



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:39 AM UTC

PDB ID : 1KJ9 / pdb_00001kj9
Title : Crystal structure of purt-encoded glycinamide ribonucleotide transformylase complexed with Mg-ATP
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

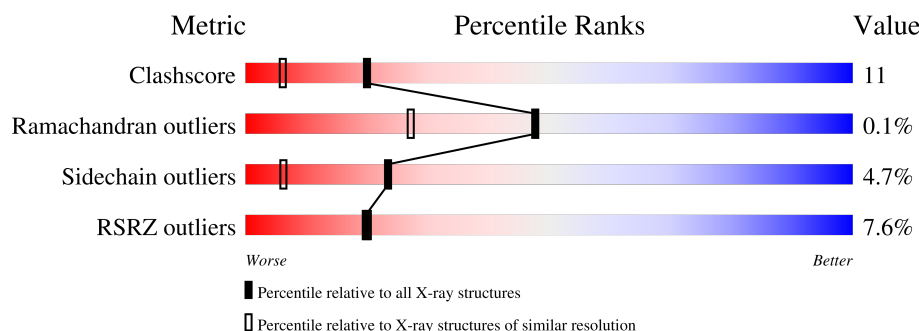
1 Overall quality at a glance

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	 % 86% 11% ..
1	B	391	 14% 72% 21% 5% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6999 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	1	0
			2947	1857	522	554	14			
1	B	387	Total	C	N	O	S	0	1	0
			2951	1859	523	555	14			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		
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	2	Total	Na	0	0
			2	2		

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

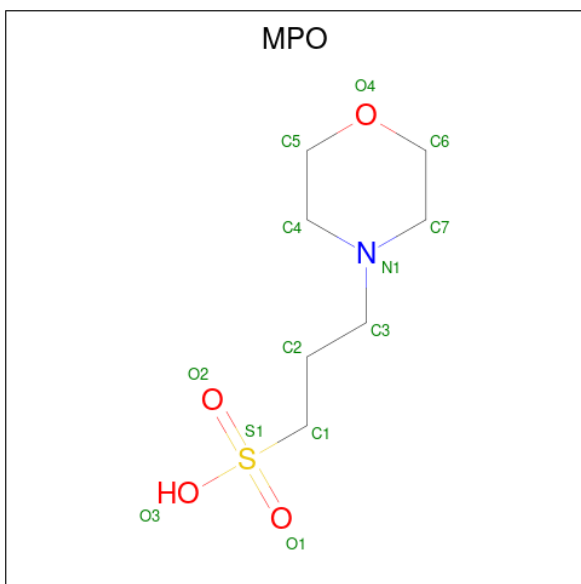
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

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



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

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

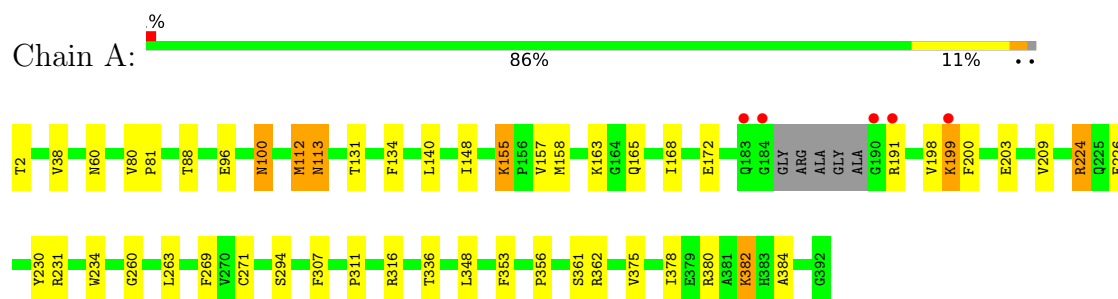
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	580	Total	O	0	0
			580	580		
8	B	413	Total	O	0	0
			413	413		

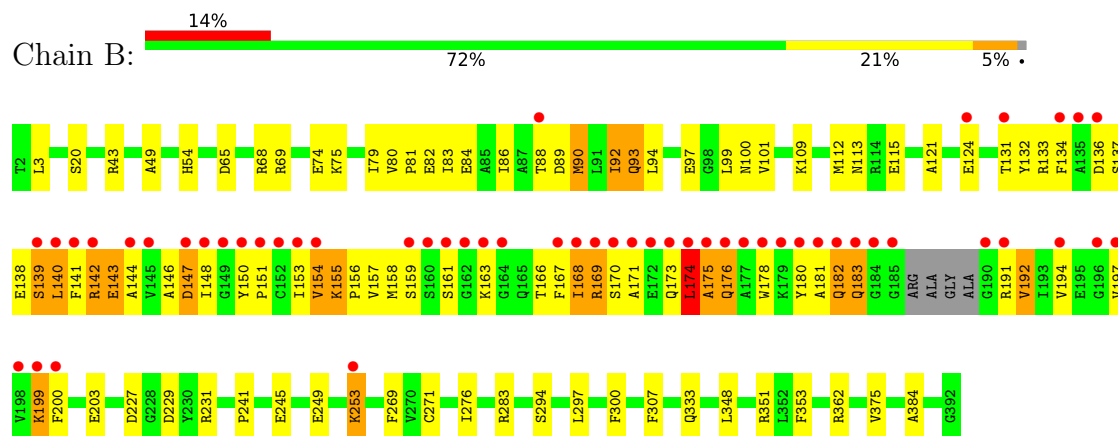
3 Residue-property plots

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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.30Å 179.50Å 75.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 30.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-1.60) 94.5 (30.00-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.182 , 0.230 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 107.4	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	6999	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: CL, MPO, ATP, EDO, MG, NA

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	0/3000	1.36	14/4065 (0.3%)
1	B	1.00	0/3004	1.42	18/4070 (0.4%)
All	All	1.00	0/6004	1.39	32/8135 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	PHE	N-CA-C	10.23	123.48	111.71
1	B	353	PHE	N-CA-C	9.23	123.81	112.54
1	B	176	GLN	CB-CA-C	-7.56	99.32	110.96
1	B	170	SER	N-CA-C	7.16	120.32	109.23
1	B	168	ILE	N-CA-C	6.74	117.34	107.37
1	B	80	VAL	N-CA-C	6.56	114.65	108.15
1	B	253	LYS	CA-CB-CG	6.49	127.09	114.10
1	B	140	LEU	CB-CA-C	6.38	121.38	110.79
1	B	199	LYS	N-CA-CB	6.06	120.59	110.53
1	A	172	GLU	CB-CA-C	-6.00	100.83	110.79
1	B	294	SER	N-CA-C	5.83	120.40	113.28
1	A	81	PRO	N-CA-CB	5.81	108.78	103.15
1	B	131	THR	N-CA-C	-5.66	102.91	110.55
1	A	168	ILE	N-CA-C	5.64	116.54	107.73
1	A	311	PRO	CB-CA-C	-5.63	103.72	111.21
1	A	113	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	294	SER	N-CA-C	5.51	120.01	113.28
1	B	227	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	300	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	253	LYS	CG-CD-CE	5.34	123.59	111.30
1	A	38	VAL	N-CA-C	5.32	115.51	107.75
1	A	224	ARG	CG-CD-NE	5.29	123.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	HIS	CA-CB-CG	-5.23	108.57	113.80
1	B	175	ALA	CA-C-N	5.20	127.51	120.65
1	B	175	ALA	C-N-CA	5.20	127.51	120.65
1	A	307	PHE	CA-CB-CG	5.19	118.99	113.80
1	B	175	ALA	N-CA-C	-5.13	105.38	110.97
1	A	80	VAL	N-CA-CB	-5.07	106.14	111.36
1	A	131	THR	N-CA-C	-5.03	103.76	110.55
1	A	198	VAL	CA-C-N	-5.02	115.34	122.77
1	A	198	VAL	C-N-CA	-5.02	115.34	122.77
1	B	121	ALA	N-CA-C	5.01	116.56	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2947	0	2968	34	0
1	B	2951	0	2971	103	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	1	0
6	A	13	0	15	0	0
7	A	20	0	29	3	0
7	B	4	0	6	0	0
8	A	580	0	0	12	0
8	B	413	0	0	17	1
All	All	6999	0	6013	137	1

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 11.

All (137) 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:141:PHE:HE1	1:B:154:VAL:HG21	1.21	1.04
1:B:156:PRO:HG2	1:B:159:SER:HB3	1.37	1.03
1:A:134:PHE:HB3	1:A:191:ARG:HE	1.21	1.01
1:A:260:GLY:H	7:A:404:EDO:H22	1.27	0.95
1:B:141:PHE:CE1	1:B:154:VAL:HG21	2.06	0.91
1:B:113:ASN:HD22	1:B:158:MET:HE2	1.38	0.85
1:B:68:ARG:HB2	1:B:90:MET:HE3	1.59	0.85
1:B:115:GLU:HG3	1:B:134:PHE:CD2	2.12	0.85
1:B:113:ASN:ND2	1:B:158:MET:HE2	1.93	0.84
1:B:43:ARG:NH2	8:B:726:HOH:O	2.03	0.81
1:A:378:ILE:O	1:A:382:LYS:HG3	1.83	0.79
1:B:115:GLU:HG3	1:B:134:PHE:CE2	2.19	0.78
1:B:137:SER:OG	1:B:140:LEU:HD12	1.84	0.77
1:B:173:GLN:HA	1:B:176:GLN:HE21	1.49	0.77
1:B:174:LEU:HD12	1:B:174:LEU:H	1.49	0.76
1:B:141:PHE:HE1	1:B:154:VAL:CG2	2.00	0.73
1:A:134:PHE:HB2	1:A:191:ARG:HH21	1.54	0.72
1:B:89:ASP:HB2	8:B:672:HOH:O	1.88	0.72
1:B:94:LEU:HB3	1:B:99:LEU:HD13	1.71	0.72
1:B:143:GLU:O	1:B:146:ALA:HB3	1.91	0.71
1:A:362:ARG:NH1	8:A:893:HOH:O	2.22	0.71
1:B:169:ARG:HH11	1:B:169:ARG:HG3	1.56	0.71
1:A:134:PHE:HB3	1:A:191:ARG:NE	2.04	0.69
1:B:174:LEU:H	1:B:174:LEU:CD1	2.04	0.69
1:B:65:ASP:O	1:B:69:ARG:HG3	1.93	0.69
1:A:260:GLY:N	7:A:404:EDO:H22	2.06	0.69
1:B:203:GLU:HG2	1:B:269:PHE:CD1	2.28	0.68
1:B:156:PRO:CG	1:B:159:SER:HB3	2.18	0.67
1:B:173:GLN:HA	1:B:176:GLN:NE2	2.10	0.66
1:B:153:ILE:CD1	1:B:197:VAL:HG22	2.25	0.66
1:B:362:ARG:NH1	8:B:607:HOH:O	2.28	0.66
1:B:178:TRP:O	1:B:182:GLN:NE2	2.29	0.65
1:B:83:ILE:O	1:B:86:ILE:HD12	1.96	0.65
1:B:138:GLU:O	1:B:142:ARG:HB2	1.98	0.63
1:A:375:VAL:HG23	8:A:697:HOH:O	1.98	0.63
1:B:88:THR:HG21	1:B:112:MET:HE2	1.81	0.63
1:B:174:LEU:HD12	1:B:174:LEU:N	2.12	0.63
1:B:161:SER:HB3	1:B:163:LYS:HE3	1.81	0.62
1:A:134:PHE:CB	1:A:191:ARG:HH21	2.13	0.61
1:B:203:GLU:HG2	1:B:269:PHE:HD1	1.66	0.61
1:B:150:TYR:HE2	1:B:168:ILE:HG22	1.66	0.61
1:B:150:TYR:CE2	1:B:168:ILE:HG22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:O	1:B:174:LEU:HD13	2.01	0.59
1:B:173:GLN:CA	1:B:176:GLN:HE21	2.15	0.59
1:B:249:GLU:O	1:B:253:LYS:HG3	2.03	0.59
1:A:112:MET:HB3	8:A:471:HOH:O	2.03	0.58
1:A:100:ASN:C	1:A:100:ASN:HD22	2.11	0.58
1:B:283:ARG:NH2	8:B:496:HOH:O	2.37	0.58
1:A:234:TRP:HZ2	8:A:885:HOH:O	1.87	0.58
1:B:159:SER:HB2	8:B:797:HOH:O	2.05	0.57
1:B:171:ALA:HA	1:B:174:LEU:HD13	1.87	0.57
1:B:147:ASP:HB2	8:B:682:HOH:O	2.05	0.56
1:B:180:TYR:HD2	1:B:183:GLN:HB2	1.70	0.56
1:B:100:ASN:ND2	8:B:551:HOH:O	2.38	0.56
1:A:60:ASN:HB2	8:A:536:HOH:O	2.06	0.55
1:B:180:TYR:HD2	1:B:183:GLN:CB	2.20	0.55
1:B:132:TYR:O	1:B:133:ARG:HD2	2.07	0.55
5:B:395:ATP:H8	5:B:395:ATP:O5'	1.91	0.54
1:B:166:THR:HB	8:B:806:HOH:O	2.09	0.53
1:A:140:LEU:HD12	8:A:684:HOH:O	2.10	0.52
1:A:199:LYS:NZ	1:A:199:LYS:HB2	2.25	0.51
1:B:79:ILE:HD11	1:B:99:LEU:HD22	1.91	0.51
1:B:199:LYS:HE2	1:B:200:PHE:O	2.09	0.51
1:B:200:PHE:HA	1:B:271[B]:CYS:SG	2.50	0.51
1:B:153:ILE:HD12	1:B:197:VAL:HG22	1.91	0.51
1:B:180:TYR:C	1:B:182:GLN:H	2.18	0.50
1:B:84:GLU:HG2	1:B:112:MET:HA	1.92	0.50
1:B:132:TYR:HA	1:B:194:VAL:O	2.12	0.50
1:B:88:THR:O	1:B:92:ILE:HD12	2.11	0.50
1:B:200:PHE:HB3	1:B:269:PHE:HB3	1.94	0.50
1:B:100:ASN:HD22	1:B:100:ASN:C	2.21	0.49
1:B:173:GLN:HG2	1:B:176:GLN:HE22	1.77	0.49
1:A:148:ILE:O	7:A:402:EDO:H11	2.12	0.49
1:B:180:TYR:CD2	1:B:183:GLN:CB	2.96	0.49
1:B:169:ARG:HG3	1:B:169:ARG:NH1	2.24	0.49
1:B:81:PRO:HB3	1:B:86:ILE:HD13	1.95	0.48
1:B:157:VAL:HG13	1:B:192:VAL:HA	1.95	0.48
1:A:157:VAL:HG11	1:A:191:ARG:HD3	1.96	0.48
1:B:153:ILE:HD11	1:B:197:VAL:HG22	1.94	0.48
1:B:68:ARG:CB	1:B:90:MET:HE3	2.38	0.47
1:B:151:PRO:HB2	1:B:167:PHE:CE2	2.49	0.47
1:B:150:TYR:HB3	1:B:151:PRO:HA	1.97	0.47
1:A:88:THR:HB	8:A:848:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:NZ	1:A:199:LYS:CB	2.78	0.47
1:A:155:LYS:HB3	1:A:165:GLN:HG2	1.96	0.47
1:B:253:LYS:HG2	8:B:493:HOH:O	2.14	0.47
1:B:297:LEU:HA	8:B:535:HOH:O	2.15	0.46
1:B:82:GLU:HB2	8:B:523:HOH:O	2.16	0.46
1:B:139:SER:O	1:B:143:GLU:HB2	2.14	0.46
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.57	0.46
1:A:200:PHE:HB3	1:A:269:PHE:HB3	1.98	0.46
1:B:153:ILE:HD12	1:B:197:VAL:CG2	2.45	0.45
1:A:96:GLU:HG3	8:A:672:HOH:O	2.15	0.45
1:B:171:ALA:C	1:B:174:LEU:HD13	2.42	0.45
1:B:134:PHE:HA	1:B:192:VAL:O	2.17	0.45
1:B:333:GLN:NE2	8:B:719:HOH:O	2.50	0.45
1:A:2:THR:HG23	8:A:924:HOH:O	2.17	0.45
1:B:68:ARG:HE	1:B:90:MET:HE1	1.81	0.45
1:A:200:PHE:HA	1:A:271[B]:CYS:SG	2.57	0.45
1:B:348:LEU:HD11	1:B:384:ALA:CB	2.47	0.44
1:B:115:GLU:OE1	1:B:191:ARG:NH1	2.51	0.44
1:B:137:SER:O	1:B:141:PHE:N	2.38	0.44
1:B:351:ARG:NH2	8:B:713:HOH:O	2.42	0.44
1:A:336:THR:HB	1:B:3:LEU:HD11	1.99	0.44
1:B:43:ARG:HH11	1:B:43:ARG:HG3	1.82	0.44
1:B:20:SER:HB3	1:B:49:ALA:HB3	2.00	0.43
1:B:241:PRO:O	1:B:245:GLU:HB2	2.17	0.43
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.84	0.43
1:B:93:GLN:O	1:B:97:GLU:HG3	2.18	0.43
1:A:348:LEU:HD11	1:A:384:ALA:CB	2.49	0.43
1:B:173:GLN:O	1:B:176:GLN:N	2.52	0.43
1:B:180:TYR:CD2	1:B:183:GLN:HB3	2.54	0.43
1:A:226:GLU:HB2	1:A:231:ARG:HG3	2.00	0.43
1:B:154:VAL:CG1	8:B:806:HOH:O	2.67	0.43
1:B:181:ALA:C	1:B:182:GLN:NE2	2.77	0.42
1:B:100:ASN:HD22	1:B:101:VAL:N	2.18	0.42
1:B:231:ARG:NH2	8:B:692:HOH:O	2.50	0.42
1:A:356:PRO:HD2	8:A:893:HOH:O	2.20	0.42
1:B:180:TYR:C	1:B:182:GLN:N	2.78	0.42
1:B:109:LYS:O	1:B:112:MET:HG3	2.20	0.41
1:B:153:ILE:HG22	1:B:155:LYS:HG2	2.01	0.41
1:B:148:ILE:HD13	1:B:148:ILE:HA	1.82	0.41
1:B:94:LEU:HD22	1:B:99:LEU:HD13	2.03	0.41
1:A:209:VAL:HG22	1:A:263:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ILE:HD12	1:B:276:ILE:N	2.35	0.41
1:A:316:ARG:HD2	8:B:582:HOH:O	2.20	0.41
1:A:203:GLU:HB2	8:A:577:HOH:O	2.20	0.41
1:B:163:LYS:HD2	8:B:683:HOH:O	2.20	0.41
1:B:174:LEU:O	1:B:175:ALA:C	2.60	0.41
1:B:348:LEU:HD11	1:B:384:ALA:HB2	2.03	0.41
1:B:136:ASP:HB3	1:B:191:ARG:HE	1.86	0.40
1:B:144:ALA:O	1:B:147:ASP:N	2.52	0.40
1:B:182:GLN:N	1:B:182:GLN:HE21	2.19	0.40
1:A:191:ARG:NH2	8:A:603:HOH:O	2.23	0.40
1:B:171:ALA:HA	1:B:174:LEU:CD1	2.51	0.40
1:B:74:GLU:O	1:B:75:LYS:C	2.61	0.40
1:B:182:GLN:NE2	1:B:182:GLN:N	2.70	0.40

All (1) 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)
8:B:509:HOH:O	8:B:509:HOH:O[2_655]	2.15	0.05

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	383/391 (98%)	373 (97%)	10 (3%)	0	100	100
1	B	384/391 (98%)	366 (95%)	17 (4%)	1 (0%)	36	20
All	All	767/782 (98%)	739 (96%)	27 (4%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/311 (100%)	300 (96%)	11 (4%)	32	11
1	B	311/311 (100%)	293 (94%)	18 (6%)	18	4
All	All	622/622 (100%)	593 (95%)	29 (5%)	23	6

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	112	MET
1	A	113	ASN
1	A	155	LYS
1	A	158	MET
1	A	163	LYS
1	A	199	LYS
1	A	224	ARG
1	A	230	TYR
1	A	361	SER
1	A	382	LYS
1	B	90	MET
1	B	92	ILE
1	B	93	GLN
1	B	124	GLU
1	B	139	SER
1	B	142	ARG
1	B	143	GLU
1	B	147	ASP
1	B	154	VAL
1	B	155	LYS
1	B	169	ARG
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	182	GLN
1	B	183	GLN
1	B	192	VAL
1	B	229	ASP
1	B	307	PHE
1	B	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	183	GLN
1	A	248	GLN
1	A	342	ASN
1	B	100	ASN
1	B	176	GLN
1	B	182	GLN
1	B	183	GLN
1	B	225	GLN
1	B	248	GLN
1	B	333	GLN
1	B	342	ASN
1	B	387	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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$
7	EDO	A	404	-	3,3,3	0.33	0	2,2,2	0.42	0
5	ATP	A	1	2	32,33,33	1.07	2 (6%)	48,52,52	1.20	5 (10%)
7	EDO	A	403	2	3,3,3	0.33	0	2,2,2	0.55	0
7	EDO	B	396	-	3,3,3	0.25	0	2,2,2	0.45	0
6	MPO	A	400	-	13,13,13	2.12	2 (15%)	17,17,17	1.32	3 (17%)
7	EDO	A	402	-	3,3,3	0.28	0	2,2,2	0.50	0
7	EDO	A	401	-	3,3,3	0.40	0	2,2,2	0.27	0
7	EDO	A	405	-	3,3,3	0.45	0	2,2,2	0.13	0
5	ATP	B	395	2	32,33,33	1.05	4 (12%)	48,52,52	1.21	4 (8%)

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
7	EDO	A	404	-	-	0/1/1/1	-
5	ATP	A	1	2	-	4/22/38/38	0/3/3/3
7	EDO	A	403	2	-	0/1/1/1	-
7	EDO	B	396	-	-	1/1/1/1	-
6	MPO	A	400	-	-	0/7/15/15	0/1/1/1
7	EDO	A	402	-	-	1/1/1/1	-
7	EDO	A	401	-	-	1/1/1/1	-
7	EDO	A	405	-	-	1/1/1/1	-
5	ATP	B	395	2	-	2/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	400	MPO	C1-S1	5.36	1.85	1.77
6	A	400	MPO	C3-N1	4.41	1.57	1.47
5	A	1	ATP	C6-N6	-2.72	1.27	1.34
5	B	395	ATP	C2-N1	2.65	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	395	ATP	C6-N6	-2.61	1.27	1.34
5	A	1	ATP	C2-N1	2.43	1.38	1.33
5	B	395	ATP	O4'-C1'	-2.19	1.36	1.42
5	B	395	ATP	C8-N7	2.03	1.35	1.31

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	ATP	C2-N1-C6	4.01	125.32	118.73
5	B	395	ATP	C5-C6-N6	3.16	131.10	123.29
5	B	395	ATP	O2B-PB-O3B	2.91	115.15	107.27
5	A	1	ATP	N3-C2-N1	-2.90	124.20	128.58
5	B	395	ATP	C2-N1-C6	2.60	122.99	118.73
5	A	1	ATP	O3'-C3'-C2'	2.56	120.03	111.82
6	A	400	MPO	O3-S1-O1	-2.46	105.23	111.40
5	B	395	ATP	N3-C2-N1	-2.42	124.92	128.58
5	A	1	ATP	C5-C6-N1	-2.29	111.71	117.51
6	A	400	MPO	O2-S1-C1	2.17	110.01	106.73
5	A	1	ATP	O2B-PB-O3B	2.09	112.92	107.27
6	A	400	MPO	O1-S1-C1	2.08	109.87	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	ATP	PB-O3B-PG-O3G
5	B	395	ATP	PB-O3B-PG-O1G
7	A	405	EDO	O1-C1-C2-O2
7	B	396	EDO	O1-C1-C2-O2
5	B	395	ATP	PG-O3B-PB-O2B
7	A	401	EDO	O1-C1-C2-O2
7	A	402	EDO	O1-C1-C2-O2
5	A	1	ATP	PG-O3B-PB-O1B
5	A	1	ATP	PB-O3B-PG-O1G
5	A	1	ATP	PG-O3B-PB-O2B

There are no ring outliers.

3 monomers are involved in 4 short contacts:

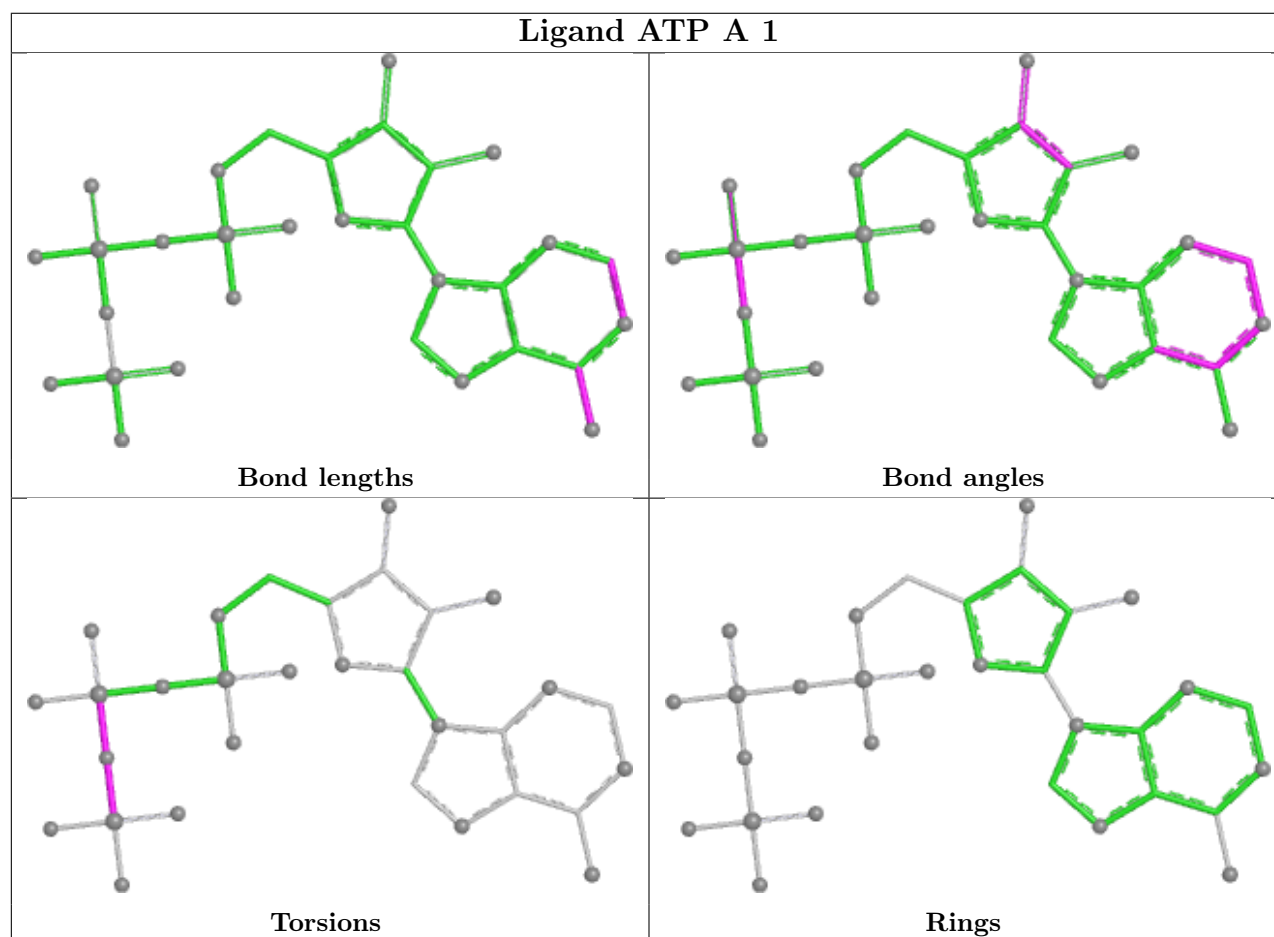
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	404	EDO	2	0

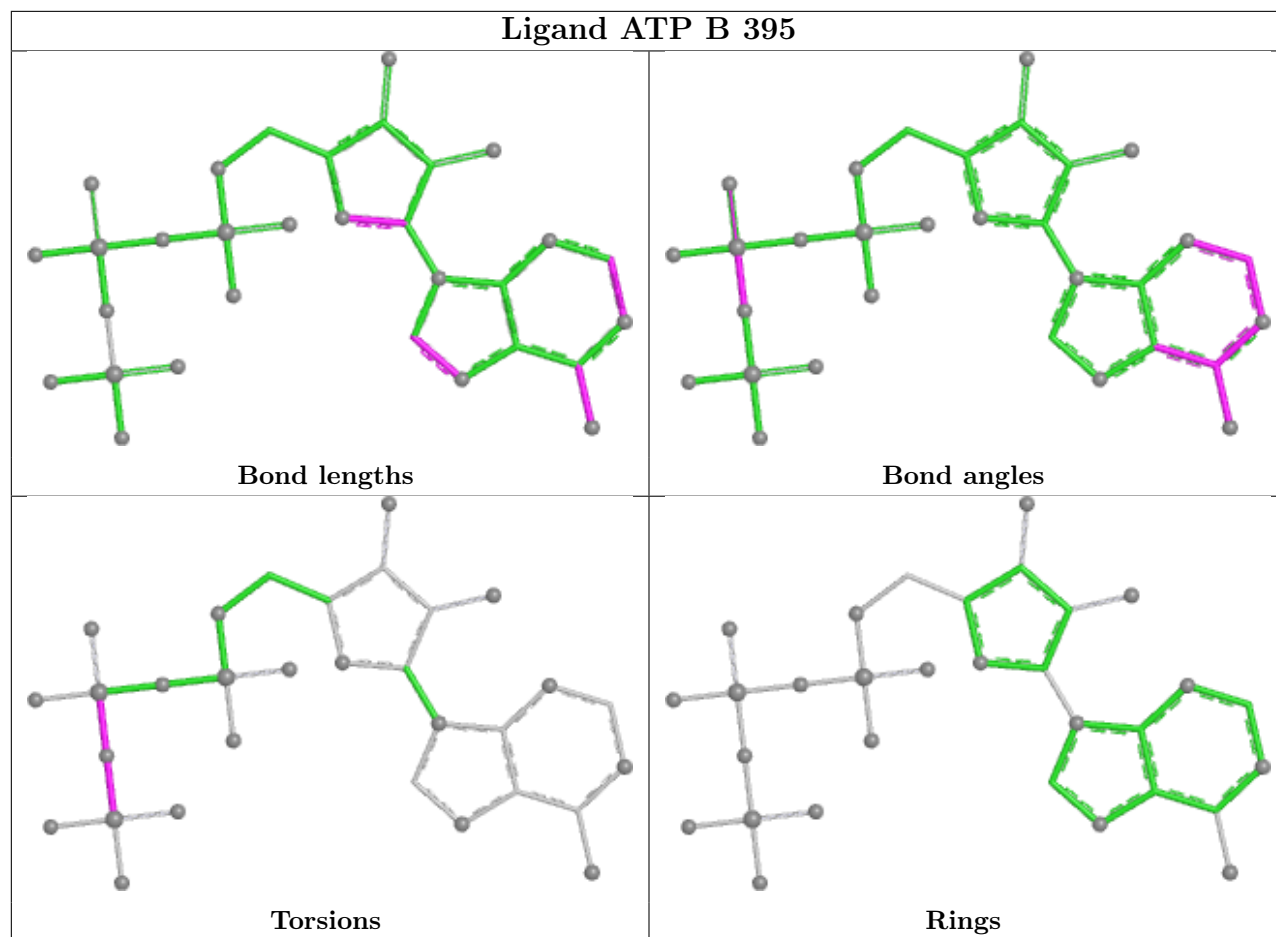
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	402	EDO	1	0
5	B	395	ATP	1	0

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.





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%)	-0.38	5 (1%) 75 79	8, 14, 40, 87	1 (0%)
1	B	387/391 (98%)	0.32	54 (13%) 6 6	10, 19, 74, 99	1 (0%)
All	All	773/782 (98%)	-0.03	59 (7%) 20 20	8, 16, 58, 99	2 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	PHE	6.9
1	B	190	GLY	6.2
1	B	175	ALA	6.2
1	A	184	GLY	5.9
1	B	185	GLY	5.9
1	B	178	TRP	5.2
1	B	148	ILE	5.0
1	B	145	VAL	5.0
1	B	150	TYR	4.5
1	B	154	VAL	4.1
1	B	149	GLY	4.1
1	B	176	GLN	4.0
1	A	190	GLY	4.0
1	B	152	CYS	4.0
1	B	184	GLY	3.9
1	B	168	ILE	3.7
1	B	167	PHE	3.6
1	B	144	ALA	3.5
1	B	162	GLY	3.5
1	B	171	ALA	3.3
1	B	163	LYS	3.3
1	B	196	GLY	3.3
1	B	140	LEU	3.3
1	A	199	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	181	ALA	3.3
1	B	199	LYS	3.2
1	B	169	ARG	3.1
1	B	198	VAL	3.0
1	B	180	TYR	3.0
1	B	194	VAL	2.9
1	A	183	GLN	2.9
1	B	177	ALA	2.9
1	B	197	VAL	2.8
1	B	179	LYS	2.8
1	B	170	SER	2.8
1	B	182	GLN	2.8
1	B	174	LEU	2.8
1	B	134	PHE	2.7
1	B	183	GLN	2.7
1	B	159	SER	2.5
1	B	172	GLU	2.5
1	B	131	THR	2.5
1	B	160	SER	2.4
1	B	151	PRO	2.4
1	B	191	ARG	2.4
1	B	164	GLY	2.3
1	B	142	ARG	2.3
1	B	139	SER	2.2
1	B	200	PHE	2.2
1	A	191	ARG	2.1
1	B	253	LYS	2.1
1	B	88	THR	2.1
1	B	124	GLU	2.1
1	B	147	ASP	2.1
1	B	153	ILE	2.1
1	B	136	ASP	2.0
1	B	161	SER	2.0
1	B	173	GLN	2.0
1	B	135	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

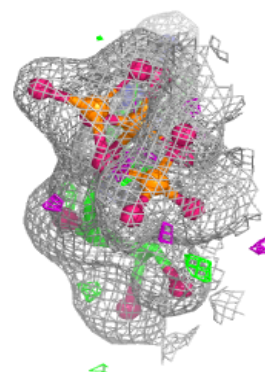
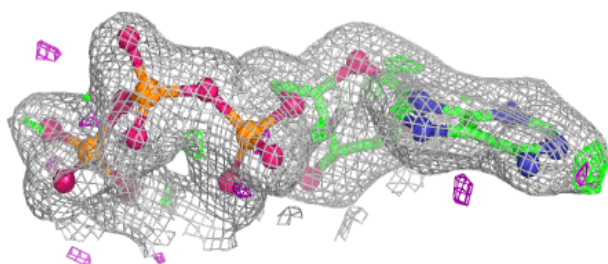
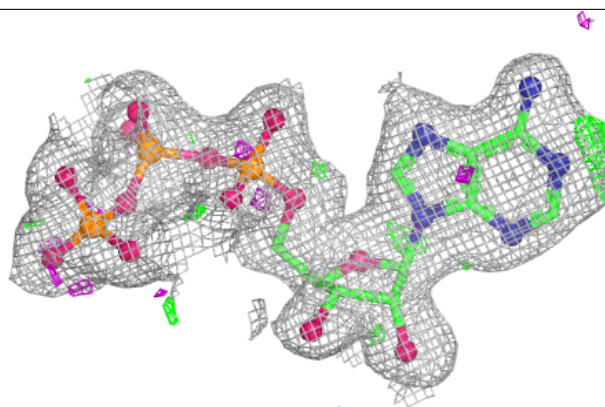
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	A	405	4/4	0.52	0.30	0,63,71,84	0
7	EDO	B	396	4/4	0.80	0.18	27,50,56,82	0
7	EDO	A	404	4/4	0.81	0.20	47,48,55,78	0
7	EDO	A	402	4/4	0.88	0.12	27,30,32,41	0
7	EDO	A	401	4/4	0.93	0.10	24,25,31,41	0
5	ATP	B	395	31/31	0.95	0.09	17,29,38,45	0
3	NA	A	397	1/1	0.96	0.08	27,27,27,27	0
2	MG	B	394	1/1	0.97	0.04	19,19,19,19	0
3	NA	A	396	1/1	0.97	0.10	24,24,24,24	0
7	EDO	A	403	4/4	0.97	0.07	13,15,17,21	0
2	MG	B	393	1/1	0.99	0.05	25,25,25,25	0
6	MPO	A	400	13/13	0.99	0.05	12,16,22,22	0
2	MG	A	393	1/1	0.99	0.06	11,11,11,11	0
2	MG	A	394	1/1	0.99	0.03	10,10,10,10	0
2	MG	A	395	1/1	0.99	0.07	18,18,18,18	0
4	CL	A	398	1/1	0.99	0.08	22,22,22,22	0
4	CL	A	399	1/1	0.99	0.13	18,18,18,18	0
5	ATP	A	1	31/31	0.99	0.04	9,12,15,16	0

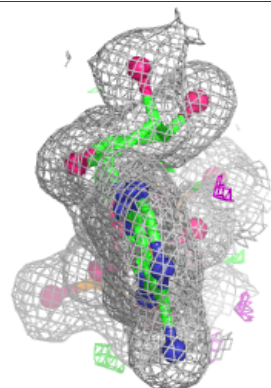
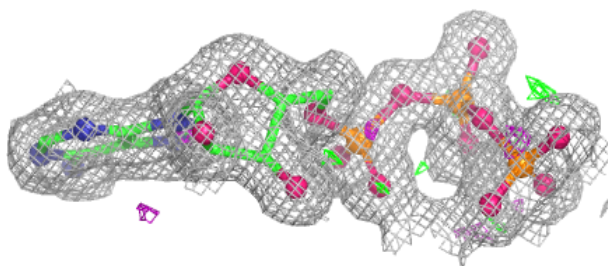
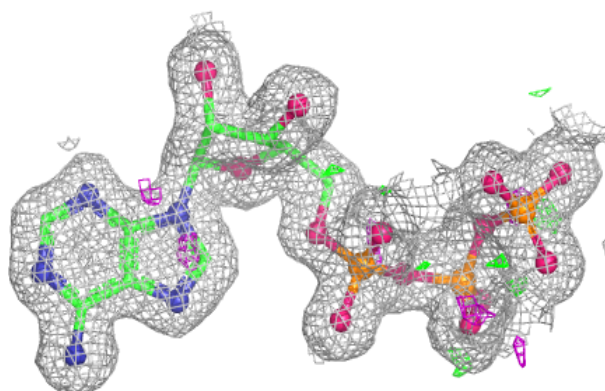
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 395:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.