Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 12:23 AM EDT

PDB ID	:	1KJ8
Title	:	Crystal Structure of PurT-Encoded Glycinamide Ribonucleotide Transformylase in Complex with Mg-ATP and GAR
Authors	:	Thoden, J.B.; Firestine, S.M.; Benkovic, S.J.; Holden, H.M.
Deposited on	:	2001-12-04
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

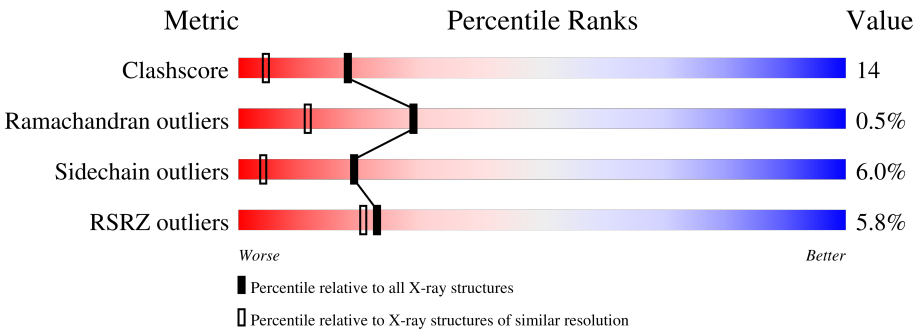
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	391	% 79% 17% • •
1	B	391	11% 65% 26% 7% • •

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
8	EDO	B	399	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6896 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 phosphoribosylglycinamide formyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	2971	1874	528	556	13	0	6	0
1	B	384	2946	1857	523	552	14	0	3	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

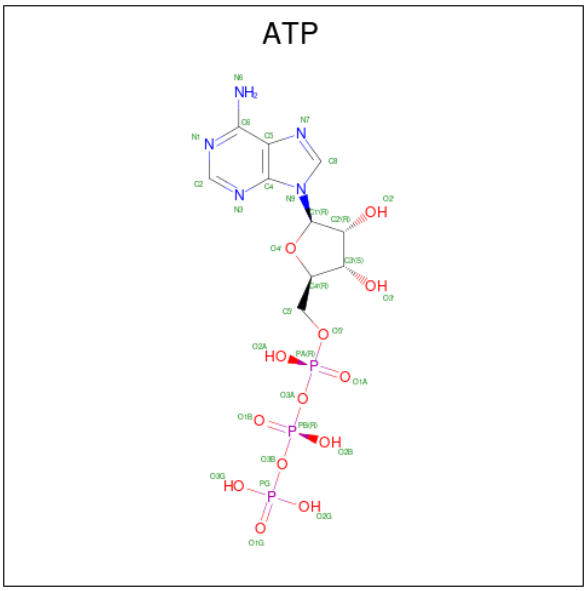
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

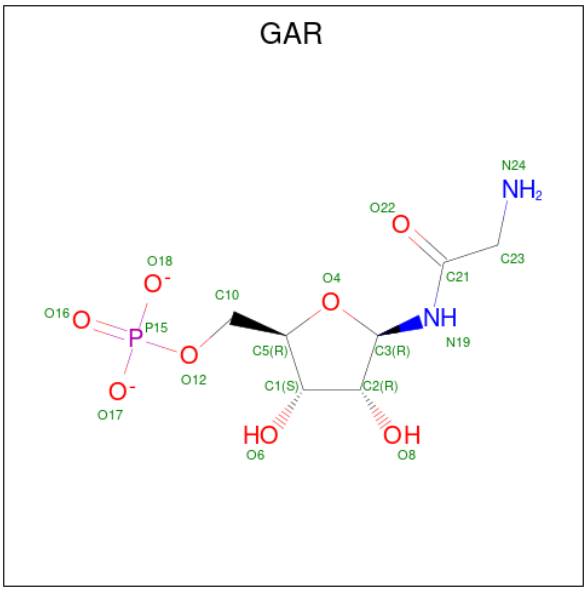
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	3	3	3	0	0
4	B	1	1	1	0	0

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



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

- Molecule 6 is GLYCINAMIDE RIBONUCLEOTIDE (three-letter code: GAR) (formula: $C_7H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	18	7	2	8	1	0	0

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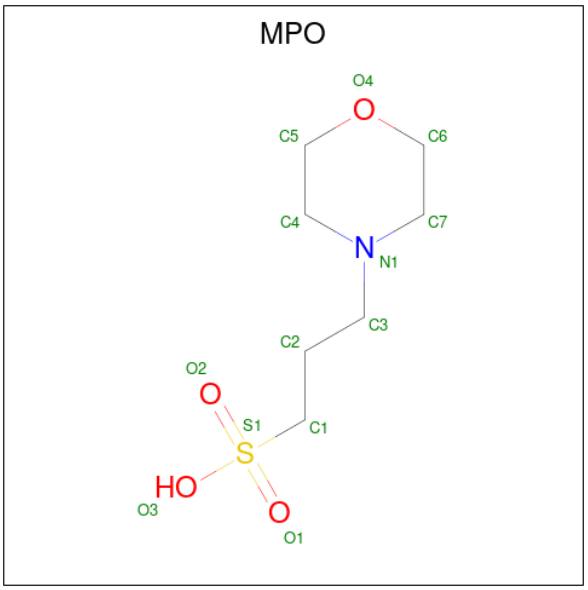
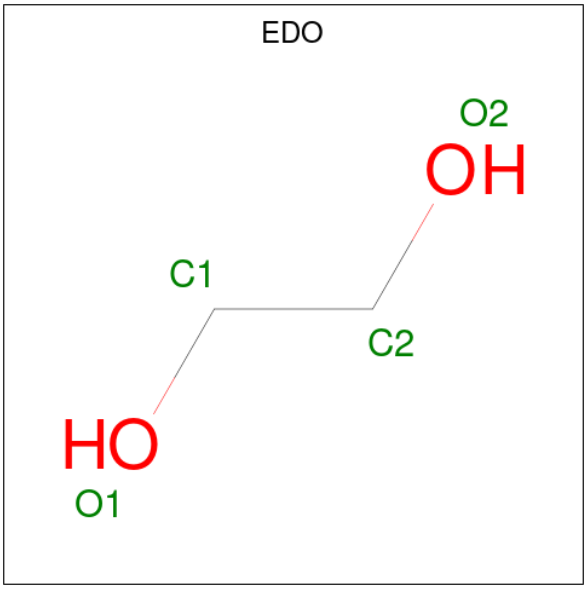
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	18	7	2	8	1	0	0

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	A	1	13	7	1	4	1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	4	2	2	0	0
			Total	C	O		
8	B	1	4	2	2	0	0
			Total	C	O		
8	B	1	4	2	2	0	0

- Molecule 9 is water.

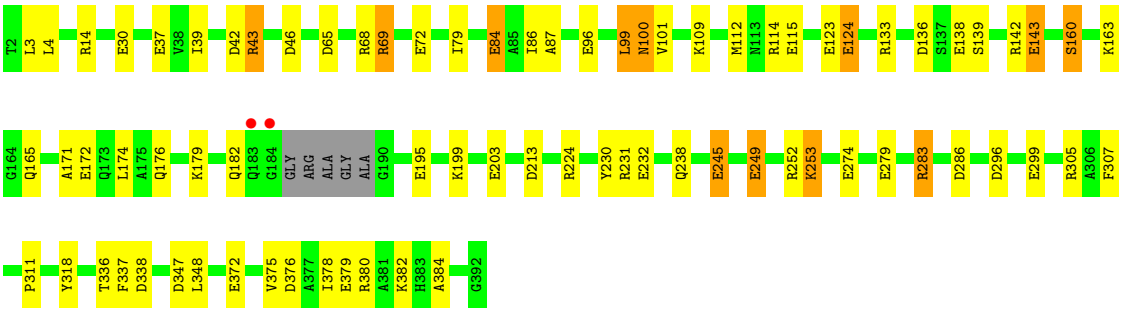
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	502	502	502	0	0
			Total	O		
9	B	344	344	344	0	0

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.

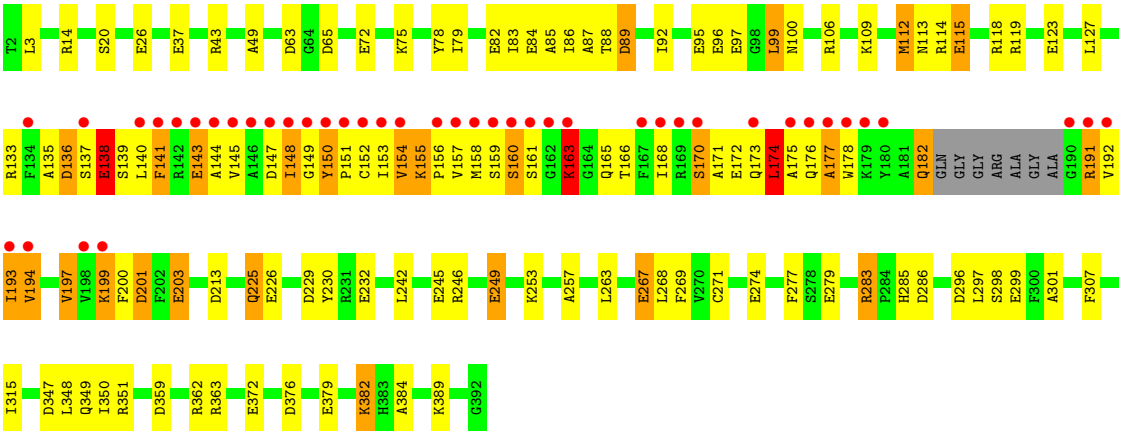
• Molecule 1: phosphoribosylglycinamide formyltransferase 2

Chain A:



• Molecule 1: phosphoribosylglycinamide formyltransferase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	62.10Å 179.30Å 75.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 69.82 – 1.54	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-1.60) 92.4 (69.82-1.54)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.34 (at 1.54Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.181 , 0.228 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 105.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6896	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, MG, MPO, ATP, GAR, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.01	21/3044 (0.7%)	1.25	30/4123 (0.7%)
1	B	1.02	21/3007 (0.7%)	1.30	31/4075 (0.8%)
All	All	1.01	42/6051 (0.7%)	1.27	61/8198 (0.7%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	GLU	CD-OE2	8.12	1.34	1.25
1	B	249	GLU	CD-OE2	8.11	1.34	1.25
1	A	172	GLU	CD-OE2	7.81	1.34	1.25
1	A	72	GLU	CD-OE2	7.68	1.34	1.25
1	B	226	GLU	CD-OE2	7.24	1.33	1.25
1	B	172	GLU	CD-OE2	6.92	1.33	1.25
1	A	84	GLU	CD-OE2	6.81	1.33	1.25
1	A	232	GLU	CD-OE2	6.69	1.33	1.25
1	B	379	GLU	CD-OE2	6.63	1.32	1.25
1	B	123	GLU	CD-OE2	6.61	1.32	1.25
1	A	96	GLU	CD-OE2	6.46	1.32	1.25
1	A	203	GLU	CD-OE2	6.43	1.32	1.25
1	B	203	GLU	CD-OE2	6.43	1.32	1.25
1	B	299	GLU	CD-OE2	6.41	1.32	1.25
1	B	72	GLU	CD-OE2	6.28	1.32	1.25
1	A	37	GLU	CD-OE2	6.26	1.32	1.25
1	A	279	GLU	CD-OE2	6.24	1.32	1.25
1	A	115	GLU	CD-OE2	6.23	1.32	1.25
1	A	123	GLU	CD-OE2	6.23	1.32	1.25
1	A	249	GLU	CD-OE2	6.21	1.32	1.25
1	B	82	GLU	CD-OE2	6.05	1.32	1.25
1	B	115	GLU	CD-OE2	6.00	1.32	1.25
1	B	372	GLU	CD-OE2	5.92	1.32	1.25
1	B	97	GLU	CD-OE2	5.89	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLU	CD-OE2	5.86	1.32	1.25
1	B	274	GLU	CD-OE2	5.78	1.32	1.25
1	B	267	GLU	CD-OE2	5.78	1.32	1.25
1	B	138	GLU	CD-OE2	5.72	1.31	1.25
1	B	279	GLU	CD-OE2	5.72	1.31	1.25
1	A	274	GLU	CD-OE2	5.70	1.31	1.25
1	B	143	GLU	CD-OE2	5.42	1.31	1.25
1	A	138	GLU	CD-OE2	5.41	1.31	1.25
1	A	379	GLU	CD-OE2	5.36	1.31	1.25
1	B	26	GLU	CD-OE2	5.35	1.31	1.25
1	A	245	GLU	CD-OE2	5.32	1.31	1.25
1	A	195	GLU	CD-OE2	5.27	1.31	1.25
1	A	124	GLU	CD-OE2	5.16	1.31	1.25
1	B	95	GLU	CD-OE2	5.13	1.31	1.25
1	B	96	GLU	CD-OE2	5.10	1.31	1.25
1	A	143	GLU	CD-OE1	-5.06	1.20	1.25
1	A	30	GLU	CD-OE2	5.03	1.31	1.25
1	A	299	GLU	CD-OE2	5.02	1.31	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	252[A]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	252[B]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	286	ASP	CB-CG-OD1	8.11	125.60	118.30
1	A	133	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	A	296	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	89	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	114	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	B	296	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	B	296	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	296	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	69	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	286	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	338	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	42	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	286	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	136	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	B	201	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	283[A]	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	283[B]	ARG	NE-CZ-NH2	-6.79	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	B	89	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	136	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	213	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	119	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	133	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	136	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	42	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	114	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	362	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	119	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	359	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	201	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	376	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	318	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	B	285	HIS	N-CA-CB	-5.55	100.60	110.60
1	B	283[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	283[B]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	231	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	224	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	46	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	347	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	380	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	283	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	63	ASP	CB-CG-OD1	5.39	123.16	118.30
1	B	347	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	65	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	136	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	376	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	B	150	TYR	C-N-CD	-5.21	109.13	120.60
1	B	118	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	213	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	351	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	376	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	252[A]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	252[B]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	65	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	213	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	43[A]	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	43[B]	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	14	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	2971	0	3001	37	0
1	B	2946	0	2970	127	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	1	0
4	B	1	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	1	0
6	A	18	0	13	0	0
6	B	18	0	13	0	0
7	A	13	0	15	0	0
8	A	4	0	6	2	0
8	B	8	0	12	10	0
9	A	502	0	0	8	1
9	B	344	0	0	9	1
All	All	6896	0	6054	164	2

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 14.

All (164) 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:156:PRO:HG2	1:B:159:SER:HB2	1.33	1.09
1:B:174:LEU:H	1:B:174:LEU:HD23	1.24	1.00
1:B:141:PHE:CE1	1:B:145:VAL:HG21	2.01	0.95
1:B:297:LEU:HA	8:B:399:EDO:H11	1.52	0.92
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.38	0.87
1:B:136:ASP:HB3	1:B:191:ARG:NH1	1.88	0.87
1:B:156:PRO:CG	1:B:159:SER:HB2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HD3	8:A:401:EDO:H22	1.59	0.83
1:B:141:PHE:HE1	1:B:145:VAL:HG21	1.43	0.81
1:B:84:GLU:OE2	1:B:112:MET:HA	1.85	0.77
1:B:141:PHE:CD2	1:B:178:TRP:HB2	2.20	0.76
1:A:160:SER:H	1:A:163:LYS:HE3	1.48	0.76
1:B:301:ALA:CB	8:B:399:EDO:H12	2.17	0.74
1:B:153:ILE:HG21	1:B:155:LYS:HE2	1.70	0.73
1:B:174:LEU:HD23	1:B:174:LEU:N	2.00	0.73
1:A:109:LYS:CD	8:A:401:EDO:H22	2.20	0.72
1:B:166:THR:O	1:B:168:ILE:HD12	1.90	0.72
1:B:154:VAL:HG23	1:B:194:VAL:HG22	1.72	0.72
1:B:148:ILE:HG21	1:B:152:CYS:HB2	1.71	0.71
1:B:149:GLY:O	1:B:152:CYS:HB3	1.90	0.71
1:B:135:ALA:HB1	1:B:140:LEU:HB3	1.72	0.70
1:B:267:GLU:HG2	9:B:529:HOH:O	1.92	0.69
1:B:114:ARG:NH1	9:B:634:HOH:O	2.26	0.68
1:B:297:LEU:HA	8:B:399:EDO:C1	2.23	0.68
1:B:141:PHE:CD1	1:B:145:VAL:HG21	2.29	0.68
1:B:182:GLN:HE21	1:B:182:GLN:N	1.92	0.68
1:A:124:GLU:HG2	9:A:858:HOH:O	1.95	0.66
1:B:153:ILE:CG2	1:B:155:LYS:HE2	2.24	0.66
1:B:298:SER:H	8:B:399:EDO:C1	2.08	0.66
1:B:173:GLN:O	1:B:176:GLN:HB2	1.96	0.66
1:B:148:ILE:HG12	1:B:194:VAL:HG12	1.77	0.66
1:B:178:TRP:O	1:B:182:GLN:NE2	2.28	0.65
1:B:106:ARG:NH1	1:B:257:ALA:O	2.28	0.65
1:B:171:ALA:O	1:B:174:LEU:HG	1.97	0.65
1:B:43:ARG:NH2	9:B:651:HOH:O	2.29	0.64
1:A:160:SER:O	1:A:163:LYS:HE3	1.96	0.64
1:A:336:THR:HB	1:B:3:LEU:HD11	1.79	0.64
1:B:154:VAL:HG23	1:B:194:VAL:CG2	2.27	0.64
1:B:166:THR:CG2	1:B:168:ILE:HD11	2.29	0.63
1:B:389:LYS:NZ	9:B:604:HOH:O	2.29	0.63
1:B:242:LEU:O	1:B:246:ARG:HG3	1.99	0.62
1:B:79:ILE:HD11	1:B:99:LEU:HD22	1.80	0.62
1:B:170:SER:N	1:B:173:GLN:OE1	2.31	0.62
1:B:144:ALA:O	1:B:147:ASP:N	2.35	0.60
1:B:156:PRO:CD	1:B:159:SER:HB2	2.30	0.60
1:B:201:ASP:OD2	1:B:201:ASP:N	2.34	0.59
1:B:160:SER:O	1:B:163:LYS:HB2	2.02	0.59
1:B:89:ASP:HB2	9:B:525:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.38	0.58
1:B:113:ASN:OD1	1:B:115:GLU:HB3	2.02	0.58
1:B:136:ASP:HB3	1:B:191:ARG:HH11	1.67	0.58
1:B:166:THR:HG22	1:B:168:ILE:CD1	2.34	0.58
1:B:145:VAL:HG13	1:B:152:CYS:SG	2.44	0.58
1:B:114:ARG:NH2	5:B:397:ATP:O3A	2.37	0.58
1:B:203:GLU:HG2	1:B:269:PHE:CD1	2.38	0.57
1:B:148:ILE:CG2	1:B:152:CYS:HB2	2.34	0.57
1:B:171:ALA:HA	1:B:174:LEU:HD21	1.87	0.57
1:B:148:ILE:HG12	1:B:194:VAL:CG1	2.35	0.56
1:A:160:SER:O	1:A:163:LYS:HG3	2.04	0.56
1:B:141:PHE:HB2	1:B:178:TRP:CE3	2.40	0.56
1:B:156:PRO:HD2	1:B:159:SER:HB2	1.88	0.56
1:A:165:GLN:OE1	9:A:901:HOH:O	2.18	0.56
1:B:141:PHE:CE2	1:B:174:LEU:HB3	2.40	0.56
1:B:144:ALA:O	1:B:147:ASP:HB2	2.06	0.56
1:B:297:LEU:CA	8:B:399:EDO:H11	2.32	0.56
1:A:245:GLU:O	1:A:249:GLU:HG3	2.06	0.56
1:B:157:VAL:HG23	1:B:158:MET:HG2	1.86	0.55
1:B:43:ARG:HH11	1:B:43:ARG:CG	2.17	0.54
1:B:166:THR:HG22	1:B:168:ILE:HD11	1.90	0.54
1:A:79:ILE:HD11	1:A:99:LEU:HD22	1.89	0.54
1:A:84:GLU:HG3	1:A:283:ARG:HH12	1.73	0.54
1:B:301:ALA:HB2	8:B:399:EDO:H12	1.90	0.54
1:A:179:LYS:O	1:A:182:GLN:HB2	2.08	0.54
1:B:127:LEU:HD21	1:B:253:LYS:HD2	1.90	0.54
1:B:348:LEU:HD11	1:B:384:ALA:CB	2.38	0.54
1:B:349[B]:GLN:HG3	1:B:350:ILE:N	2.22	0.54
1:B:137:SER:O	1:B:141:PHE:N	2.30	0.53
1:A:142:ARG:HB2	9:A:751:HOH:O	2.08	0.53
1:B:88:THR:OG1	1:B:109:LYS:HG3	2.09	0.53
1:B:232:GLU:OE1	1:B:382:LYS:HD2	2.09	0.53
1:B:182:GLN:N	1:B:182:GLN:NE2	2.57	0.52
1:A:86:ILE:HG22	1:A:87:ALA:N	2.23	0.52
1:A:43[B]:ARG:NH2	9:A:513:HOH:O	2.38	0.52
1:B:135:ALA:O	1:B:191:ARG:HD3	2.09	0.52
1:B:137:SER:O	1:B:140:LEU:N	2.42	0.52
1:B:268:LEU:HD23	1:B:277:PHE:HA	1.90	0.52
1:B:141:PHE:CZ	1:B:174:LEU:HB3	2.45	0.52
1:A:65:ASP:O	1:A:69:ARG:HG3	2.10	0.52
1:B:86:ILE:HG22	1:B:87:ALA:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.40	0.51
1:B:203:GLU:HG2	1:B:269:PHE:HD1	1.75	0.51
1:B:145:VAL:CG2	1:B:194:VAL:HG21	2.40	0.51
1:B:173:GLN:O	1:B:176:GLN:N	2.43	0.51
1:B:174:LEU:HA	1:B:177:ALA:HB3	1.92	0.51
1:B:191:ARG:CD	1:B:192:VAL:N	2.73	0.51
1:A:171:ALA:HA	1:A:174:LEU:HG	1.92	0.50
1:A:375:VAL:HG23	9:A:468:HOH:O	2.12	0.50
1:B:191:ARG:HD2	1:B:192:VAL:N	2.27	0.50
1:A:176:GLN:NE2	9:A:775:HOH:O	2.41	0.50
1:B:232:GLU:CD	1:B:382:LYS:HD2	2.32	0.50
1:B:136:ASP:OD1	1:B:136:ASP:N	2.45	0.49
1:B:137:SER:OG	1:B:140:LEU:HD12	2.11	0.49
1:B:173:GLN:O	1:B:175:ALA:N	2.46	0.49
1:A:100:ASN:C	1:A:100:ASN:HD22	2.15	0.48
1:B:200:PHE:HA	1:B:271[B]:CYS:SG	2.53	0.48
1:B:150:TYR:HE2	1:B:168:ILE:CG2	2.27	0.48
1:B:150:TYR:HD2	1:B:168:ILE:O	1.97	0.48
1:B:348:LEU:HD11	1:B:384:ALA:HB2	1.95	0.47
1:A:100:ASN:HD22	1:A:101:VAL:N	2.12	0.47
1:A:165:GLN:HG3	9:A:770:HOH:O	2.13	0.47
1:B:193:ILE:HG13	1:B:194:VAL:N	2.28	0.47
1:B:151:PRO:HG2	1:B:197:VAL:HB	1.97	0.47
1:B:315:ILE:HA	9:B:643:HOH:O	2.15	0.47
1:B:135:ALA:HB1	1:B:140:LEU:CB	2.44	0.47
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.55	0.46
1:B:298:SER:H	8:B:399:EDO:H11	1.78	0.46
1:A:378:ILE:O	1:A:382:LYS:HG3	2.15	0.46
1:B:249:GLU:HG2	1:B:253:LYS:HE2	1.97	0.46
1:A:139:SER:O	1:A:143:GLU:HG3	2.15	0.46
1:A:305:ARG:HD3	1:A:311:PRO:O	2.15	0.46
1:A:160:SER:H	1:A:163:LYS:CE	2.25	0.45
1:B:43:ARG:HG3	1:B:43:ARG:NH1	2.15	0.45
1:B:225:GLN:HE21	1:B:225:GLN:HB3	1.59	0.45
1:B:92:ILE:CD1	1:B:109:LYS:HD2	2.46	0.45
1:B:200:PHE:CZ	1:B:203:GLU:HG3	2.51	0.45
1:B:145:VAL:HG22	1:B:194:VAL:HG21	1.97	0.45
1:B:141:PHE:CD1	1:B:145:VAL:CG2	2.98	0.45
1:A:253:LYS:HE3	1:A:253:LYS:HB3	1.57	0.45
1:B:150:TYR:CD2	1:B:168:ILE:HG22	2.52	0.45
1:A:84:GLU:HG3	1:A:283:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:CG	1:B:43:ARG:NH1	2.79	0.44
1:A:337:PHE:O	1:B:3:LEU:HD12	2.16	0.44
1:B:166:THR:HB	1:B:168:ILE:HD11	1.99	0.44
1:B:156:PRO:HG2	1:B:159:SER:CB	2.25	0.44
1:B:194:VAL:HG12	1:B:194:VAL:O	2.17	0.44
1:B:83:ILE:HD12	1:B:85:ALA:HB3	1.99	0.44
1:B:84:GLU:HG3	9:B:545:HOH:O	2.18	0.44
1:B:141:PHE:HD2	1:B:178:TRP:HB2	1.74	0.43
1:B:150:TYR:HA	1:B:151:PRO:C	2.39	0.43
1:B:199:LYS:HD2	1:B:199:LYS:HA	1.79	0.43
1:B:75:LYS:HA	1:B:75:LYS:HE2	2.01	0.43
1:B:141:PHE:O	1:B:145:VAL:HG23	2.18	0.43
1:B:14:ARG:HG2	1:B:37:GLU:HB3	2.01	0.43
1:B:301:ALA:HB3	8:B:399:EDO:H12	1.97	0.42
1:A:39:ILE:HD12	1:A:39:ILE:N	2.35	0.42
1:B:20:SER:HB3	1:B:49:ALA:HB3	2.00	0.42
1:B:173:GLN:C	1:B:175:ALA:H	2.23	0.42
1:B:283[B]:ARG:NH2	9:B:679:HOH:O	2.52	0.41
1:B:156:PRO:HD2	1:B:159:SER:CB	2.49	0.41
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.89	0.41
1:B:78:TYR:CD2	1:B:100:ASN:ND2	2.89	0.41
1:B:298:SER:H	8:B:399:EDO:C2	2.34	0.41
1:A:86:ILE:CG2	1:A:87:ALA:N	2.84	0.41
1:B:136:ASP:OD1	1:B:140:LEU:HD13	2.21	0.41
1:B:200:PHE:CE2	1:B:203:GLU:HG3	2.55	0.41
1:A:3[A]:LEU:HD23	1:A:4:LEU:N	2.36	0.41
1:A:179:LYS:O	1:A:182:GLN:N	2.45	0.41
1:B:137:SER:O	1:B:138:GLU:C	2.59	0.41
8:B:399:EDO:H21	9:B:614:HOH:O	2.20	0.40
1:B:141:PHE:CE2	1:B:178:TRP:HB2	2.56	0.40
1:B:153:ILE:CG2	1:B:154:VAL:N	2.84	0.40
4:A:397:CL:CL	9:A:732:HOH:O	2.60	0.40
1:B:92:ILE:CD1	1:B:109:LYS:CD	2.99	0.40

All (2) 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)
9:B:477:HOH:O	9:B:477:HOH:O[2_655]	2.10	0.10
9:A:521:HOH:O	9:A:755:HOH:O[4_556]	2.17	0.03

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	388/391 (99%)	376 (97%)	12 (3%)	0	100 100
1	B	383/391 (98%)	365 (95%)	14 (4%)	4 (1%)	15 3
All	All	771/782 (99%)	741 (96%)	26 (3%)	4 (0%)	29 11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	LYS
1	B	174	LEU
1	B	177	ALA
1	B	197	VAL

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	316/311 (102%)	306 (97%)	10 (3%)	39 15
1	B	312/311 (100%)	285 (91%)	27 (9%)	10 1
All	All	628/622 (101%)	591 (94%)	37 (6%)	19 4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	99	LEU

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	112	MET
1	A	160	SER
1	A	199	LYS
1	A	230	TYR
1	A	238	GLN
1	A	253	LYS
1	A	307	PHE
1	B	99	LEU
1	B	112	MET
1	B	133	ARG
1	B	138	GLU
1	B	139	SER
1	B	141	PHE
1	B	143	GLU
1	B	148	ILE
1	B	154	VAL
1	B	155	LYS
1	B	160	SER
1	B	161	SER
1	B	163	LYS
1	B	165	GLN
1	B	170	SER
1	B	174	LEU
1	B	182	GLN
1	B	191	ARG
1	B	193	ILE
1	B	194	VAL
1	B	199	LYS
1	B	225	GLN
1	B	229	ASP
1	B	230	TYR
1	B	263	LEU
1	B	307	PHE
1	B	382	LYS

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

Mol	Chain	Res	Type
1	A	100	ASN
1	A	182	GLN
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	238	GLN
1	A	248	GLN
1	B	176	GLN
1	B	182	GLN
1	B	225	GLN
1	B	248	GLN
1	B	329	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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	GAR	B	398	-	17,18,18	0.76	1 (5%)	21,26,26	0.95	1 (4%)
5	ATP	A	1	2	26,33,33	0.89	0	31,52,52	1.81	4 (12%)
8	EDO	B	400	-	3,3,3	0.33	0	2,2,2	0.39	0
8	EDO	B	399	-	3,3,3	0.56	0	2,2,2	0.20	0
5	ATP	B	397	2	26,33,33	0.93	2 (7%)	31,52,52	1.72	5 (16%)
6	GAR	A	399	-	17,18,18	0.76	0	21,26,26	1.14	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	EDO	A	401	-	3,3,3	0.60	0	2,2,2	0.06	0
7	MPO	A	400	-	13,13,13	2.03	3 (23%)	17,17,17	1.53	4 (23%)

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	GAR	B	398	-	-	0/12/28/28	0/1/1/1
5	ATP	A	1	2	-	3/18/38/38	0/3/3/3
8	EDO	B	400	-	-	1/1/1/1	-
8	EDO	B	399	-	-	1/1/1/1	-
5	ATP	B	397	2	-	11/18/38/38	0/3/3/3
6	GAR	A	399	-	-	0/12/28/28	0/1/1/1
8	EDO	A	401	-	-	0/1/1/1	-
7	MPO	A	400	-	-	0/7/15/15	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	400	MPO	C1-S1	4.86	1.84	1.77
7	A	400	MPO	C3-N1	4.52	1.57	1.47
5	B	397	ATP	C2-N1	2.58	1.38	1.33
5	B	397	ATP	O4'-C1'	-2.25	1.37	1.41
6	B	398	GAR	O4-C3	-2.19	1.39	1.43
7	A	400	MPO	O1-S1	2.06	1.51	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	397	ATP	C5-C6-N6	6.19	129.76	120.35
5	A	1	ATP	C5-C6-N6	5.18	128.22	120.35
5	A	1	ATP	C2-N1-C6	4.91	127.14	118.75
5	A	1	ATP	C5-C6-N1	-4.25	110.72	120.35
5	A	1	ATP	N3-C2-N1	-4.06	122.33	128.68
7	A	400	MPO	O1-S1-C1	3.96	111.68	106.92
5	B	397	ATP	C5-C6-N1	-3.43	112.57	120.35
5	B	397	ATP	C2-N1-C6	2.94	123.78	118.75
6	B	398	GAR	C10-C5-C1	2.48	124.49	115.18
5	B	397	ATP	C2'-C3'-C4'	-2.44	97.91	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	397	ATP	N3-C2-N1	-2.35	125.01	128.68
7	A	400	MPO	C2-C1-S1	-2.29	109.73	113.25
7	A	400	MPO	O2-S1-C1	2.29	109.67	106.92
7	A	400	MPO	C2-C3-N1	-2.26	108.15	113.84
6	A	399	GAR	O17-P15-O12	2.17	112.50	106.73
6	A	399	GAR	C3-N19-C21	2.04	126.05	122.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	ATP	PB-O3B-PG-O3G
5	B	397	ATP	PB-O3B-PG-O2G
5	B	397	ATP	PB-O3B-PG-O3G
5	B	397	ATP	PB-O3A-PA-O5'
8	B	399	EDO	O1-C1-C2-O2
5	B	397	ATP	O4'-C4'-C5'-O5'
5	B	397	ATP	C5'-O5'-PA-O3A
5	B	397	ATP	C5'-O5'-PA-O1A
5	B	397	ATP	PG-O3B-PB-O2B
5	B	397	ATP	C4'-C5'-O5'-PA
5	B	397	ATP	C3'-C4'-C5'-O5'
5	B	397	ATP	PB-O3B-PG-O1G
8	B	400	EDO	O1-C1-C2-O2
5	A	1	ATP	PG-O3B-PB-O2B
5	B	397	ATP	PG-O3B-PB-O1B
5	A	1	ATP	PB-O3B-PG-O1G

There are no ring outliers.

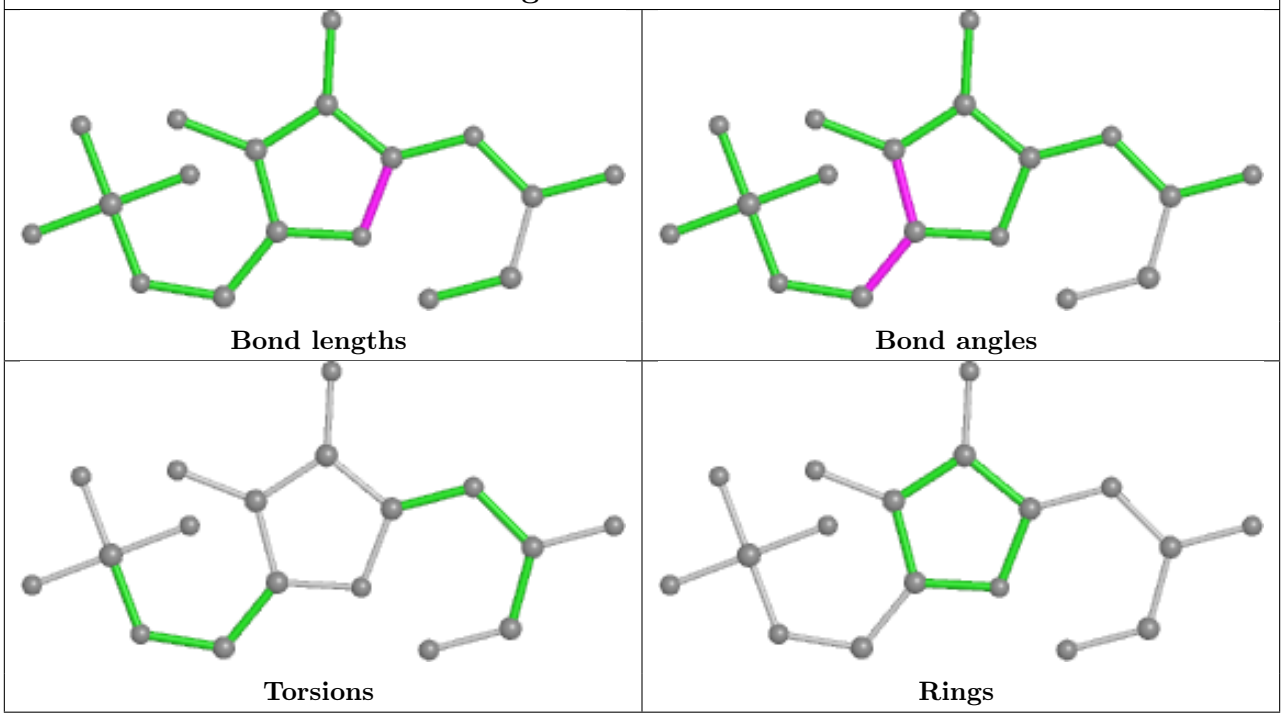
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	399	EDO	10	0
5	B	397	ATP	1	0
8	A	401	EDO	2	0

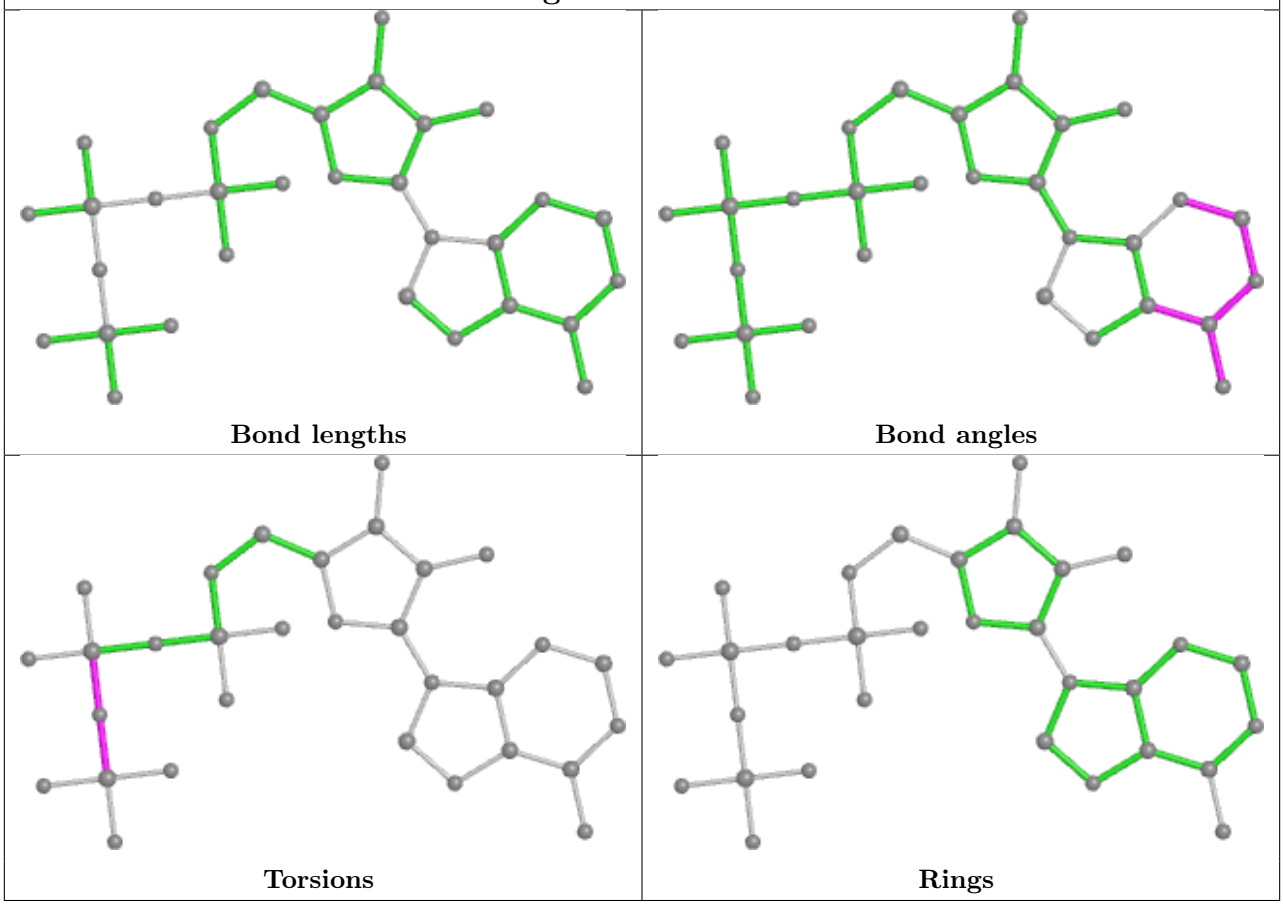
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

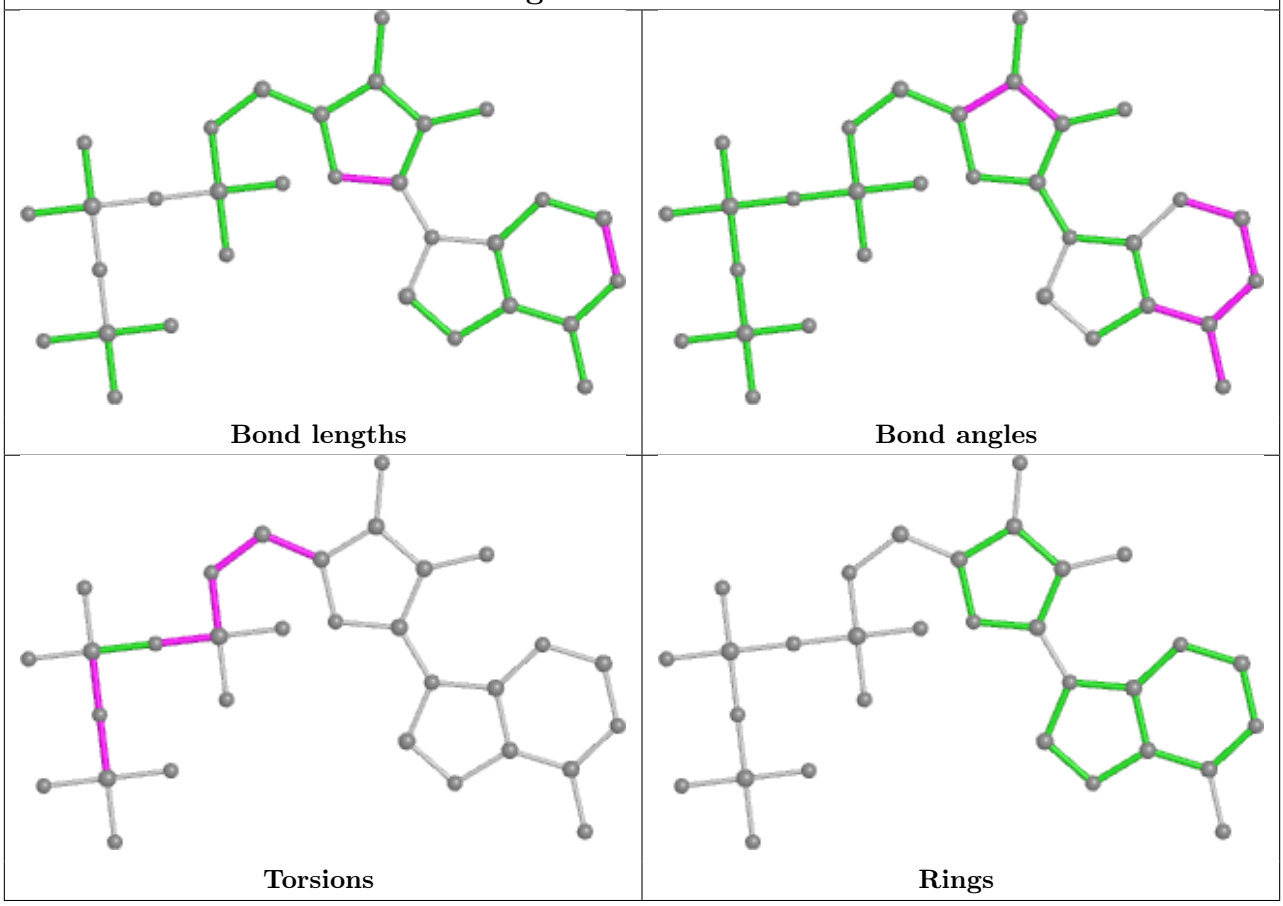
Ligand GAR B 398



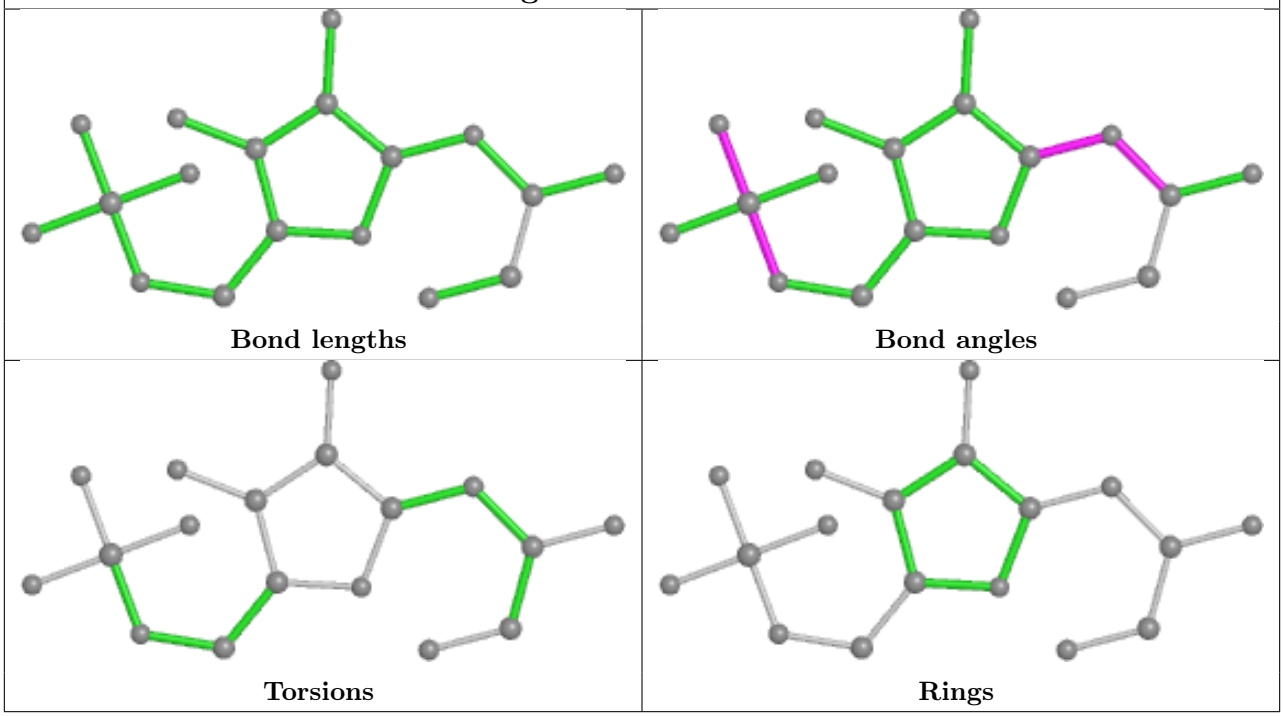
Ligand ATP A 1



Ligand ATP B 397



Ligand GAR A 399



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	386/391 (98%)	-0.72	2 (0%) 91 90	9, 16, 40, 91	0
1	B	384/391 (98%)	0.00	43 (11%) 5 4	10, 19, 85, 99	0
All	All	770/782 (98%)	-0.36	45 (5%) 23 20	9, 17, 71, 99	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	11.3
1	B	150	TYR	9.6
1	B	159	SER	9.1
1	B	141	PHE	8.5
1	B	160	SER	8.3
1	B	148	ILE	7.8
1	B	167	PHE	7.6
1	B	168	ILE	7.1
1	B	178	TRP	6.5
1	B	176	GLN	6.5
1	B	162	GLY	6.2
1	B	137	SER	6.1
1	B	169	ARG	6.1
1	B	149	GLY	5.4
1	B	191	ARG	5.2
1	B	140	LEU	4.9
1	B	154	VAL	4.7
1	B	152	CYS	4.6
1	B	177	ALA	4.5
1	B	145	VAL	4.3
1	B	193	ILE	4.3
1	B	194	VAL	4.2
1	B	161	SER	3.9
1	B	142	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	3.9
1	B	192	VAL	3.9
1	B	173	GLN	3.7
1	B	158	MET	3.6
1	B	163	LYS	3.5
1	B	170	SER	3.4
1	A	184	GLY	3.3
1	B	179	LYS	3.3
1	B	180	TYR	3.3
1	B	151	PRO	3.2
1	B	147	ASP	2.8
1	B	199	LYS	2.8
1	B	190	GLY	2.7
1	B	153	ILE	2.5
1	B	143	GLU	2.4
1	B	198	VAL	2.4
1	B	156	PRO	2.3
1	A	183	GLN	2.1
1	B	134	PHE	2.1
1	B	157	VAL	2.1
1	B	146	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ATP	B	397	31/31	0.51	0.16	0,39,92,97	0
8	EDO	B	399	4/4	0.72	0.25	45,56,61,64	0

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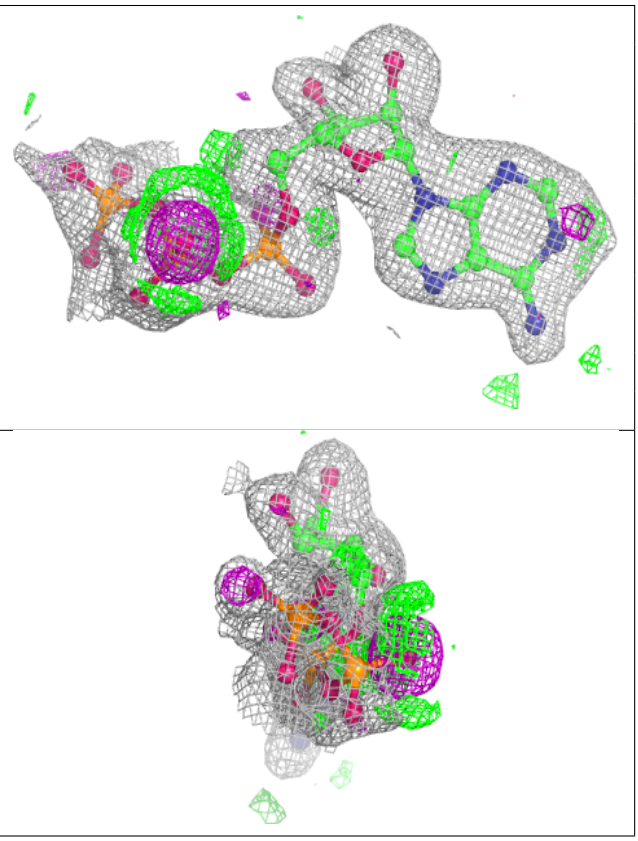
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	EDO	A	401	4/4	0.81	0.18	47,60,60,62	0
8	EDO	B	400	4/4	0.84	0.17	33,36,55,58	0
2	MG	B	394	1/1	0.91	0.09	39,39,39,39	0
2	MG	B	393	1/1	0.93	0.15	51,51,51,51	0
3	NA	B	395	1/1	0.96	0.09	23,23,23,23	0
4	CL	B	396	1/1	0.96	0.07	35,35,35,35	0
3	NA	A	395	1/1	0.96	0.08	29,29,29,29	0
4	CL	A	398	1/1	0.97	0.08	34,34,34,34	0
7	MPO	A	400	13/13	0.98	0.06	17,24,31,32	0
4	CL	A	397	1/1	0.98	0.07	25,25,25,25	0
6	GAR	B	398	18/18	0.99	0.05	10,14,21,29	0
2	MG	A	393	1/1	0.99	0.04	16,16,16,16	0
5	ATP	A	1	31/31	0.99	0.05	8,14,19,23	0
4	CL	A	396	1/1	0.99	0.04	21,21,21,21	0
6	GAR	A	399	18/18	0.99	0.06	11,15,17,20	0
2	MG	A	394	1/1	1.00	0.04	12,12,12,12	0

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

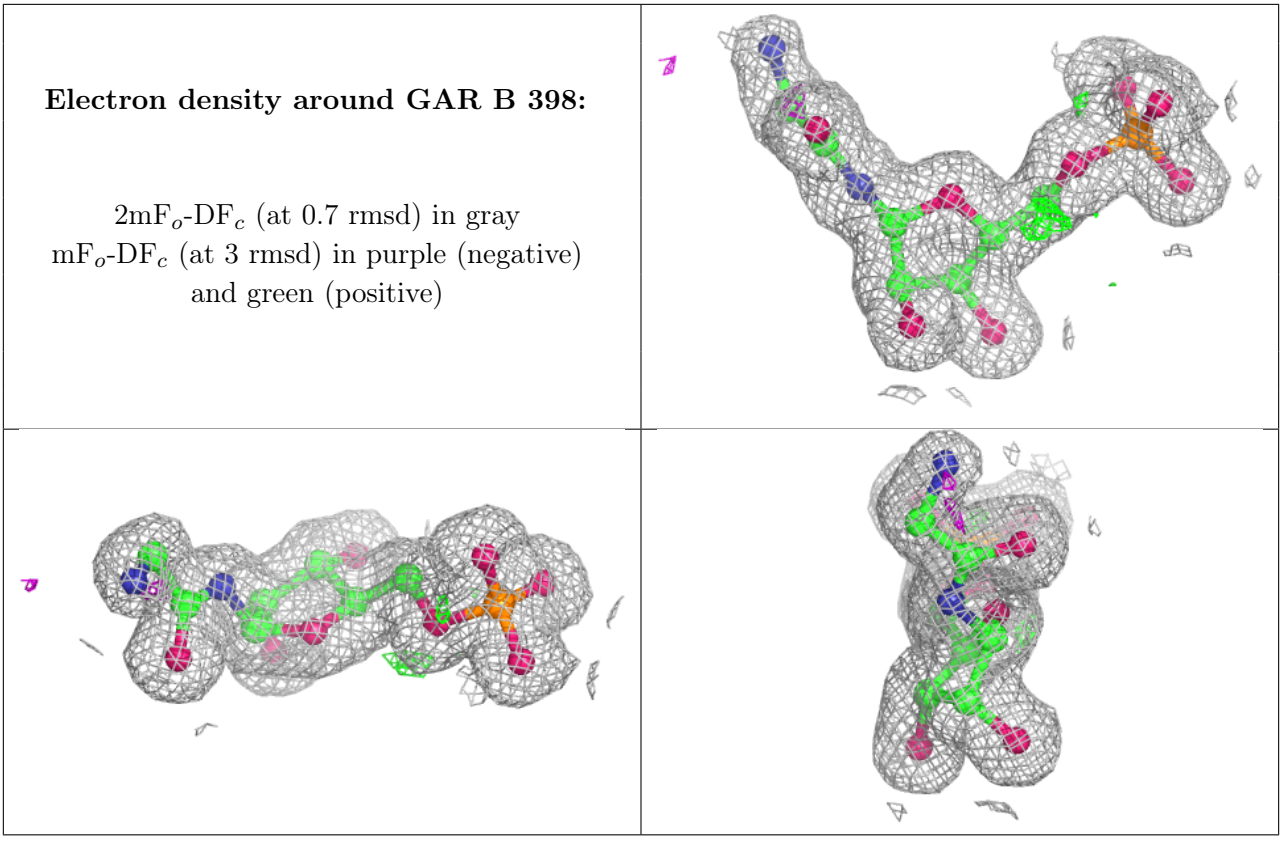
Electron density around ATP B 397:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



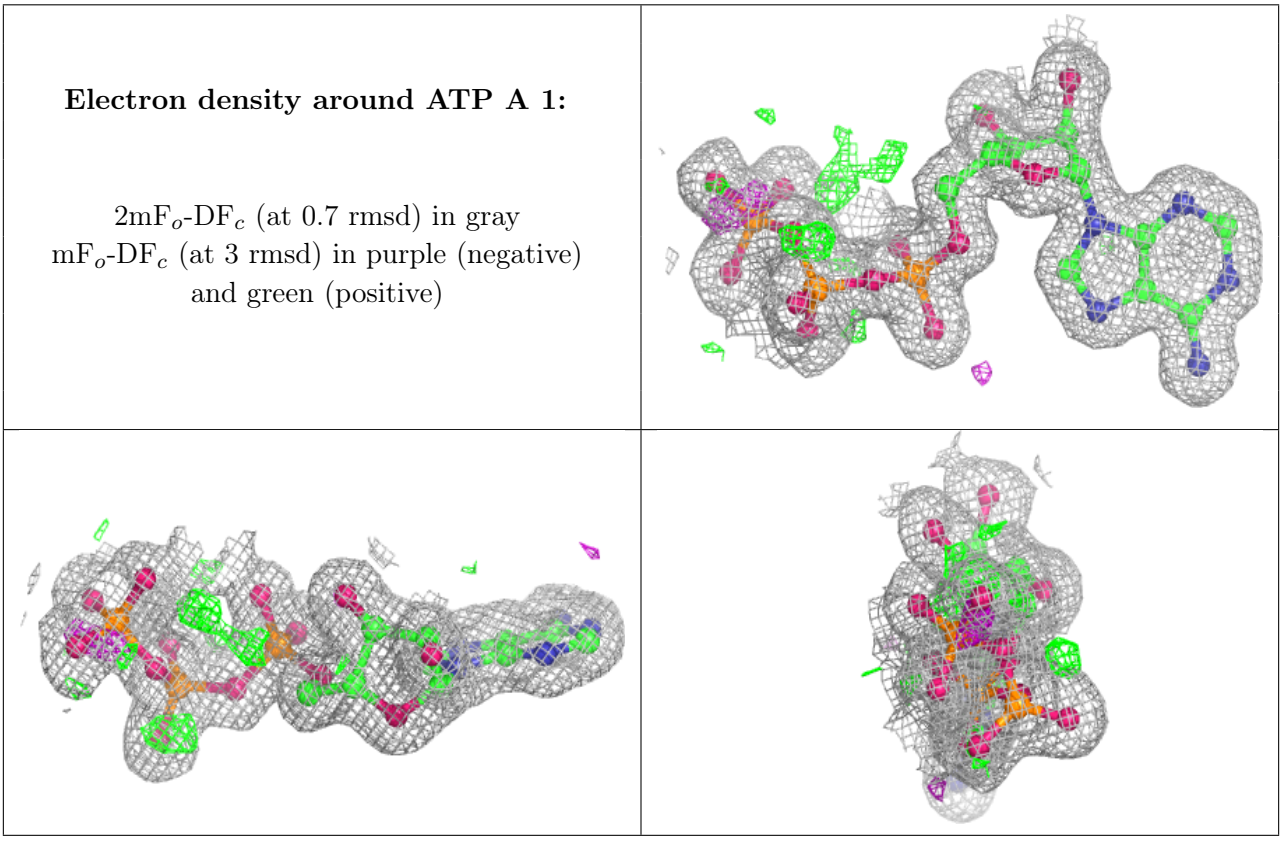
Electron density around GAR B 398:

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



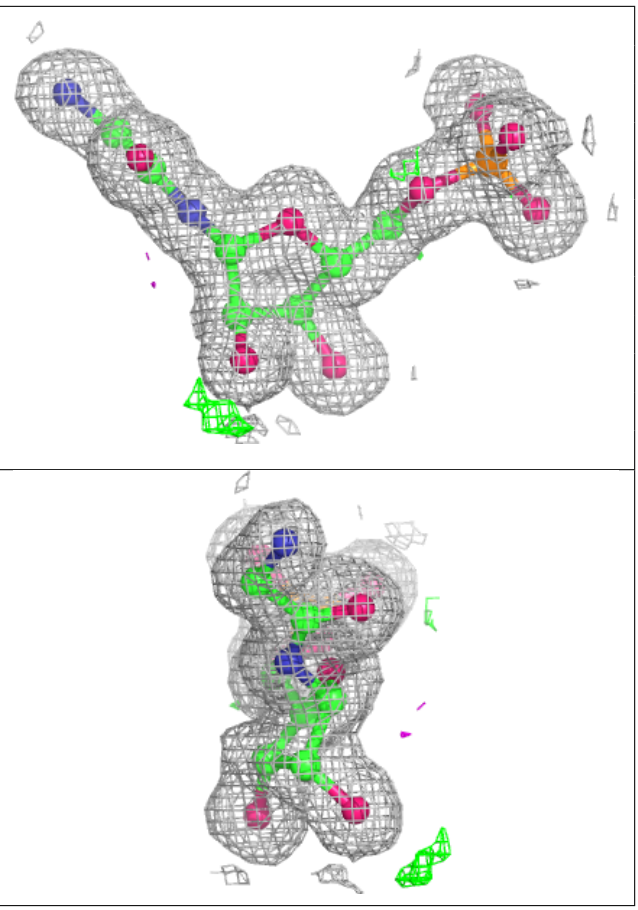
Electron density around ATP A 1:

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



Electron density around GAR A 399:

$2mF_o$-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.