



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:33 AM UTC

PDB ID : 1KJ8 / pdb_00001kj8
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

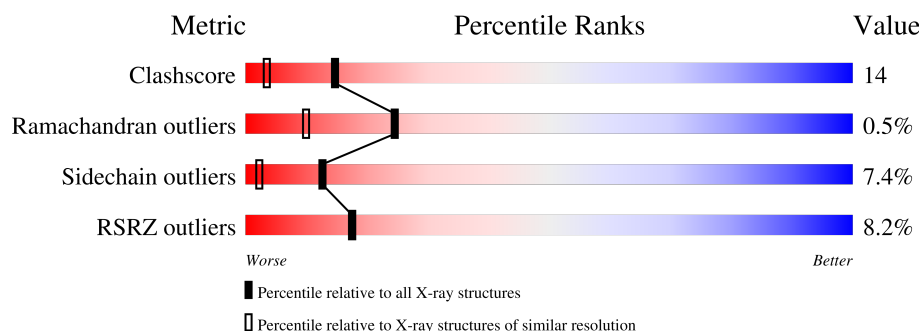
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	 84% 13% ..
1	B	391	 15% 69% 21% 6% ..

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

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
1	A	386	Total	C	N	O	S	0	6	0
			2971	1874	528	556	13			
1	B	384	Total	C	N	O	S	0	3	0
			2946	1857	523	552	14			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

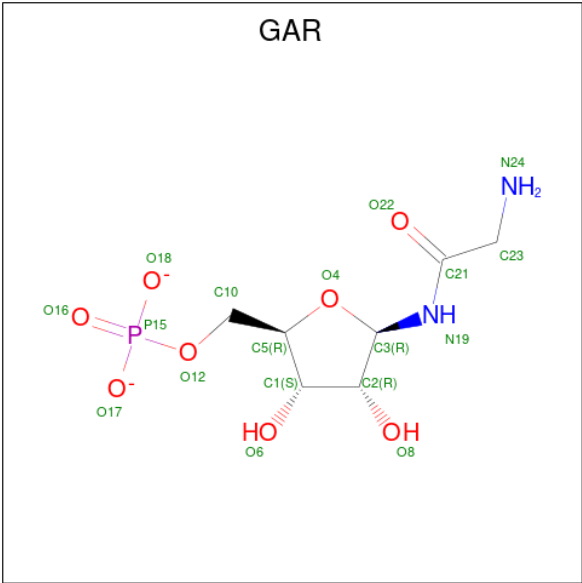
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	1	Total	Cl	0	0
			1	1		

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



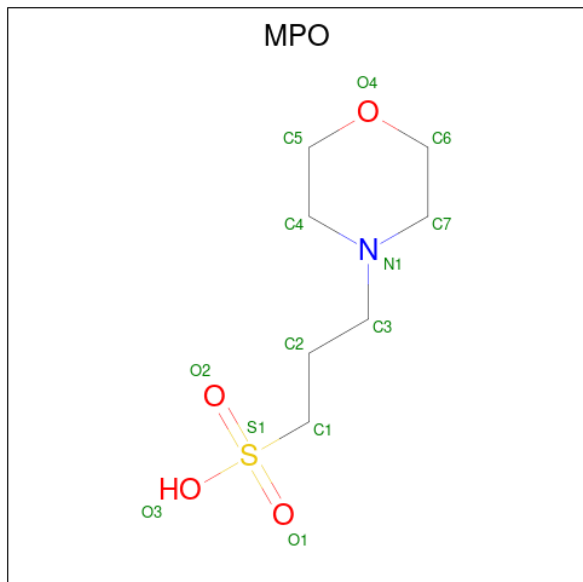
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is GLYCINAMIDE RIBONUCLEOTIDE (CCD ID: GAR) (formula: $C_7H_{13}N_2O_8P$).



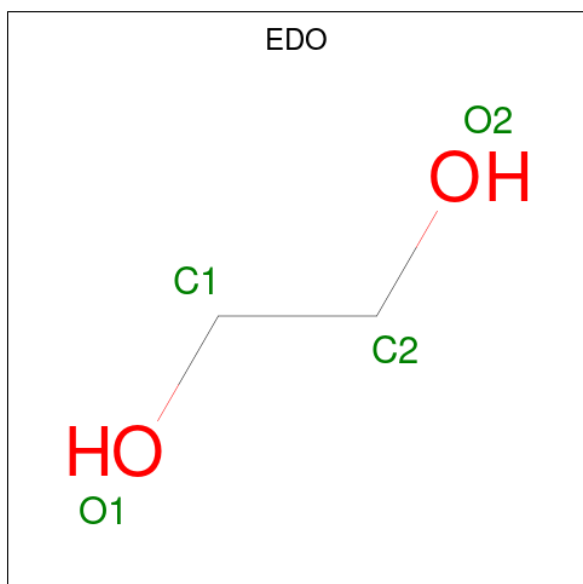
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			18	7	2	8	1		
6	B	1	Total	C	N	O	P	0	0
			18	7	2	8	1		

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



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

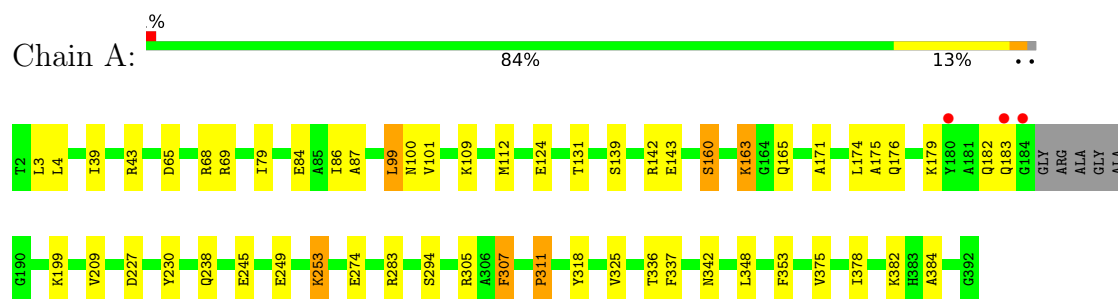
- Molecule 9 is water.

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

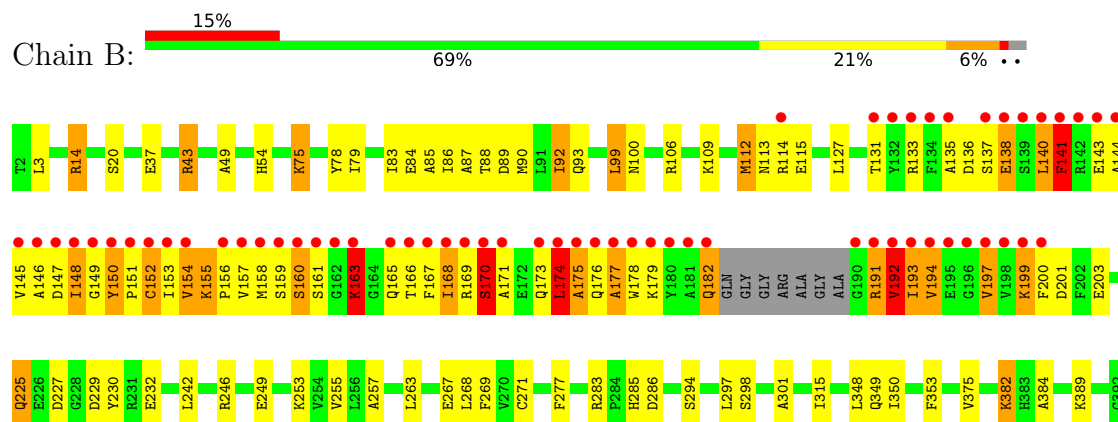
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: phosphoribosylglycinamide formyltransferase 2



- Molecule 1: phosphoribosylglycinamide formyltransferase 2



4 Data and refinement statistics

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 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-1.60) 96.7 (30.00-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 1.54Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.181 , 0.228 (Not available) , (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)	0.36 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	0/3044	1.35	10/4123 (0.2%)
1	B	1.10	0/3007	1.47	24/4075 (0.6%)
All	All	1.11	0/6051	1.41	34/8198 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	VAL	N-CA-C	10.08	123.26	108.65
1	B	353	PHE	N-CA-C	9.80	122.98	111.71
1	B	168	ILE	N-CA-C	9.15	120.92	107.37
1	A	353	PHE	N-CA-C	8.42	122.66	112.38
1	B	170	SER	N-CA-C	8.29	122.91	109.40
1	A	227	ASP	N-CA-C	-6.79	104.30	112.58
1	B	175	ALA	N-CA-C	-6.61	102.72	111.24
1	B	54	HIS	CA-CB-CG	-6.39	107.41	113.80
1	A	325	VAL	N-CA-C	6.22	118.08	109.80
1	B	227	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	285	HIS	N-CA-CB	-5.88	100.60	110.83
1	B	192	VAL	CA-C-O	5.78	127.30	121.64
1	B	152	CYS	N-CA-C	5.59	117.59	108.76
1	A	131	THR	N-CA-C	-5.57	103.18	110.53
1	B	169	ARG	N-CA-C	-5.56	106.63	113.41
1	B	131	THR	CA-C-N	-5.54	113.50	122.36
1	B	131	THR	C-N-CA	-5.54	113.50	122.36
1	A	342	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	318	TYR	N-CA-C	5.44	119.78	113.20
1	B	141	PHE	CA-C-N	5.43	128.34	120.79
1	B	141	PHE	C-N-CA	5.43	128.34	120.79
1	B	140	LEU	CB-CA-C	5.33	119.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	PRO	CB-CA-C	-5.31	104.14	111.21
1	B	90	MET	N-CA-C	-5.31	105.67	111.82
1	A	307	PHE	CA-CB-CG	5.29	119.09	113.80
1	B	14	ARG	N-CA-C	5.26	117.54	109.07
1	A	175	ALA	N-CA-C	5.22	116.78	111.14
1	B	150	TYR	C-N-CD	-5.21	109.13	120.60
1	B	167	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	174	LEU	N-CA-CB	5.14	119.17	110.49
1	B	141	PHE	O-C-N	5.13	127.57	122.08
1	B	286	ASP	N-CA-C	5.08	117.21	111.11
1	B	294	SER	N-CA-C	5.02	119.40	113.28
1	A	294	SER	N-CA-C	5.00	119.39	113.28

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	131	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6896	0	6054	168	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 (168) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:201:ASP:OD2	1:B:201:ASP:N	2.34	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:B:232:GLU:CD	1:B:382:LYS:HD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:100:ASN:C	1:A:100:ASN:HD22	2.15	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
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: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: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:150:TYR:HA	1:B:151:PRO:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:173:GLN:C	1:B:175:ALA:H	2.23	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:137:SER:O	1:B:138:GLU:C	2.59	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
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: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:154:VAL:C	1:B:155:LYS:HG2	2.44	0.42
1:B:141:PHE:CD1	1:B:141:PHE:C	2.96	0.42
1:B:173:GLN:C	1:B:175:ALA:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:144:ALA:C	1:B:146:ALA:N	2.77	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/391 (99%)	376 (97%)	12 (3%)	0	100	100
1	B	383/391 (98%)	365 (95%)	14 (4%)	4 (1%)	12	3
All	All	771/782 (99%)	741 (96%)	26 (3%)	4 (0%)	24	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	LYS

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/311 (102%)	303 (96%)	13 (4%)	27	8
1	B	312/311 (100%)	279 (89%)	33 (11%)	6	1
All	All	628/622 (101%)	582 (93%)	46 (7%)	13	2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	99	LEU
1	A	112	MET
1	A	160	SER
1	A	163	LYS
1	A	183	GLN
1	A	199	LYS
1	A	209	VAL
1	A	230	TYR
1	A	238	GLN
1	A	253	LYS
1	A	274	GLU
1	A	307	PHE
1	B	43	ARG
1	B	75	LYS
1	B	92	ILE
1	B	93	GLN
1	B	99	LEU
1	B	112	MET
1	B	133	ARG

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Mol	Chain	Res	Type
1	B	138	GLU
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	179	LYS
1	B	182	GLN
1	B	191	ARG
1	B	192	VAL
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	255	VAL
1	B	263	LEU
1	B	375	VAL
1	B	382	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	100	ASN
1	A	183	GLN
1	B	176	GLN
1	B	182	GLN
1	B	225	GLN
1	B	248	GLN
1	B	329	GLN
1	B	383	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
5	ATP	A	1	2	32,33,33	1.08	2 (6%)	48,52,52	1.36	3 (6%)
8	EDO	A	401	-	3,3,3	0.57	0	2,2,2	0.06	0
8	EDO	B	400	-	3,3,3	0.32	0	2,2,2	0.42	0
8	EDO	B	399	-	3,3,3	0.54	0	2,2,2	0.13	0
7	MPO	A	400	-	13,13,13	2.06	3 (23%)	17,17,17	1.39	3 (17%)
5	ATP	B	397	2	32,33,33	1.12	3 (9%)	48,52,52	1.16	5 (10%)
6	GAR	B	398	-	17,18,18	0.74	1 (5%)	22,26,26	1.29	3 (13%)
6	GAR	A	399	-	17,18,18	0.74	0	22,26,26	1.33	2 (9%)

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
5	ATP	A	1	2	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	A	401	-	-	0/1/1/1	-
8	EDO	B	400	-	-	1/1/1/1	-
8	EDO	B	399	-	-	1/1/1/1	-
7	MPO	A	400	-	-	0/7/15/15	0/1/1/1
5	ATP	B	397	2	-	10/22/38/38	0/3/3/3
6	GAR	B	398	-	-	0/12/28/28	0/1/1/1
6	GAR	A	399	-	-	0/12/28/28	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	400	MPO	C1-S1	4.87	1.84	1.77
7	A	400	MPO	C3-N1	4.58	1.57	1.47
5	B	397	ATP	C6-N6	-2.72	1.27	1.34
5	B	397	ATP	C2-N1	2.68	1.38	1.33
5	A	1	ATP	C6-N6	-2.54	1.27	1.34
5	B	397	ATP	C8-N7	2.15	1.35	1.31
7	A	400	MPO	O1-S1	2.12	1.51	1.45
5	A	1	ATP	C2-N1	2.06	1.37	1.33
6	B	398	GAR	O4-C3	-2.04	1.39	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	ATP	C2-N1-C6	5.12	127.14	118.73
5	A	1	ATP	N3-C2-N1	-4.13	122.33	128.58
6	B	398	GAR	O4-C3-N19	-3.57	106.19	110.22
6	A	399	GAR	O4-C3-N19	-3.32	106.46	110.22
7	A	400	MPO	O1-S1-C1	3.28	111.68	106.73
5	B	397	ATP	C2-N1-C6	3.07	123.78	118.73
5	A	1	ATP	C5-C6-N1	-2.68	110.72	117.51
5	B	397	ATP	C5-C6-N6	2.62	129.76	123.29
6	B	398	GAR	C10-C5-C1	2.58	124.49	115.21
5	B	397	ATP	C2'-C3'-C4'	-2.43	97.91	102.61
5	B	397	ATP	N3-C2-N1	-2.36	125.01	128.58
6	B	398	GAR	C2-C3-N19	-2.30	109.13	112.02
7	A	400	MPO	C2-C1-S1	-2.29	109.73	113.25
6	A	399	GAR	O17-P15-O12	2.24	112.50	106.67
5	B	397	ATP	C5-C4-N9	2.13	108.13	105.81
7	A	400	MPO	C2-C3-N1	-2.06	108.15	113.93

There are no chirality outliers.

All (16) torsion outliers are listed below:

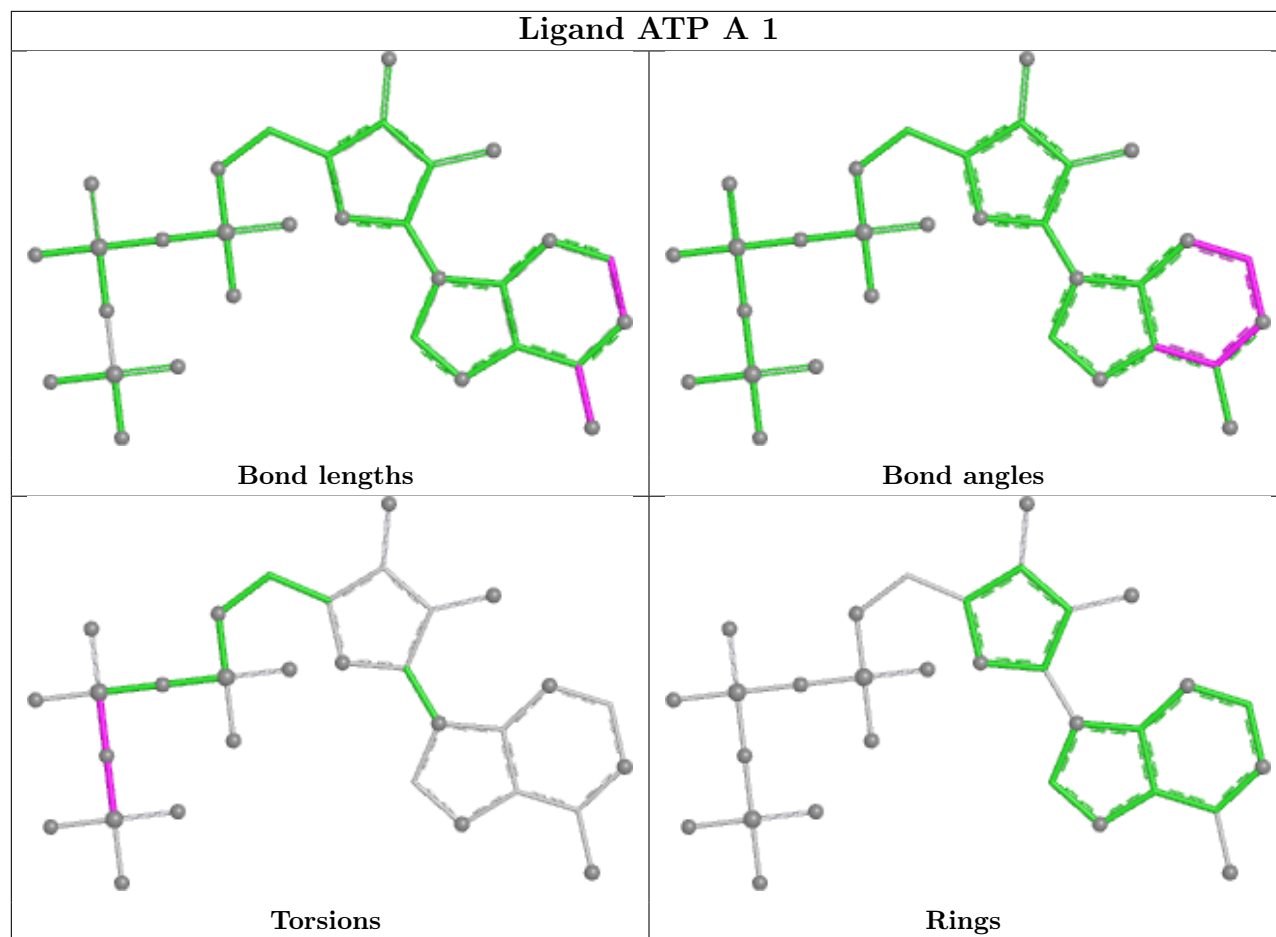
Mol	Chain	Res	Type	Atoms
5	A	1	ATP	PB-O3B-PG-O3G
5	B	397	ATP	PB-O3B-PG-O2G
5	B	397	ATP	PB-O3B-PG-O3G
5	B	397	ATP	PB-O3A-PA-O5'
5	B	397	ATP	O4'-C4'-C5'-O5'
8	B	399	EDO	O1-C1-C2-O2
5	B	397	ATP	C5'-O5'-PA-O1A
5	B	397	ATP	PG-O3B-PB-O2B
5	B	397	ATP	C4'-C5'-O5'-PA
8	B	400	EDO	O1-C1-C2-O2
5	B	397	ATP	PB-O3B-PG-O1G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

There are no ring outliers.

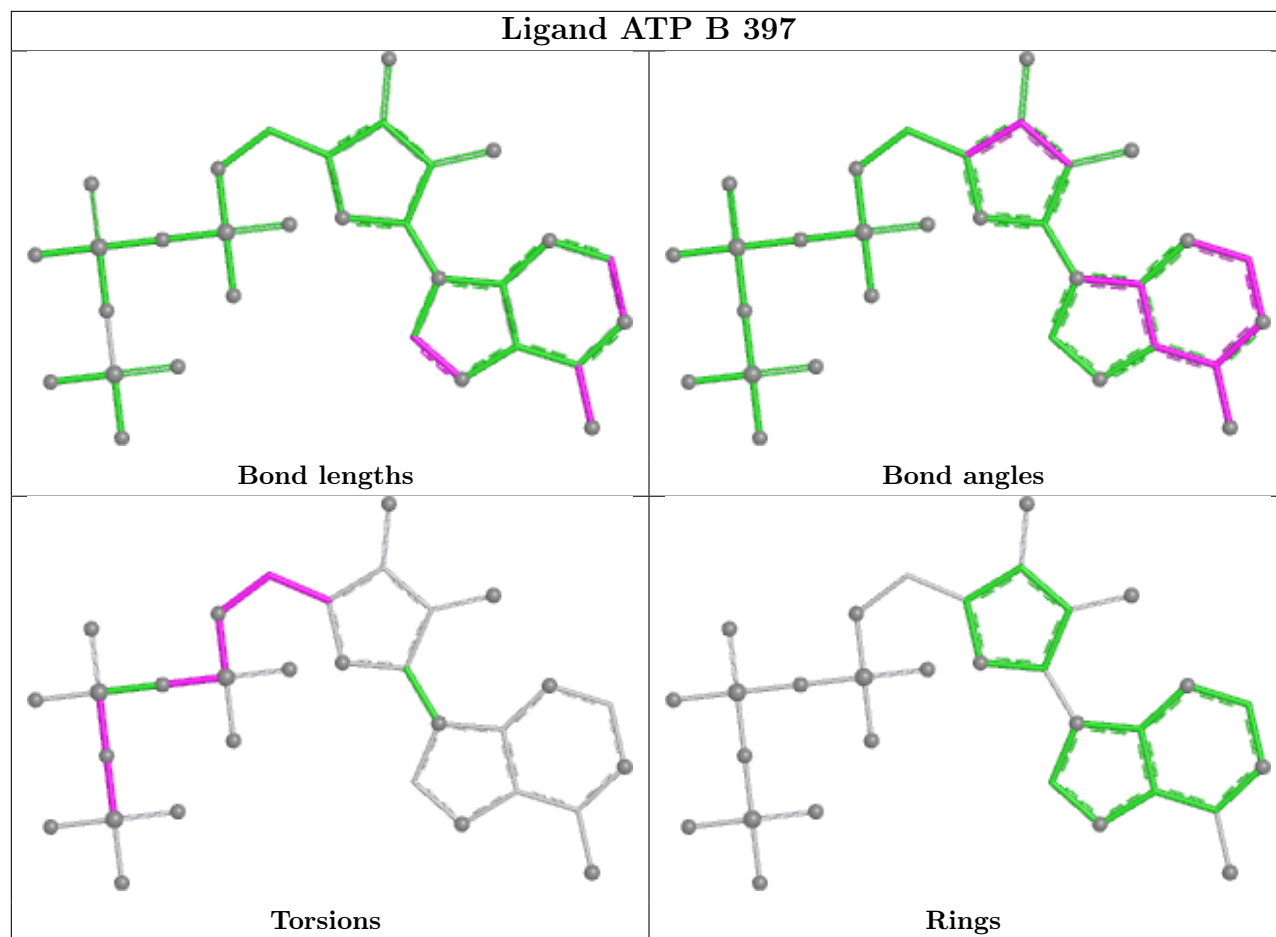
3 monomers are involved in 13 short contacts:

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

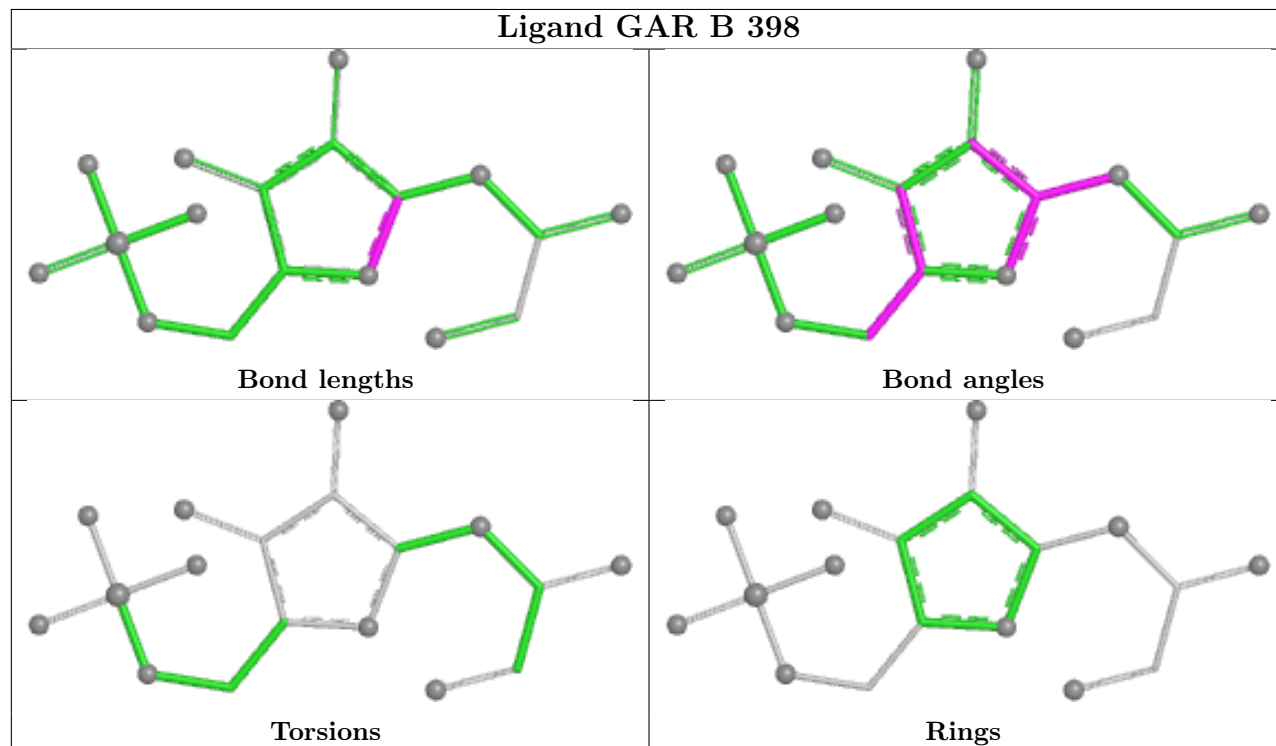
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

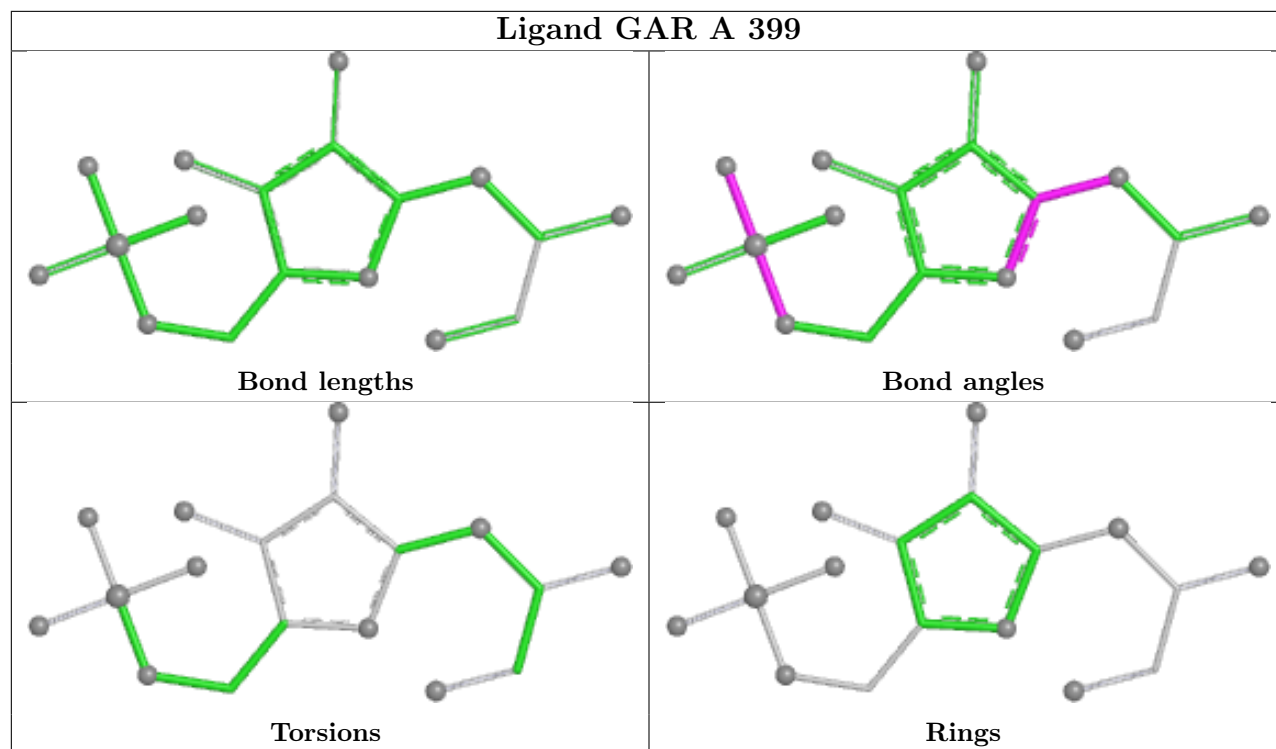


Ligand ATP B 397



Ligand GAR B 398





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/391 (98%)	-0.34	3 (0%) 82 86	9, 16, 40, 91	6 (1%)
1	B	384/391 (98%)	0.44	60 (15%) 5 4	10, 19, 85, 99	3 (0%)
All	All	770/782 (98%)	0.05	63 (8%) 17 17	9, 17, 71, 99	9 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	175	ALA	8.3
1	B	193	ILE	6.9
1	B	154	VAL	6.8
1	B	168	ILE	6.6
1	B	194	VAL	6.6
1	B	141	PHE	6.3
1	B	192	VAL	6.2
1	B	148	ILE	6.0
1	B	177	ALA	6.0
1	A	184	GLY	5.7
1	B	178	TRP	5.6
1	B	140	LEU	5.5
1	B	150	TYR	5.5
1	B	181	ALA	5.4
1	B	167	PHE	5.1
1	B	152	CYS	5.0
1	B	159	SER	5.0
1	B	162	GLY	4.9
1	B	166	THR	4.8
1	B	196	GLY	4.7
1	B	174	LEU	4.5
1	B	144	ALA	4.4
1	B	160	SER	4.4
1	B	180	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	190	GLY	4.2
1	B	176	GLN	4.2
1	B	191	ARG	4.1
1	B	145	VAL	4.1
1	B	157	VAL	4.1
1	B	149	GLY	4.0
1	B	171	ALA	4.0
1	B	146	ALA	3.8
1	B	151	PRO	3.7
1	B	135	ALA	3.7
1	B	169	ARG	3.7
1	B	137	SER	3.7
1	B	156	PRO	3.6
1	B	198	VAL	3.5
1	B	163	LYS	3.4
1	B	134	PHE	3.4
1	B	161	SER	3.3
1	B	153	ILE	3.2
1	B	158	MET	3.1
1	B	139	SER	3.1
1	B	142	ARG	3.1
1	B	173	GLN	3.0
1	B	170	SER	2.9
1	B	197	VAL	2.9
1	A	183	GLN	2.9
1	B	147	ASP	2.9
1	B	195	GLU	2.9
1	B	143	GLU	2.7
1	B	132	TYR	2.7
1	B	199	LYS	2.7
1	B	133	ARG	2.5
1	B	165	GLN	2.5
1	B	138	GLU	2.5
1	B	114	ARG	2.4
1	B	200	PHE	2.4
1	B	182	GLN	2.2
1	B	131	THR	2.2
1	A	180	TYR	2.2
1	B	179	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

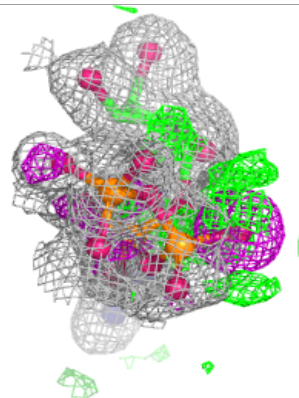
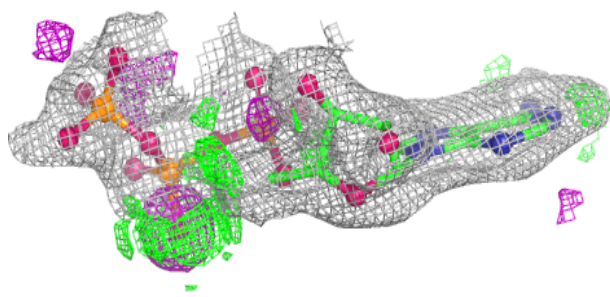
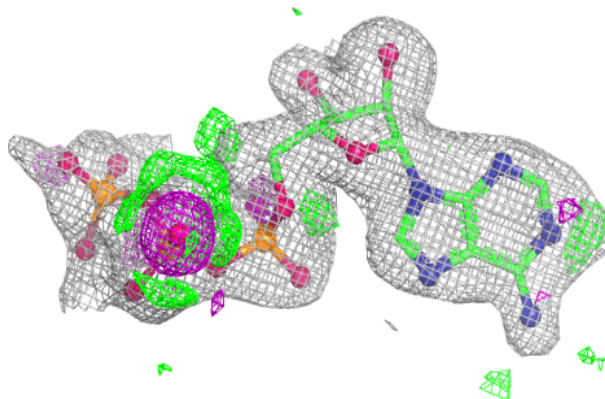
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ATP	B	397	31/31	0.64	0.15	0,39,92,97	0
2	MG	B	393	1/1	0.80	0.13	51,51,51,51	0
8	EDO	B	400	4/4	0.81	0.19	33,36,55,58	0
8	EDO	A	401	4/4	0.82	0.16	47,60,60,62	0
8	EDO	B	399	4/4	0.83	0.20	45,56,61,64	0
2	MG	B	394	1/1	0.90	0.12	39,39,39,39	0
3	NA	A	395	1/1	0.94	0.08	29,29,29,29	0
4	CL	B	396	1/1	0.95	0.10	35,35,35,35	0
4	CL	A	398	1/1	0.96	0.10	34,34,34,34	0
3	NA	B	395	1/1	0.97	0.04	23,23,23,23	0
6	GAR	B	398	18/18	0.98	0.05	10,14,21,29	0
7	MPO	A	400	13/13	0.98	0.07	17,24,31,32	0
5	ATP	A	1	31/31	0.98	0.04	8,14,19,23	0
4	CL	A	397	1/1	0.98	0.08	25,25,25,25	0
6	GAR	A	399	18/18	0.98	0.04	11,15,17,20	0
4	CL	A	396	1/1	0.99	0.10	21,21,21,21	0
2	MG	A	393	1/1	0.99	0.06	16,16,16,16	0
2	MG	A	394	1/1	0.99	0.04	12,12,12,12	0

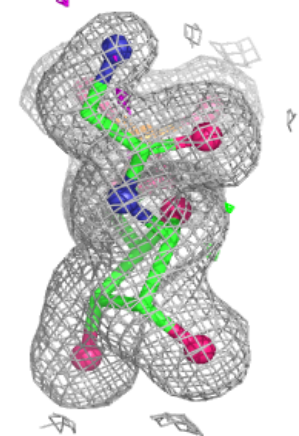
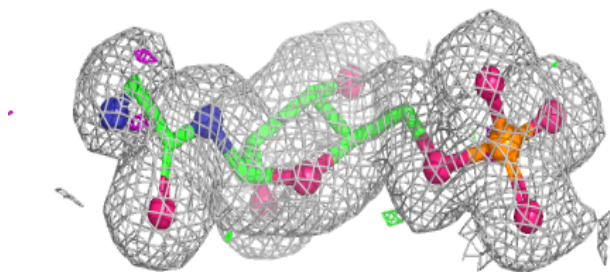
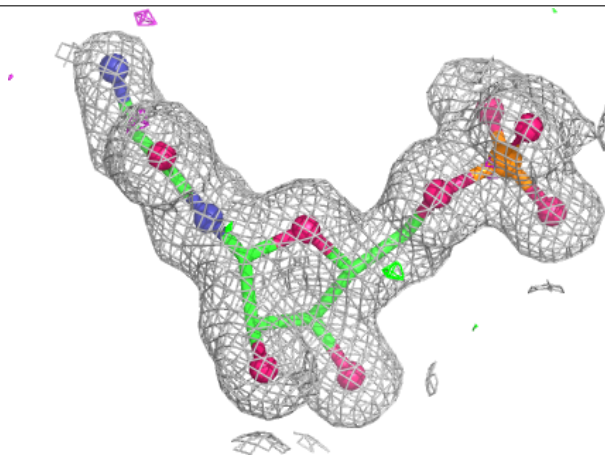
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

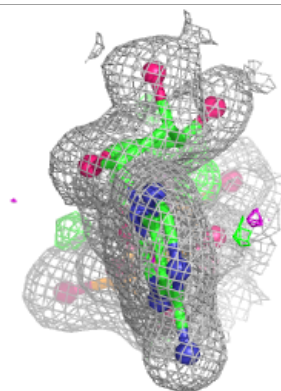
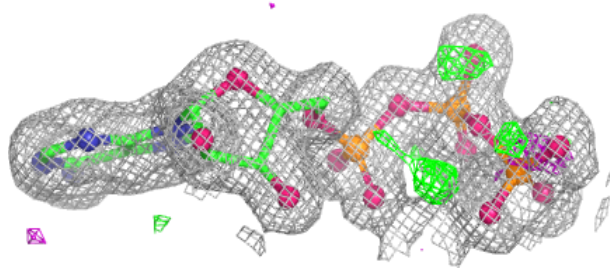
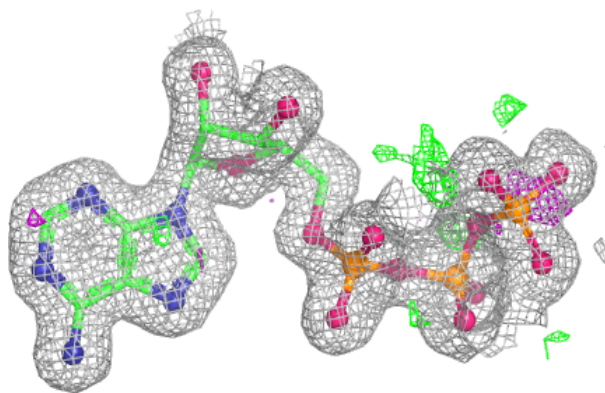
**Electron density around GAR B 398:**

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

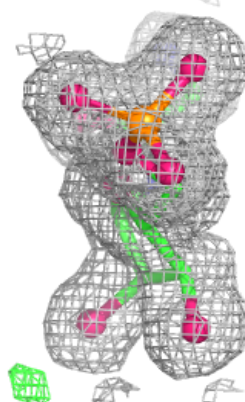
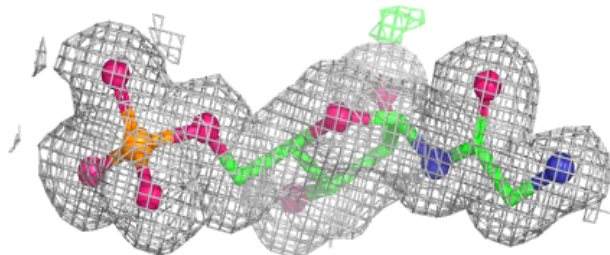
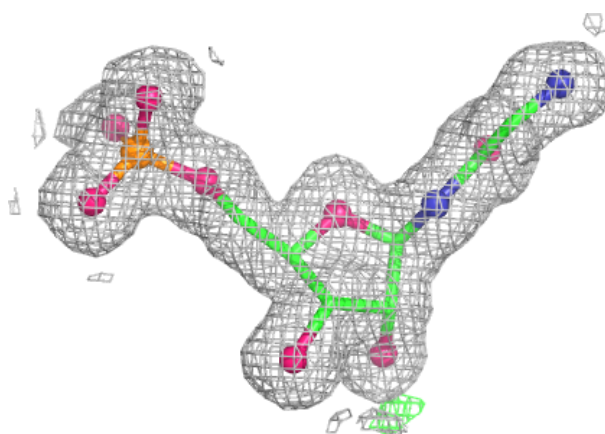


Electron density around ATP A 1:

$2mF_o-DF_c$ (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.