:266:SER:HB3	1.76	0.51
1:E:41:ALA:HB2	1:E:47:ARG:O	2.11	0.51
1:D:15:TRP:CZ2	1:C:253:ALA:HB2	2.46	0.51
1:C:409:LEU:N	1:C:409:LEU:HD12	2.26	0.50
1:C:407:SER:O	1:C:409:LEU:HD12	2.12	0.50
1:E:313:THR:HB	1:E:314:PRO:HD3	1.93	0.50
1:B:312:ALA:HB3	1:B:480:ARG:NH2	2.27	0.50
1:A:487:GLU:OE2	1:A:546:TYR:CZ	2.65	0.50
1:C:476:PRO:O	1:C:479:ARG:HG2	2.13	0.49
1:D:309:TYR:CD2	1:D:480:ARG:NH2	2.81	0.49
1:C:407:SER:CB	1:C:409:LEU:HD13	2.43	0.49
1:C:115:GLU:OE1	1:C:566:ASN:OD1	2.31	0.48
1:A:489:MET:HE1	1:A:576:SER:HB2	1.95	0.48
1:E:489:MET:HE1	1:E:576:SER:HB2	1.95	0.48
1:A:533:GLN:HG2	1:A:543:PHE:CZ	2.48	0.48
1:A:192:ARG:CZ	1:A:349:LEU:HD23	2.44	0.48
1:E:411:PRO:HB2	1:E:516:LEU:HD13	1.96	0.48
1:C:0:HIS:O	1:C:4:THR:HG23	2.13	0.48
1:A:301:PHE:CZ	1:A:570:VAL:HG22	2.48	0.47
1:D:309:TYR:CG	1:D:480:ARG:NH2	2.83	0.47
1:C:417:HIS:HD2	1:C:452:VAL:HG11	1.79	0.47
1:C:319:TRP:CG	1:C:478:VAL:HG21	2.49	0.47
1:D:526:ALA:HB2	1:D:589:LEU:HD22	1.97	0.46
1:E:301:PHE:HZ	1:E:570:VAL:HG22	1.80	0.46
1:A:300:GLY:HA3	1:A:569:MET:HG3	1.97	0.46
1:E:270:TYR:HB3	1:E:279:PHE:HB3	1.98	0.46
1:E:300:GLY:HA3	1:E:569:MET:HG3	1.97	0.46
1:C:489:MET:CE	1:C:579:LEU:HD12	2.45	0.46
1:B:478:VAL:O	1:B:481:VAL:HG22	2.16	0.46
1:A:487:GLU:OE2	1:A:546:TYR:OH	2.31	0.46
1:D:313:THR:HB	1:D:314:PRO:HD3	1.97	0.45
1:D:352:GLU:O	1:A:51:ARG:NH1	2.50	0.45
1:B:300:GLY:CA	1:B:569:MET:HG3	2.45	0.45
1:B:339:ARG:NH2	1:B:371:GLU:OE2	2.34	0.45
1:D:33:GLU:OE1	1:D:557:CYS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PRO:O	1:A:490:LYS:HG3	2.15	0.45
1:B:491:LEU:HD22	1:B:546:TYR:HB3	1.97	0.45
1:D:478:VAL:HG12	1:D:478:VAL:O	2.17	0.44
1:A:149:MET:HA	1:A:149:MET:CE	2.47	0.44
1:D:168:ASP:OD1	1:D:168:ASP:N	2.50	0.44
1:D:300:GLY:CA	1:D:569:MET:HG3	2.46	0.44
1:A:478:VAL:O	1:A:481:VAL:HG22	2.17	0.44
1:A:533:GLN:HG2	1:A:543:PHE:CE2	2.52	0.44
1:A:581:LEU:HD12	1:A:581:LEU:N	2.32	0.44
1:C:301:PHE:HZ	1:C:570:VAL:HG22	1.81	0.44
1:A:33:GLU:OE1	1:A:557:CYS:HB3	2.17	0.44
1:D:212:GLY:O	1:D:216:VAL:HG23	2.18	0.44
1:B:355:THR:HB	1:B:359:SER:HB2	2.00	0.44
1:D:196:THR:HG21	1:D:311:GLU:O	2.17	0.44
1:D:270:TYR:HB3	1:D:279:PHE:HB3	2.00	0.43
6:E:610:MPD:HM1	6:E:610:MPD:O4	2.18	0.43
1:D:303:ARG:NH1	3:D:612:ATP:H5'1	2.33	0.43
1:E:182:ARG:NH1	1:E:267:ASP:O	2.50	0.43
1:E:310:MET:HA	1:E:310:MET:HE2	2.00	0.43
1:A:135:ALA:HB1	1:A:406:ARG:NH2	2.33	0.43
1:E:41:ALA:HB2	1:E:47:ARG:HB3	2.01	0.43
1:E:149:MET:HG3	1:E:274:GLN:NE2	2.34	0.43
1:C:33:GLU:OE1	1:C:557:CYS:HB3	2.19	0.43
1:C:270:TYR:HB3	1:C:279:PHE:HB3	2.00	0.43
1:E:212:GLY:O	1:E:216:VAL:HG23	2.18	0.43
1:A:146:GLU:OE2	1:A:274:GLN:HG3	2.18	0.43
1:D:111:VAL:HG12	1:D:566:ASN:HD21	1.81	0.43
1:B:323:LEU:HD23	1:B:323:LEU:C	2.39	0.43
1:C:44:GLN:HG3	1:C:47:ARG:NH2	2.32	0.43
1:E:60:ARG:NH2	2:E:602:SO4:O4	2.50	0.42
1:C:526:ALA:HB2	1:C:589:LEU:HD22	2.01	0.42
1:A:368:LEU:C	1:A:368:LEU:HD12	2.40	0.42
1:E:163:LEU:HD12	1:E:297:LEU:HD23	2.00	0.42
1:C:427:LEU:CD2	1:C:548:LEU:HD11	2.50	0.42
1:A:197:ALA:HB1	1:A:201:ILE:HB	2.01	0.42
1:D:238:VAL:HG12	1:D:239:HIS:O	2.20	0.42
1:A:203:TYR:O	1:A:207:VAL:HG22	2.20	0.42
1:D:570:VAL:HG13	1:D:575:PRO:HA	2.01	0.42
1:D:238:VAL:HG11	1:D:247:LEU:HD12	2.02	0.41
1:E:478:VAL:O	1:E:481:VAL:HG22	2.20	0.41
1:C:125:TYR:O	1:C:128:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:556:SER:CB	1:C:581:LEU:HD21	2.45	0.41
1:E:541:ASP:OD1	1:E:544:ARG:NH2	2.54	0.41
1:D:135:ALA:O	1:D:139:GLU:HG2	2.20	0.41
1:D:388:ALA:O	1:D:399:VAL:HB	2.21	0.41
1:B:358:TYR:OH	1:B:573:ALA:CB	2.65	0.41
1:B:440:HIS:CE1	1:B:442:GLU:HB3	2.56	0.41
1:C:415:LEU:HD23	1:C:524:THR:HB	2.02	0.41
1:C:440:HIS:CE1	1:C:442:GLU:HB3	2.56	0.41
1:D:477:GLU:H	1:D:477:GLU:CD	2.22	0.41
1:B:309:TYR:HE1	1:B:480:ARG:CD	2.34	0.41
1:A:125:TYR:O	1:A:128:THR:HB	2.21	0.41
1:B:270:TYR:HB3	1:B:279:PHE:HB3	2.04	0.40
1:C:236:ILE:HG12	1:C:344:VAL:HG21	2.03	0.40
1:B:381:GLU:HA	1:B:448:LEU:O	2.21	0.40
1:B:0:HIS:O	1:B:4:THR:HG23	2.21	0.40
1:C:313:THR:HB	1:C:314:PRO:HD3	2.03	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	590/612 (96%)	576 (98%)	14 (2%)	0	100	100
1	B	591/612 (97%)	578 (98%)	13 (2%)	0	100	100
1	C	590/612 (96%)	579 (98%)	11 (2%)	0	100	100
1	D	591/612 (97%)	578 (98%)	13 (2%)	0	100	100
1	E	591/612 (97%)	577 (98%)	14 (2%)	0	100	100
All	All	2953/3060 (96%)	2888 (98%)	65 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	483/504 (96%)	478 (99%)	5 (1%)	76 87
1	B	481/504 (95%)	479 (100%)	2 (0%)	91 96
1	C	482/504 (96%)	479 (99%)	3 (1%)	86 94
1	D	484/504 (96%)	479 (99%)	5 (1%)	76 87
1	E	484/504 (96%)	481 (99%)	3 (1%)	86 94
All	All	2414/2520 (96%)	2396 (99%)	18 (1%)	84 92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	47	ARG
1	D	220	ASP
1	D	378	ARG
1	D	397	ARG
1	D	567	ARG
1	B	220	ASP
1	B	586	ARG
1	E	208	ARG
1	E	220	ASP
1	E	357	ARG
1	A	139	GLU
1	A	208	ARG
1	A	347	ARG
1	A	357	ARG
1	A	568	GLN
1	C	220	ASP
1	C	357	ARG
1	C	397	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	209	GLN
1	D	566	ASN
1	B	209	GLN
1	B	326	ASN
1	B	566	ASN
1	E	274	GLN
1	A	566	ASN
1	C	326	ASN
1	C	417	HIS
1	C	533	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 65 ligands modelled in this entry, 10 are monoatomic - leaving 55 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	$\#\|Z\| > 2$
2	SO4	A	601	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	B	604	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	B	608	-	4,4,4	0.13	0	6,6,6	0.07	0
6	MPD	D	618	-	7,7,7	0.98	1 (14%)	9,10,10	0.44	0
2	SO4	C	602	-	4,4,4	0.16	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	606	-	4,4,4	0.31	0	6,6,6	0.31	0
2	SO4	C	601	-	4,4,4	0.18	0	6,6,6	0.16	0
2	SO4	D	602	-	4,4,4	0.11	0	6,6,6	0.06	0
2	SO4	A	602	-	4,4,4	0.27	0	6,6,6	0.28	0
3	ATP	A	612	4	26,33,33	1.48	1 (3%)	31,52,52	1.61	6 (19%)
2	SO4	A	603	-	4,4,4	0.11	0	6,6,6	0.20	0
2	SO4	A	609	-	4,4,4	0.19	0	6,6,6	0.13	0
6	MPD	B	612	-	7,7,7	0.94	1 (14%)	9,10,10	0.37	0
5	B3P	A	615	-	18,18,18	0.58	0	21,23,23	1.21	4 (19%)
2	SO4	D	609	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	D	608	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	E	602	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	E	603	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	D	610	-	4,4,4	0.12	0	6,6,6	0.15	0
2	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	B	605	-	4,4,4	0.10	0	6,6,6	0.11	0
2	SO4	D	604	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	A	608	-	4,4,4	0.17	0	6,6,6	0.11	0
2	SO4	A	610	-	4,4,4	0.33	0	6,6,6	0.30	0
2	SO4	D	611	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	611	-	4,4,4	0.20	0	6,6,6	0.10	0
2	SO4	D	606	-	4,4,4	0.43	0	6,6,6	0.38	0
3	ATP	B	609	4	26,33,33	1.32	4 (15%)	31,52,52	1.41	6 (19%)
2	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	603	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	E	605	-	4,4,4	0.16	0	6,6,6	0.17	0
6	MPD	A	616	-	7,7,7	0.64	0	9,10,10	0.53	0
6	MPD	D	616	-	7,7,7	0.80	0	9,10,10	0.32	0
2	SO4	E	606	-	4,4,4	0.12	0	6,6,6	0.17	0
6	MPD	C	609	-	7,7,7	0.98	1 (14%)	9,10,10	0.44	0
2	SO4	B	607	-	4,4,4	0.36	0	6,6,6	0.26	0
2	SO4	D	607	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	A	607	-	4,4,4	0.39	0	6,6,6	0.12	0
6	MPD	C	608	-	7,7,7	0.64	0	9,10,10	0.24	0
3	ATP	C	604	4	26,33,33	1.34	3 (11%)	31,52,52	1.48	7 (22%)
6	MPD	E	610	-	7,7,7	1.10	1 (14%)	9,10,10	0.42	0
2	SO4	E	601	-	4,4,4	0.21	0	6,6,6	0.20	0
5	B3P	C	607	-	18,18,18	0.65	0	21,23,23	1.14	2 (9%)
2	SO4	E	604	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	D	603	-	4,4,4	0.10	0	6,6,6	0.37	0
5	B3P	D	615	-	18,18,18	0.43	0	21,23,23	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	601	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	D	601	-	4,4,4	0.16	0	6,6,6	0.20	0
3	ATP	E	607	4	26,33,33	1.26	3 (11%)	31,52,52	1.03	2 (6%)
2	SO4	A	605	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	B	602	-	4,4,4	0.19	0	6,6,6	0.22	0
2	SO4	B	603	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	D	605	-	4,4,4	0.16	0	6,6,6	0.13	0
3	ATP	D	612	4	26,33,33	1.50	3 (11%)	31,52,52	1.66	7 (22%)
6	MPD	D	617	-	7,7,7	0.91	1 (14%)	9,10,10	0.41	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
6	MPD	C	608	-	-	1/5/5/5	-
3	ATP	B	609	4	-	2/18/38/38	0/3/3/3
5	B3P	D	615	-	-	3/28/28/28	-
3	ATP	C	604	4	-	3/18/38/38	0/3/3/3
6	MPD	D	618	-	-	0/5/5/5	-
5	B3P	C	607	-	-	3/28/28/28	-
3	ATP	E	607	4	-	1/18/38/38	0/3/3/3
3	ATP	A	612	4	-	4/18/38/38	0/3/3/3
6	MPD	B	612	-	-	0/5/5/5	-
6	MPD	D	616	-	-	0/5/5/5	-
6	MPD	A	616	-	-	0/5/5/5	-
5	B3P	A	615	-	-	10/28/28/28	-
6	MPD	C	609	-	-	0/5/5/5	-
6	MPD	E	610	-	-	0/5/5/5	-
3	ATP	D	612	4	-	4/18/38/38	0/3/3/3
6	MPD	D	617	-	-	0/5/5/5	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	612	ATP	O4'-C1'	5.26	1.48	1.41
3	D	612	ATP	O4'-C1'	4.71	1.47	1.41
3	C	604	ATP	O4'-C1'	3.28	1.45	1.41
3	E	607	ATP	O4'-C1'	3.20	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	609	ATP	C2-N3	3.12	1.37	1.32
3	E	607	ATP	C2-N3	2.85	1.36	1.32
3	C	604	ATP	C2-N3	2.69	1.36	1.32
3	B	609	ATP	C5-C4	2.67	1.48	1.40
6	E	610	MPD	O2-C2	-2.58	1.38	1.44
3	C	604	ATP	O5'-C5'	-2.52	1.35	1.44
3	D	612	ATP	O5'-C5'	-2.50	1.35	1.44
6	D	618	MPD	O2-C2	-2.40	1.38	1.44
3	B	609	ATP	PG-O3G	-2.37	1.45	1.54
6	C	609	MPD	O2-C2	-2.34	1.38	1.44
3	D	612	ATP	C3'-C4'	2.26	1.58	1.53
6	B	612	MPD	O2-C2	-2.23	1.39	1.44
6	D	617	MPD	O2-C2	-2.22	1.39	1.44
3	E	607	ATP	C5-C4	2.12	1.46	1.40
3	B	609	ATP	O4'-C1'	2.05	1.43	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	612	ATP	O4'-C4'-C5'	4.16	123.05	109.37
3	A	612	ATP	N3-C2-N1	-3.78	122.78	128.68
3	D	612	ATP	N3-C2-N1	-3.77	122.79	128.68
3	C	604	ATP	O4'-C4'-C5'	3.37	120.47	109.37
3	B	609	ATP	C4-C5-N7	-3.00	106.28	109.40
3	C	604	ATP	O5'-PA-O1A	2.98	120.71	109.07
5	A	615	B3P	C3-N1-C4	-2.92	111.94	116.08
3	D	612	ATP	C5'-C4'-C3'	-2.90	104.33	115.18
3	C	604	ATP	O3'-C3'-C4'	-2.86	102.77	111.05
3	A	612	ATP	C4-C5-N7	-2.86	106.42	109.40
3	B	609	ATP	O2A-PA-O1A	2.82	126.18	112.24
3	A	612	ATP	O3'-C3'-C4'	-2.72	103.19	111.05
3	A	612	ATP	O4'-C4'-C5'	2.61	117.97	109.37
3	B	609	ATP	N3-C2-N1	-2.61	124.59	128.68
3	A	612	ATP	O3'-C3'-C2'	2.49	119.86	111.82
3	D	612	ATP	O3G-PG-O2G	2.36	116.66	107.64
3	B	609	ATP	C2'-C3'-C4'	2.32	107.14	102.64
3	C	604	ATP	N3-C2-N1	-2.25	125.16	128.68
3	C	604	ATP	C4-C5-N7	-2.23	107.07	109.40
3	B	609	ATP	O4'-C4'-C3'	-2.22	100.73	105.11
3	A	612	ATP	O2A-PA-O5'	-2.21	97.49	107.75
5	A	615	B3P	O4-C5-C4	-2.21	107.17	111.63
3	C	604	ATP	C5'-C4'-C3'	-2.20	106.95	115.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	607	ATP	O2A-PA-O1A	2.18	123.03	112.24
3	D	612	ATP	O2'-C2'-C1'	2.16	118.83	110.85
3	D	612	ATP	O2A-PA-O1A	2.14	122.84	112.24
5	C	607	B3P	C7-C4-C5	-2.13	105.54	110.04
3	E	607	ATP	N3-C2-N1	-2.11	125.38	128.68
3	B	609	ATP	PA-O3A-PB	-2.10	125.64	132.83
3	D	612	ATP	PB-O3B-PG	-2.06	125.75	132.83
3	C	604	ATP	O3'-C3'-C2'	2.05	118.46	111.82
5	A	615	B3P	C2-N2-C8	-2.05	113.17	116.08
5	C	607	B3P	O6-C7-C4	-2.04	107.50	111.63
5	A	615	B3P	O2-C10-C8	-2.04	107.50	111.63

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	612	ATP	C5'-O5'-PA-O1A
3	A	612	ATP	C5'-O5'-PA-O1A
3	C	604	ATP	C5'-O5'-PA-O1A
5	A	615	B3P	N1-C4-C7-O6
5	C	607	B3P	C7-C4-N1-C3
5	A	615	B3P	C3-C1-C2-N2
5	A	615	B3P	C1-C3-N1-C4
5	A	615	B3P	C5-C4-C7-O6
5	D	615	B3P	C5-C4-N1-C3
5	A	615	B3P	C9-C8-N2-C2
5	C	607	B3P	C5-C4-N1-C3
5	A	615	B3P	O3-C11-C8-C10
6	C	608	MPD	O2-C2-C3-C4
3	D	612	ATP	C5'-O5'-PA-O3A
3	C	604	ATP	C5'-O5'-PA-O3A
3	A	612	ATP	PB-O3A-PA-O1A
3	A	612	ATP	C5'-O5'-PA-O2A
5	D	615	B3P	C7-C4-N1-C3
5	C	607	B3P	C6-C4-N1-C3
5	A	615	B3P	C2-C1-C3-N1
5	A	615	B3P	O3-C11-C8-N2
3	D	612	ATP	O4'-C4'-C5'-O5'
5	D	615	B3P	C11-C8-C9-O1
5	A	615	B3P	C6-C4-C7-O6
5	A	615	B3P	O3-C11-C8-C9
3	C	604	ATP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	D	612	ATP	C3'-C4'-C5'-O5'
3	A	612	ATP	C5'-O5'-PA-O3A
3	B	609	ATP	O4'-C4'-C5'-O5'
3	B	609	ATP	C3'-C4'-C5'-O5'
3	E	607	ATP	O4'-C4'-C5'-O5'

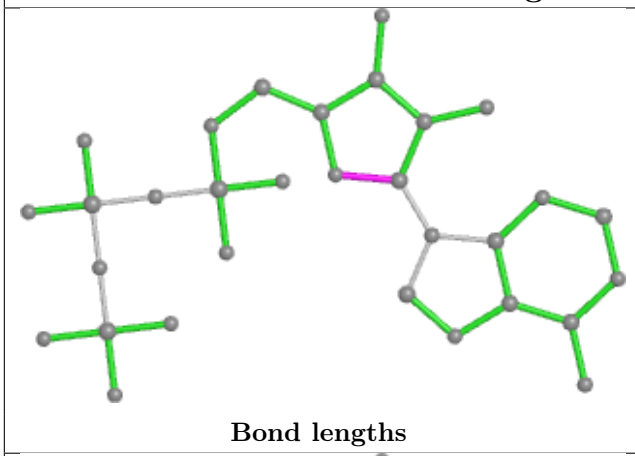
There are no ring outliers.

5 monomers are involved in 8 short contacts:

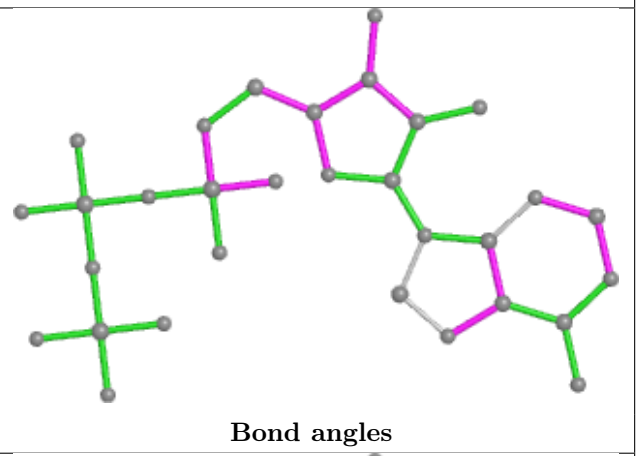
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	602	SO4	3	0
6	D	616	MPD	1	0
6	C	609	MPD	1	0
6	E	610	MPD	2	0
3	D	612	ATP	1	0

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

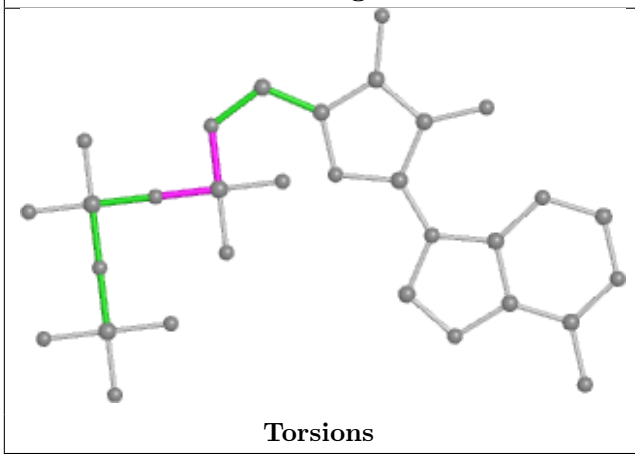
Ligand ATP A 612



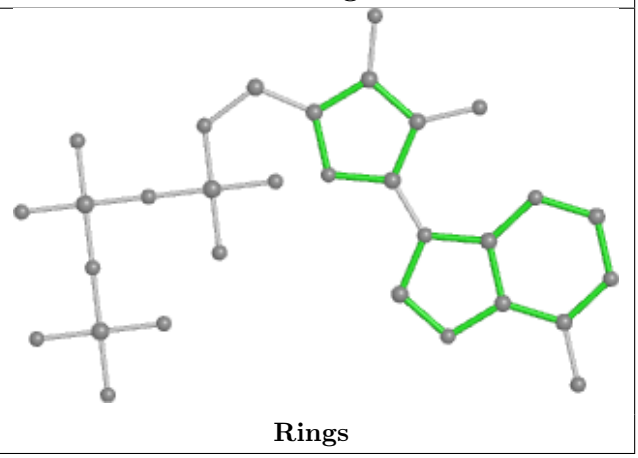
Bond lengths



Bond angles

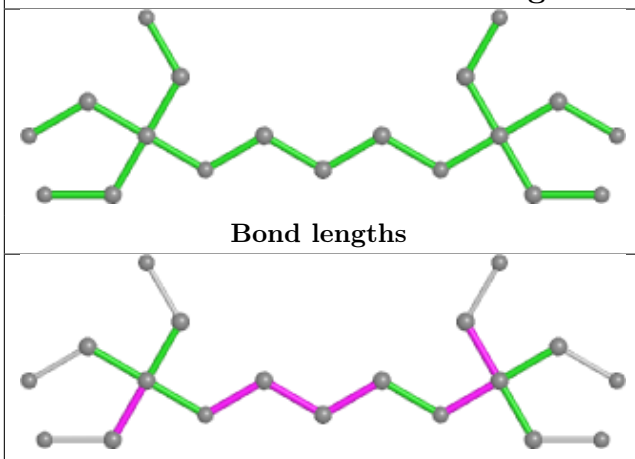


Torsions



Rings

Ligand B3P A 615



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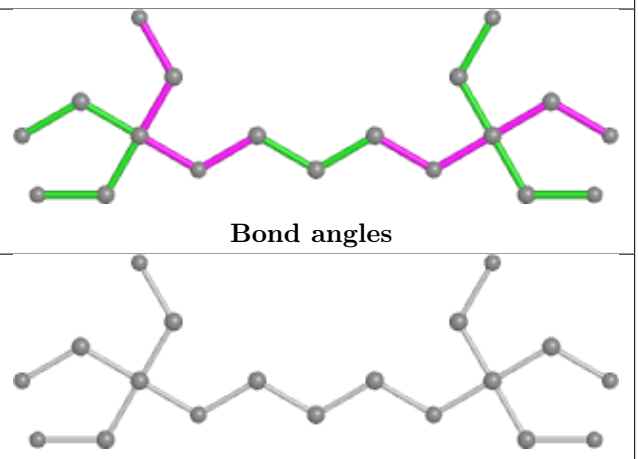
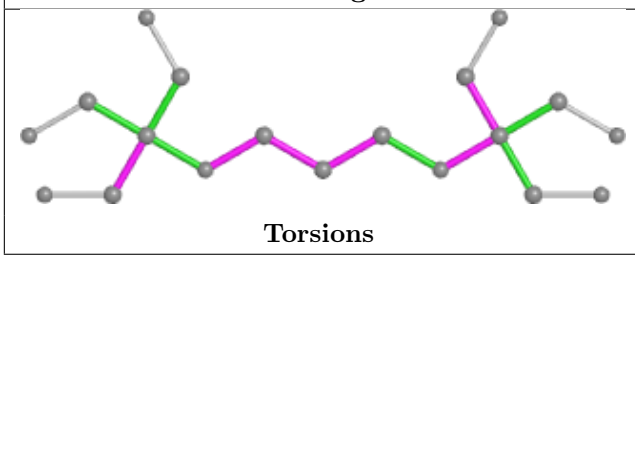


Bond angles



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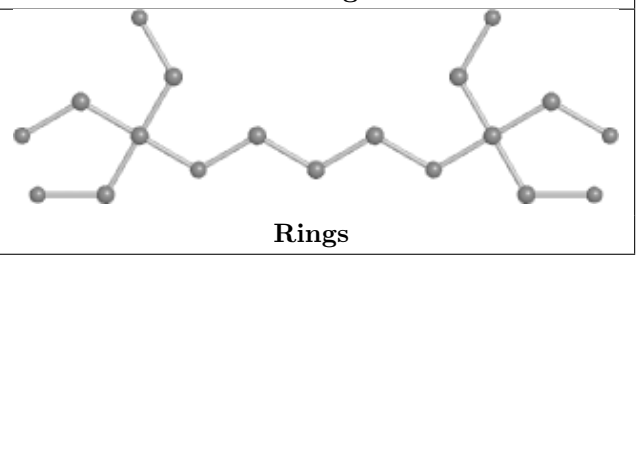
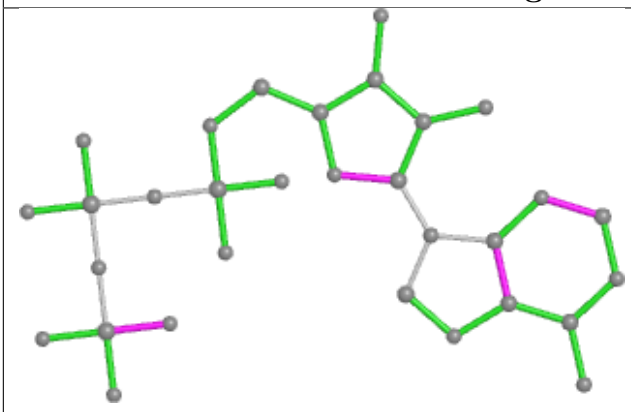
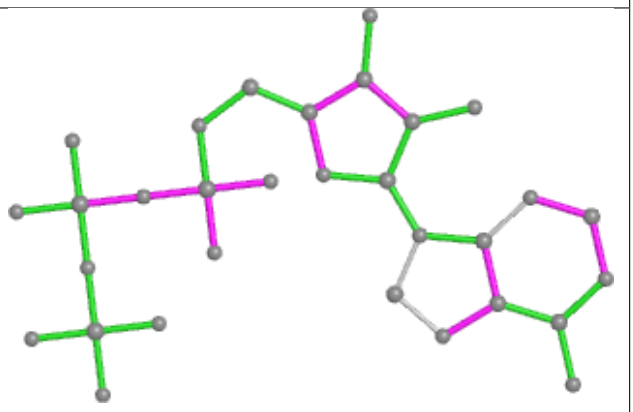


Rings

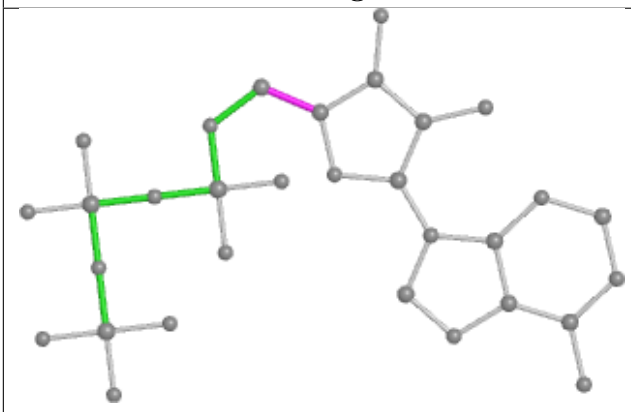
Ligand ATP B 609



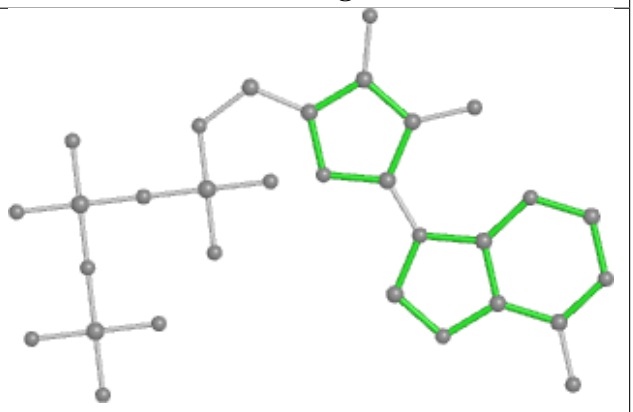
Bond lengths



Bond angles

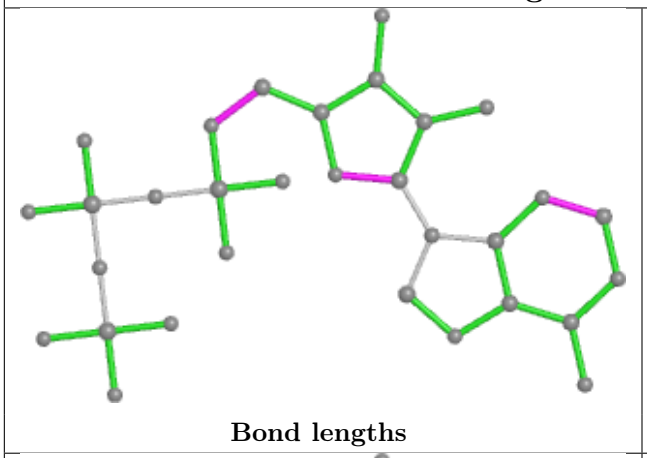


Torsions

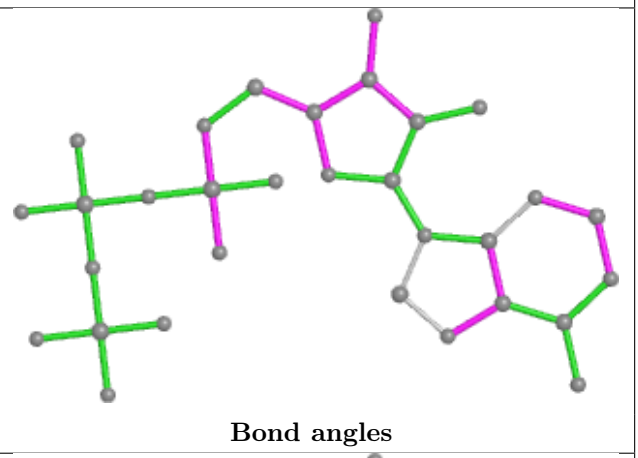


Rings

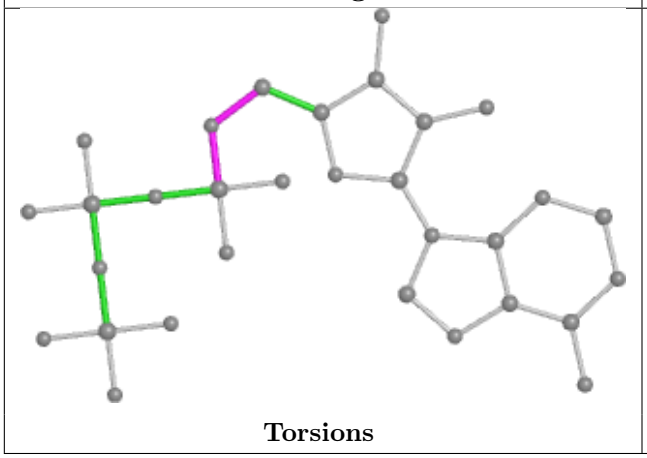
Ligand ATP C 604



Bond lengths



Bond angles



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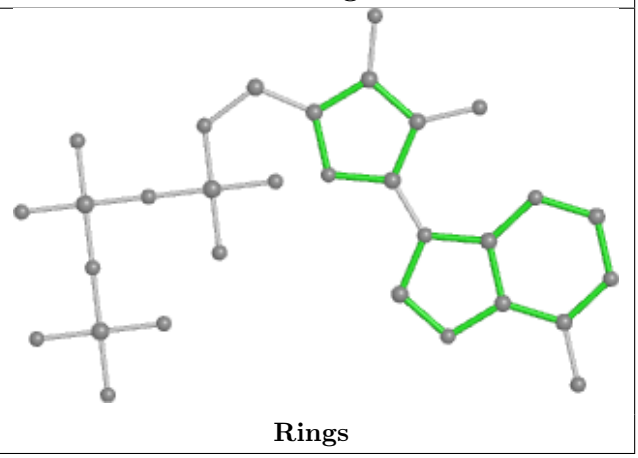
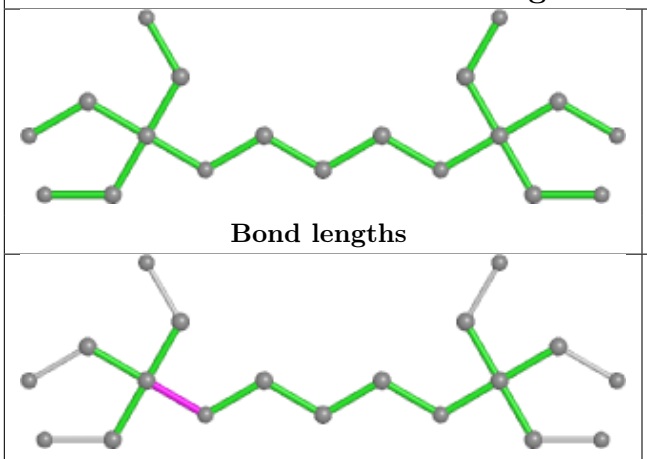
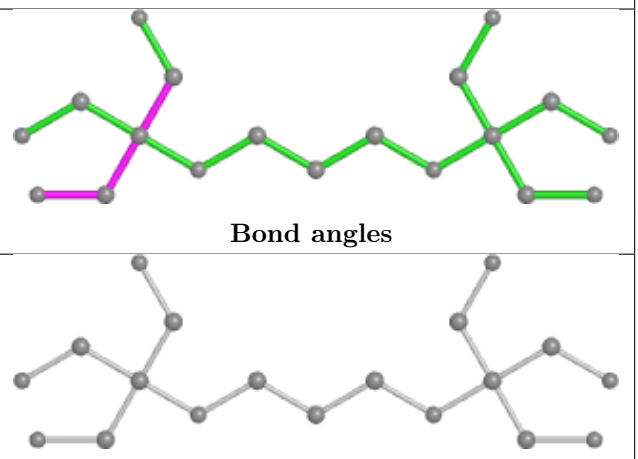


Rings

Ligand B3P C 607



Bond lengths



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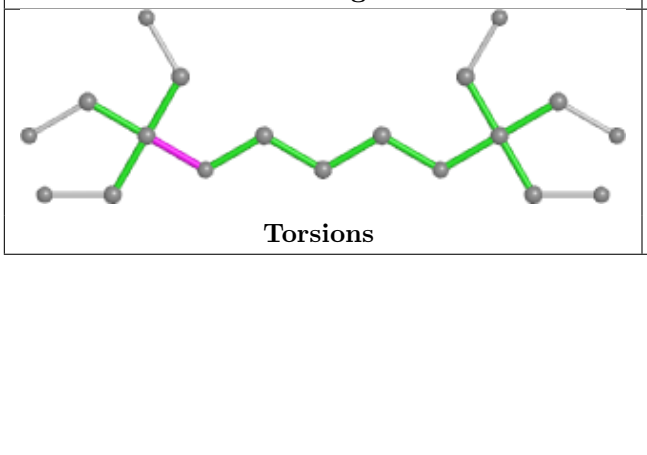

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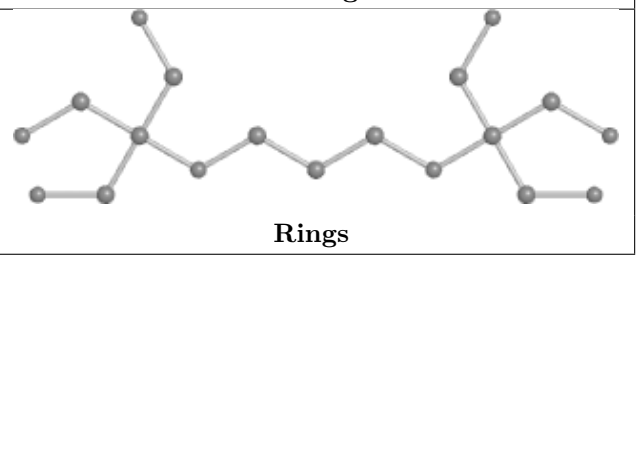
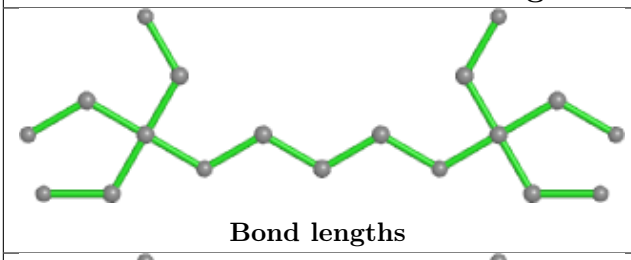


Rings

Ligand B3P D 615



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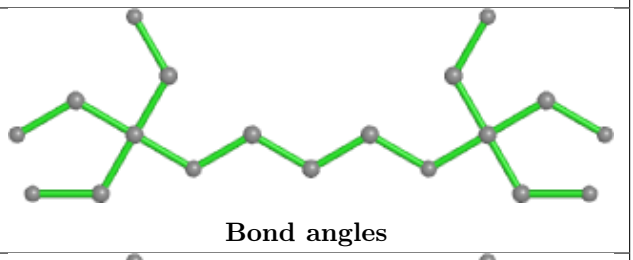
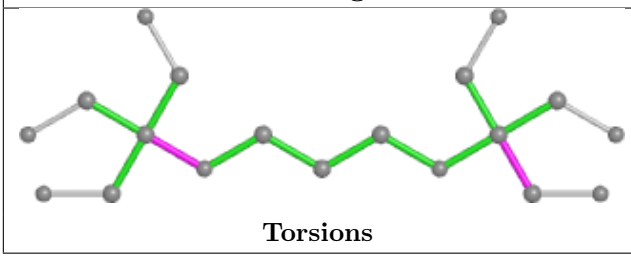


Bond angles



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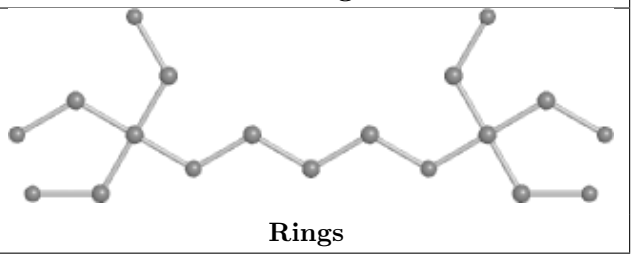
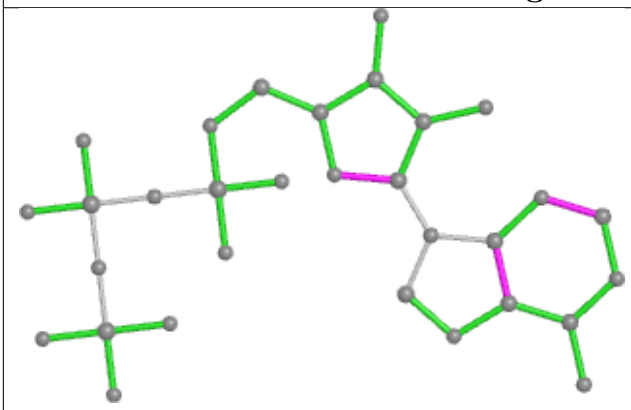
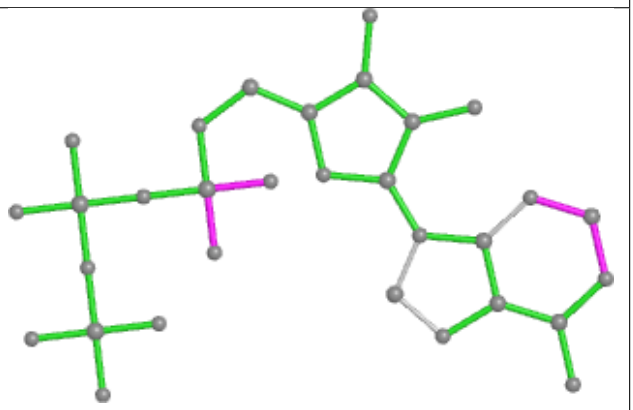


Rings

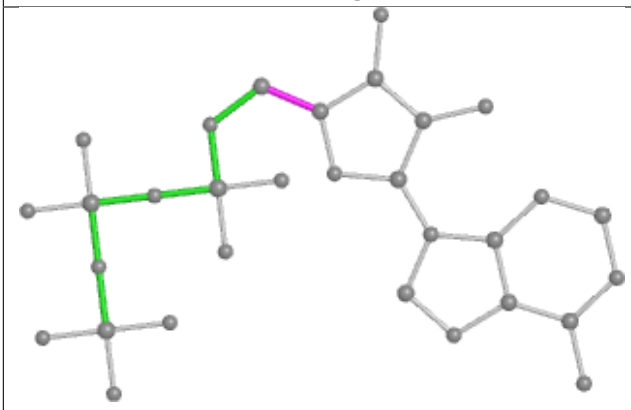
Ligand ATP E 607



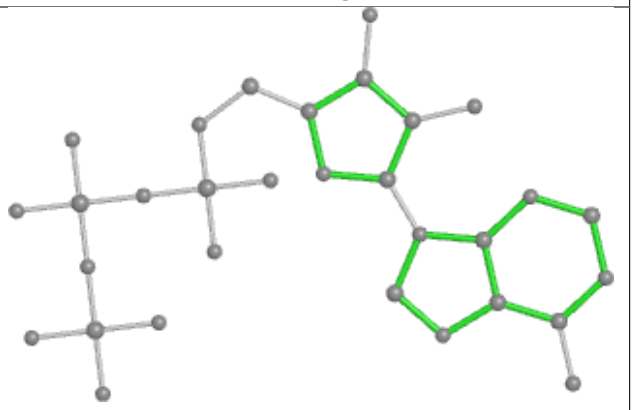
Bond lengths



Bond angles

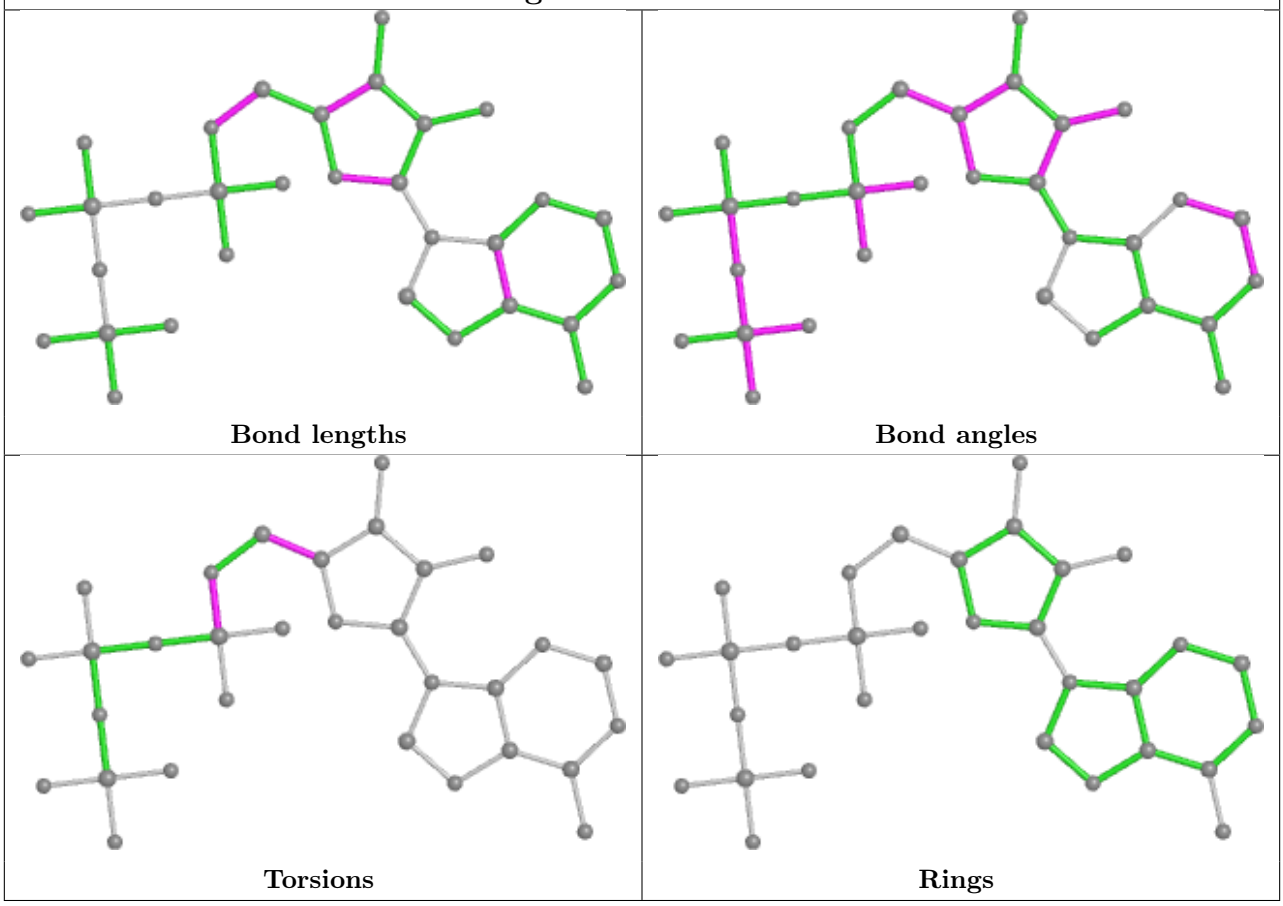


Torsions



Rings

Ligand ATP D 612



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	592/612 (96%)	0.04	8 (1%)	75	80	36, 50, 72, 88	0
1	B	593/612 (96%)	-0.03	10 (1%)	70	76	37, 49, 68, 86	0
1	C	592/612 (96%)	0.17	21 (3%)	44	51	39, 58, 79, 101	0
1	D	593/612 (96%)	-0.03	14 (2%)	59	66	40, 51, 72, 98	0
1	E	593/612 (96%)	-0.09	13 (2%)	62	69	43, 55, 75, 90	0
All	All	2963/3060 (96%)	0.01	66 (2%)	62	69	36, 52, 74, 101	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	8.5
1	D	42	ASP	7.4
1	B	41	ALA	6.7
1	E	42	ASP	6.7
1	C	1	MET	5.7
1	D	43	GLY	5.7
1	C	43	GLY	5.6
1	B	1	MET	5.1
1	E	1	MET	4.9
1	C	473	VAL	4.2
1	B	42	ASP	4.1
1	C	358	TYR	4.1
1	D	45	ASP	4.0
1	A	1	MET	4.0
1	D	0	HIS	4.0
1	E	0	HIS	3.9
1	C	208	ARG	3.9
1	D	44	GLN	3.8
1	E	41	ALA	3.8
1	E	43	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	41	ALA	3.7
1	A	0	HIS	3.6
1	A	591	GLY	3.4
1	C	44	GLN	3.2
1	C	539	LEU	3.2
1	B	43	GLY	3.2
1	D	591	GLY	3.2
1	A	544	ARG	3.0
1	C	213	GLU	2.9
1	E	45	ASP	2.9
1	B	47	ARG	2.9
1	D	217	GLU	2.9
1	B	358	TYR	2.8
1	D	219	PHE	2.7
1	D	216	VAL	2.7
1	C	0	HIS	2.7
1	D	212	GLY	2.6
1	A	208	ARG	2.6
1	C	586	ARG	2.6
1	C	590	ALA	2.6
1	D	309	TYR	2.6
1	B	40	PRO	2.5
1	A	476	PRO	2.5
1	E	408	GLY	2.5
1	E	591	GLY	2.4
1	C	42	ASP	2.4
1	D	213	GLU	2.3
1	B	44	GLN	2.3
1	C	378	ARG	2.3
1	B	473	VAL	2.3
1	E	213	GLU	2.3
1	E	586	ARG	2.3
1	C	472	ALA	2.2
1	C	267	ASP	2.2
1	E	44	GLN	2.2
1	A	523	ARG	2.2
1	E	46	GLY	2.2
1	C	216	VAL	2.1
1	A	217	GLU	2.1
1	C	217	GLU	2.1
1	B	275	SER	2.0
1	C	534	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	471	ASP	2.0
1	C	409	LEU	2.0
1	E	473	VAL	2.0
1	C	296	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MPD	C	608	8/8	0.61	0.34	86,103,107,108	0
2	SO4	A	611	5/5	0.70	0.41	100,103,104,105	0
2	SO4	B	603	5/5	0.70	0.25	102,103,105,106	0
2	SO4	A	605	5/5	0.72	0.36	99,103,104,105	0
6	MPD	A	616	8/8	0.74	0.50	75,90,96,100	0
2	SO4	A	608	5/5	0.75	0.34	102,104,105,106	0
2	SO4	D	608	5/5	0.75	0.45	106,109,110,110	0
2	SO4	A	606	5/5	0.78	0.30	95,99,99,101	0
2	SO4	E	606	5/5	0.80	0.26	94,94,97,98	0
2	SO4	A	603	5/5	0.80	0.24	93,98,101,103	0
2	SO4	D	604	5/5	0.82	0.41	98,98,101,101	0
2	SO4	E	605	5/5	0.82	0.40	93,95,99,102	0
6	MPD	D	617	8/8	0.83	0.41	83,100,109,109	0
2	SO4	B	606	5/5	0.83	0.23	86,87,92,94	0
6	MPD	D	616	8/8	0.83	0.42	68,89,100,100	0
6	MPD	E	610	8/8	0.84	0.29	87,104,111,114	0
2	SO4	B	607	5/5	0.85	0.21	84,88,90,91	0
2	SO4	A	610	5/5	0.85	0.20	90,91,91,94	0
5	B3P	D	615	19/19	0.86	0.15	73,88,90,91	45

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	609	5/5	0.86	0.27	100,101,102,102	0
2	SO4	C	603	5/5	0.86	0.25	90,92,95,95	0
2	SO4	D	607	5/5	0.87	0.18	90,90,94,95	0
2	SO4	A	604	5/5	0.87	0.27	103,103,106,106	0
2	SO4	E	604	5/5	0.87	0.28	95,97,99,99	0
2	SO4	B	605	5/5	0.88	0.23	98,98,100,101	0
5	B3P	A	615	19/19	0.88	0.38	63,82,89,97	0
6	MPD	B	612	8/8	0.88	0.42	84,102,105,105	0
2	SO4	D	602	5/5	0.89	0.39	109,110,112,113	0
2	SO4	D	606	5/5	0.89	0.30	76,79,86,88	0
2	SO4	D	609	5/5	0.89	0.38	101,102,104,105	0
2	SO4	D	611	5/5	0.89	0.38	96,98,98,99	0
2	SO4	E	601	5/5	0.89	0.24	101,102,103,104	0
2	SO4	A	601	5/5	0.90	0.21	93,96,98,99	0
2	SO4	A	602	5/5	0.90	0.29	81,83,86,92	0
2	SO4	A	607	5/5	0.90	0.39	85,88,90,93	0
4	MG	C	605	1/1	0.90	0.33	44,44,44,44	0
2	SO4	B	604	5/5	0.90	0.43	98,99,101,101	0
2	SO4	B	608	5/5	0.90	0.40	97,100,101,103	0
2	SO4	D	601	5/5	0.91	0.29	86,91,93,97	0
5	B3P	C	607	19/19	0.91	0.25	61,75,91,98	0
2	SO4	C	601	5/5	0.92	0.19	92,95,96,98	0
2	SO4	C	602	5/5	0.92	0.25	94,95,97,98	0
2	SO4	B	601	5/5	0.92	0.24	92,93,96,96	0
6	MPD	D	618	8/8	0.92	0.36	82,99,102,104	0
6	MPD	C	609	8/8	0.92	0.24	75,90,95,95	0
2	SO4	D	603	5/5	0.93	0.39	79,88,90,91	0
2	SO4	D	610	5/5	0.93	0.37	104,105,109,109	0
4	MG	C	606	1/1	0.94	0.18	53,53,53,53	0
4	MG	D	614	1/1	0.94	0.14	49,49,49,49	0
2	SO4	B	602	5/5	0.94	0.24	87,89,91,92	0
2	SO4	E	602	5/5	0.95	0.34	90,92,95,97	0
2	SO4	E	603	5/5	0.95	0.15	93,94,97,98	0
4	MG	E	609	1/1	0.95	0.16	50,50,50,50	0
2	SO4	D	605	5/5	0.95	0.16	95,98,99,100	0
4	MG	A	614	1/1	0.96	0.19	46,46,46,46	0
4	MG	B	611	1/1	0.96	0.22	50,50,50,50	0
3	ATP	D	612	31/31	0.98	0.20	40,46,58,62	0
3	ATP	E	607	31/31	0.98	0.17	46,50,60,64	0
3	ATP	A	612	31/31	0.98	0.23	39,47,61,71	0
4	MG	A	613	1/1	0.98	0.26	36,36,36,36	0
3	ATP	C	604	31/31	0.98	0.20	44,50,59,65	0

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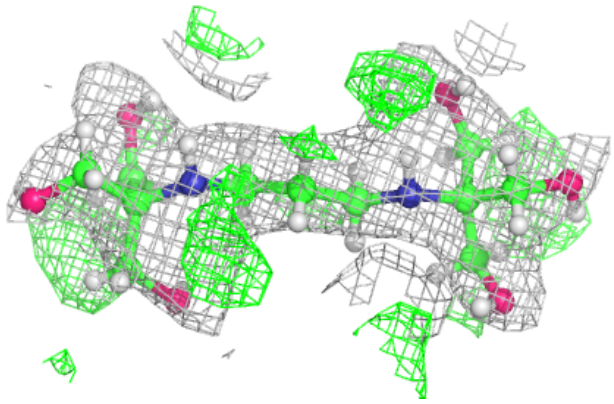
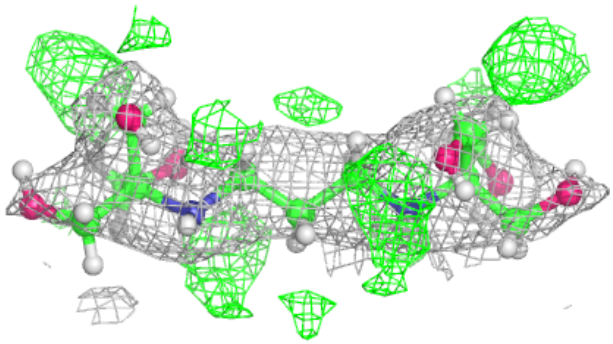
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	613	1/1	0.98	0.21	35,35,35,35	0
3	ATP	B	609	31/31	0.99	0.22	38,44,52,53	0
4	MG	E	608	1/1	0.99	0.28	43,43,43,43	0
4	MG	B	610	1/1	0.99	0.25	33,33,33,33	0

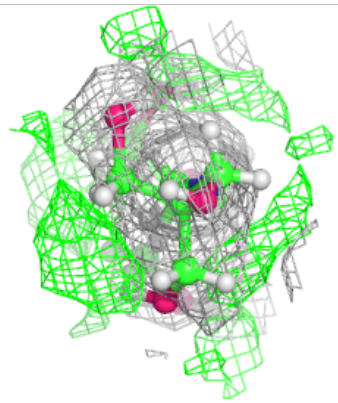
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P D 615:

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

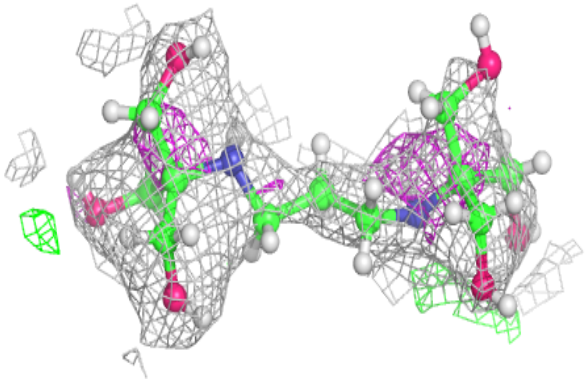


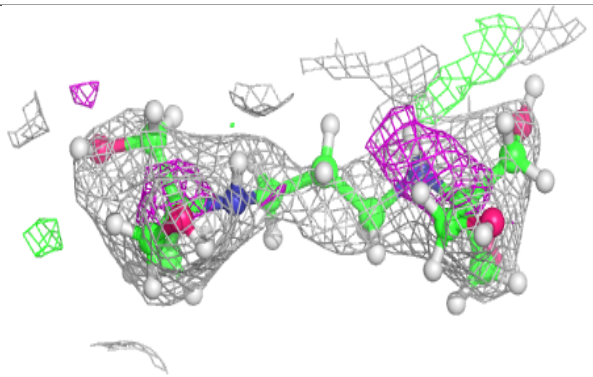


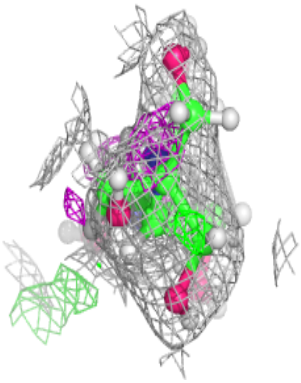


Electron density around B3P A 615:

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

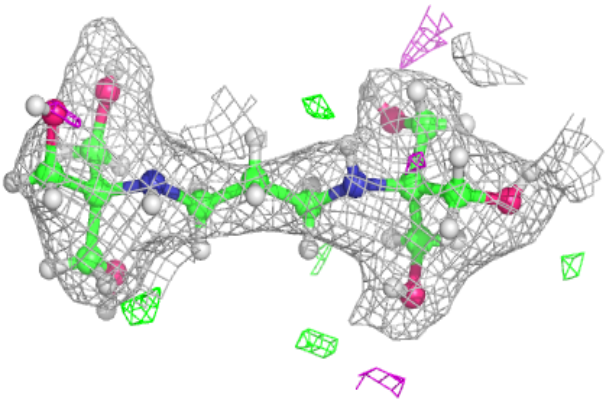


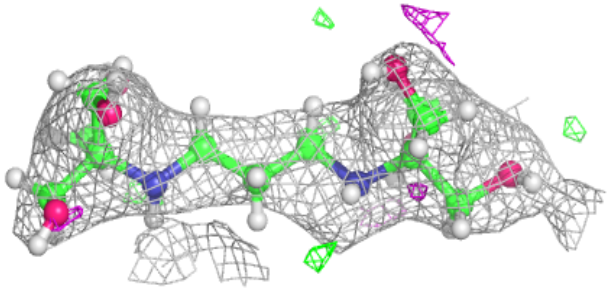


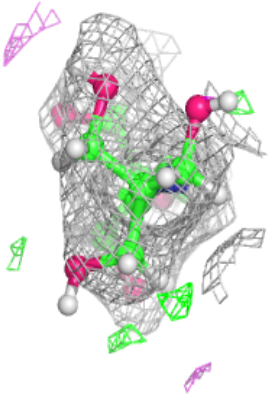


Electron density around B3P C 607:

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

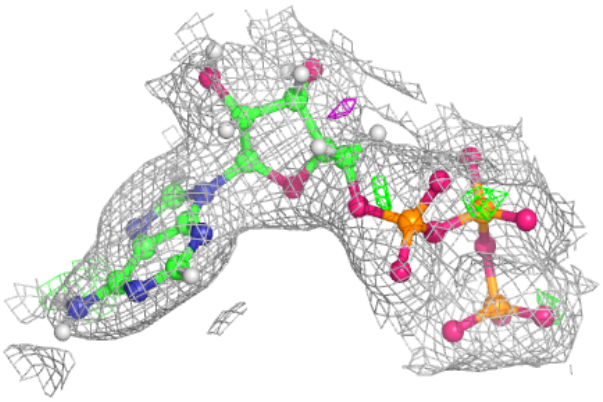


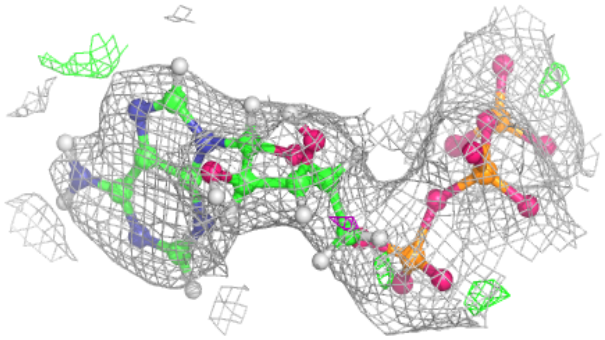


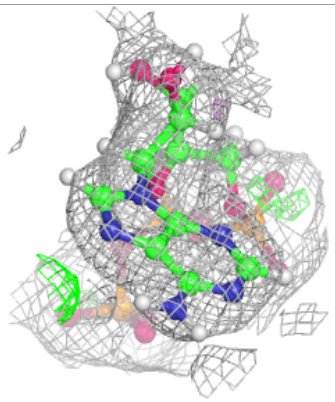


Electron density around ATP D 612:

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

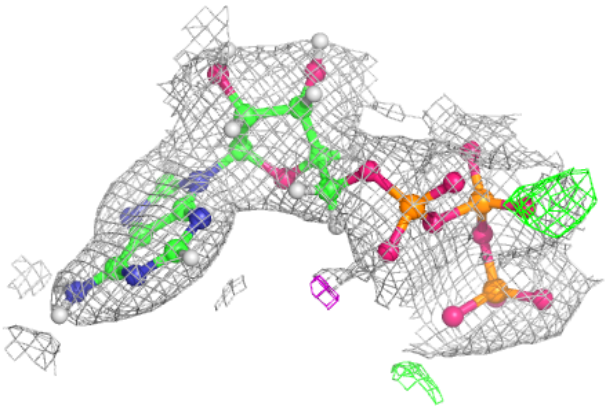


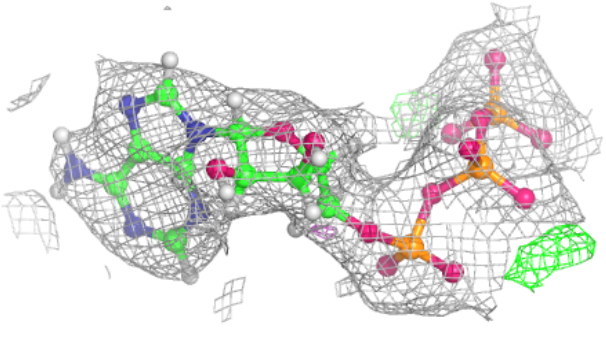


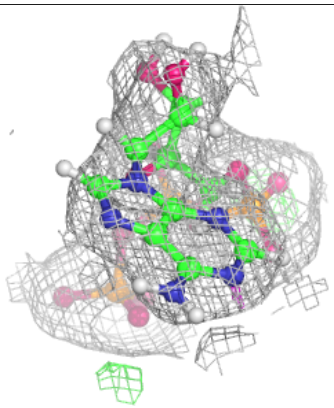


Electron density around ATP E 607:

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

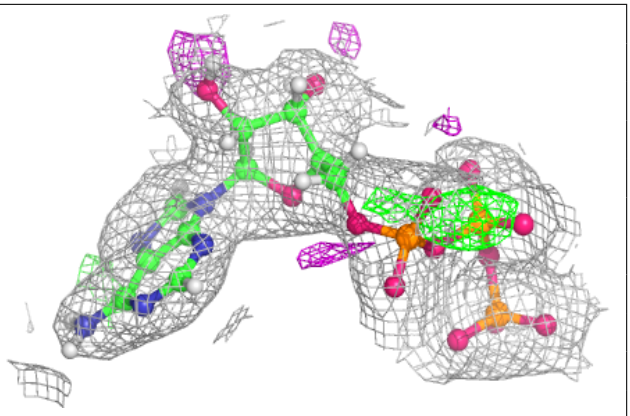


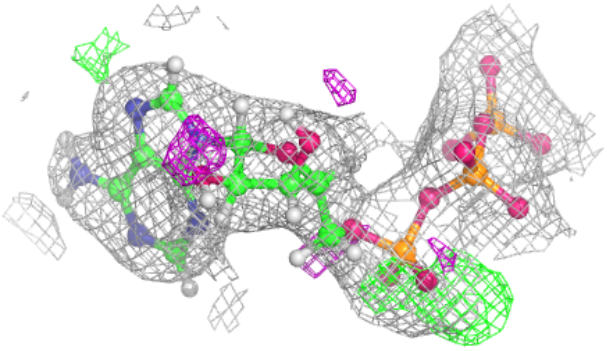


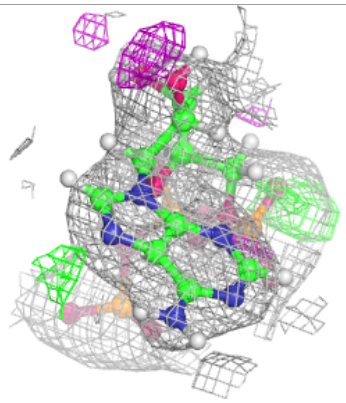


Electron density around ATP A 612:

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

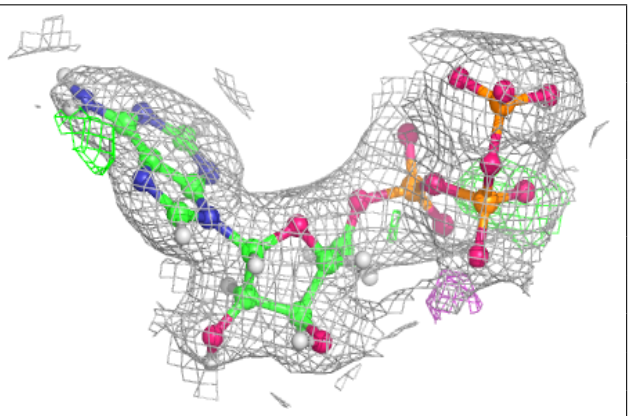


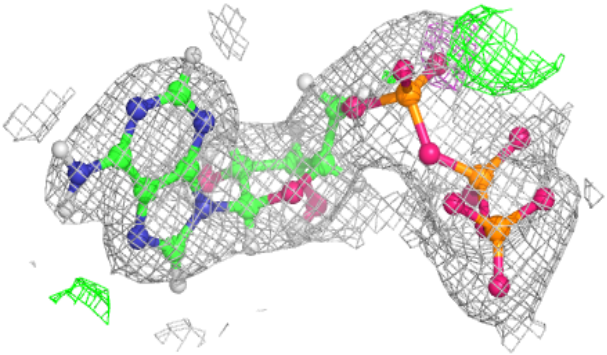


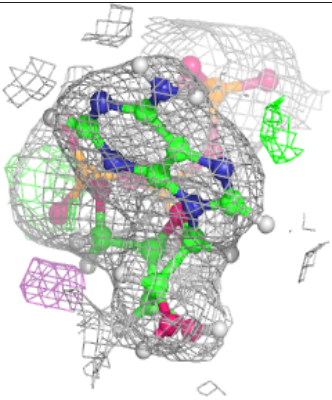


Electron density around ATP C 604:

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

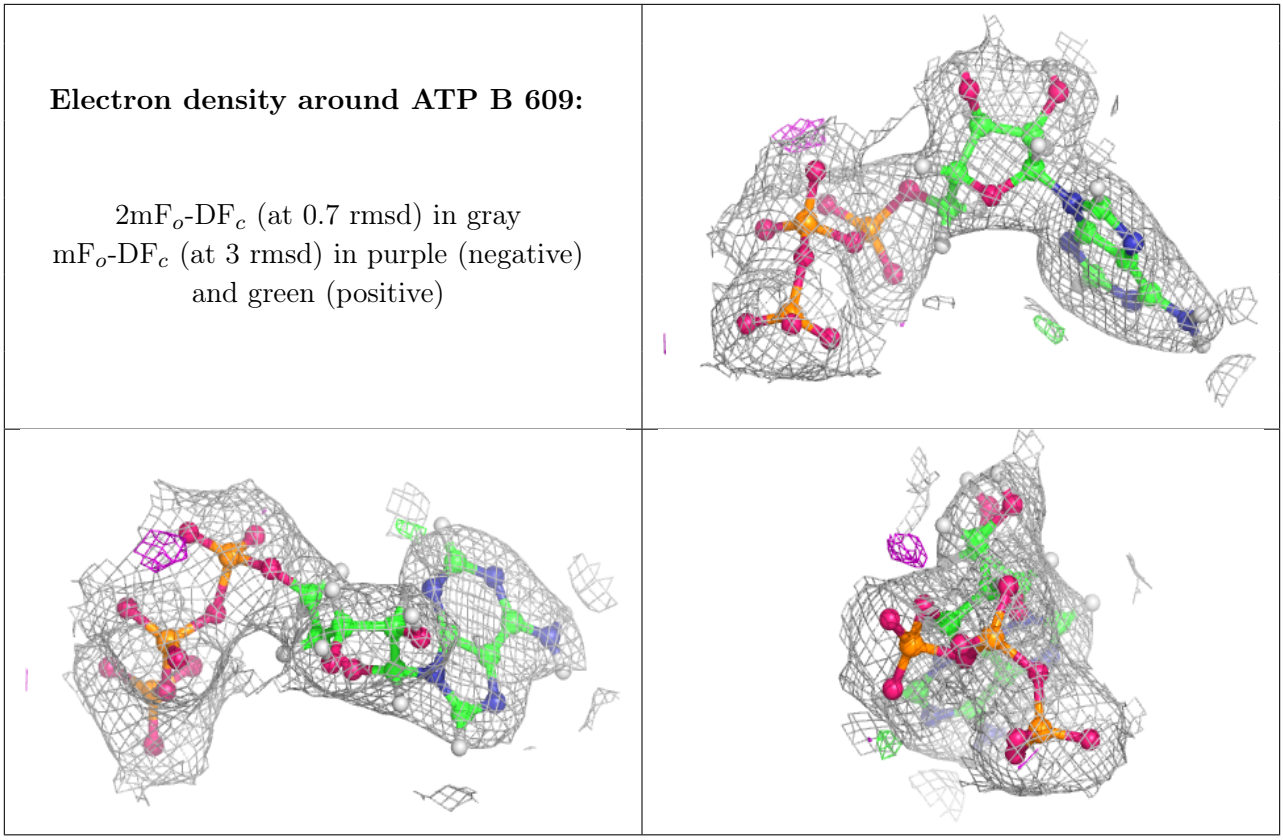






Electron density around ATP B 609:

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



6.5 Other polymers (i)

There are no such residues in this entry.