



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 PM UTC

PDB ID : 6JT8 / pdb_00006jt8
Title : Crystal structure of 450-451_deletion mutant of FGAM Synthetase
Authors : Sharma, N.; Ahalawat, N.; Sandhu, P.; Mondal, J.; Anand, R.
Deposited on : 2019-04-10
Resolution : 1.90 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

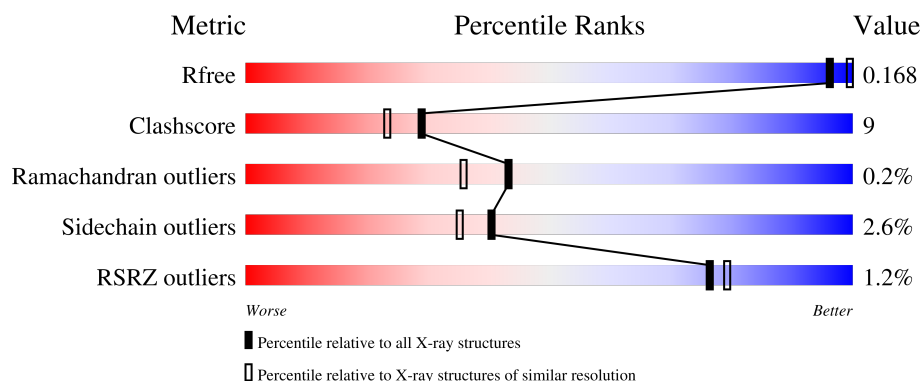
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1301	

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
5	GOL	A	1333	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1342	-	X	-	-
5	GOL	A	1343	-	-	X	-
5	GOL	A	1347	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11874 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 Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1288	Total	C	N	O	S	0	44	0
			10249	6430	1820	1946	53			

There are 10 discrepancies between the modelled and reference sequences:

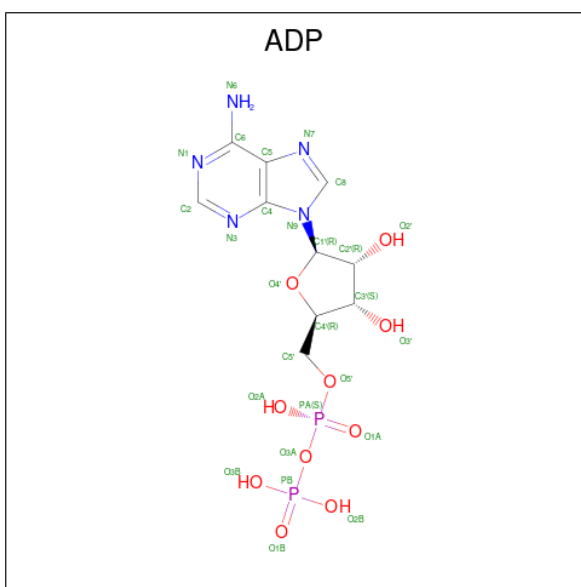
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-6	LEU	-	expression tag	UNP A0A0D6F9Y3
A	-5	VAL	-	expression tag	UNP A0A0D6F9Y3
A	-4	PRO	-	expression tag	UNP A0A0D6F9Y3
A	-3	ARG	-	expression tag	UNP A0A0D6F9Y3
A	-2	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-1	SER	-	expression tag	UNP A0A0D6F9Y3
A	0	HIS	-	expression tag	UNP A0A0D6F9Y3
A	?	-	GLY	deletion	UNP A0A0D6F9Y3
A	?	-	GLY	deletion	UNP A0A0D6F9Y3

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



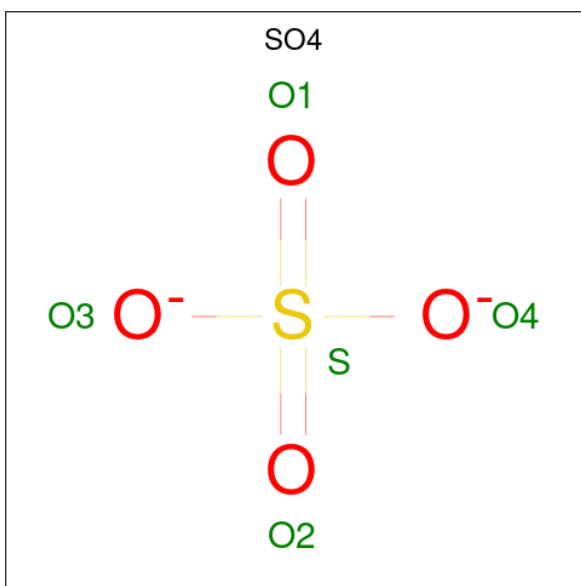
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		

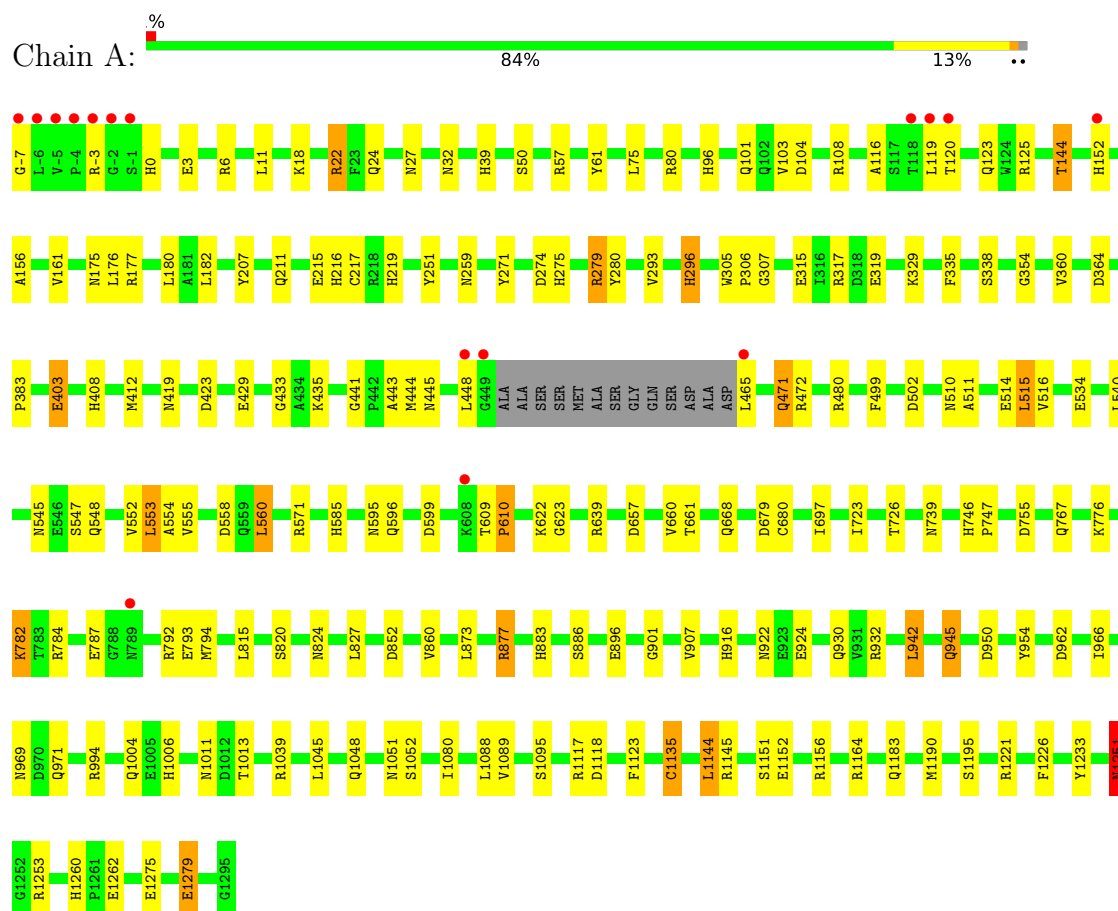
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1358	Total	O	0	0
			1358	1358		

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: Phosphoribosylformylglycinamide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	147.15Å 147.15Å 141.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.17 – 1.90 48.17 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.17-1.90) 99.9 (48.17-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.125 , 0.159 0.139 , 0.168	Depositor DCC
R_{free} test set	6856 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11874	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, ADP, EDO, MG, CYG

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	1.35	34/10471 (0.3%)	1.09	13/14209 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	877[A]	ARG	CA-C	8.81	1.64	1.53
1	A	877[B]	ARG	CA-C	8.81	1.64	1.53
1	A	932	ARG	C-O	-6.74	1.15	1.23
1	A	1123	PHE	C-O	-6.68	1.16	1.24
1	A	1251	ASN	N-CA	6.65	1.54	1.46
1	A	1039	ARG	C-O	-6.41	1.18	1.24
1	A	1118	ASP	C-O	-6.27	1.16	1.24
1	A	480	ARG	C-O	-6.17	1.17	1.24
1	A	1144	LEU	CA-C	-6.15	1.44	1.52
1	A	994	ARG	C-O	-5.93	1.17	1.24
1	A	32	ASN	CG-OD1	5.92	1.34	1.23
1	A	11	LEU	C-O	-5.80	1.16	1.23
1	A	57	ARG	C-O	-5.78	1.17	1.24
1	A	639	ARG	C-O	-5.72	1.17	1.24
1	A	697	ILE	C-O	5.63	1.29	1.24
1	A	1221	ARG	C-O	-5.53	1.17	1.23
1	A	558	ASP	C-O	-5.50	1.17	1.24
1	A	433	GLY	CA-C	5.41	1.59	1.51
1	A	755	ASP	N-CA	-5.34	1.39	1.46
1	A	962	ASP	C-O	-5.34	1.16	1.24
1	A	279	ARG	C-O	-5.34	1.17	1.23
1	A	403	GLU	C-O	-5.29	1.18	1.23
1	A	971	GLN	CA-C	5.28	1.58	1.52
1	A	161	VAL	N-CA	-5.27	1.39	1.46
1	A	207	TYR	N-CA	5.26	1.52	1.46
1	A	1080	ILE	C-O	-5.25	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ALA	CA-CB	-5.23	1.48	1.53
1	A	554	ALA	N-CA	5.21	1.52	1.46
1	A	50	SER	CA-C	5.15	1.59	1.52
1	A	6	ARG	CA-C	-5.14	1.46	1.52
1	A	794	MET	N-CA	5.13	1.52	1.46
1	A	502	ASP	C-O	-5.13	1.17	1.23
1	A	610	PRO	CA-C	5.10	1.58	1.52
1	A	423	ASP	N-CA	5.02	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	THR	CA-C-N	-6.61	112.84	119.92
1	A	609	THR	C-N-CA	-6.61	112.84	119.92
1	A	1156	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	A	511	ALA	N-CA-C	5.85	117.65	111.28
1	A	877[A]	ARG	CA-C-O	5.78	128.16	121.28
1	A	877[B]	ARG	CA-C-O	5.78	128.16	121.28
1	A	0	HIS	N-CA-C	-5.75	101.01	109.18
1	A	156	ALA	CA-C-N	-5.21	115.37	120.52
1	A	156	ALA	C-N-CA	-5.21	115.37	120.52
1	A	571	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	A	448	LEU	N-CA-C	5.11	119.16	111.96
1	A	441	GLY	CA-C-N	5.10	125.10	119.90
1	A	441	GLY	C-N-CA	5.10	125.10	119.90

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	10249	0	10011	168	0
2	A	44	0	66	6	0
3	A	27	0	12	1	0
4	A	85	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	108	0	141	37	0
6	A	3	0	0	0	0
7	A	1358	0	0	66	0
All	All	11874	0	10230	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (181) 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:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:HD11	1.05	1.03
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:HD11	1.88	1.02
1:A:1164:ARG:HH22	5:A:1331:GOL:H12	1.25	0.96
5:A:1337:GOL:H32	7:A:2113:HOH:O	1.65	0.95
1:A:176[B]:LEU:HD21	7:A:2372:HOH:O	1.71	0.90
1:A:429:GLU:HG3	7:A:2562:HOH:O	1.72	0.90
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:CD1	2.00	0.87
1:A:1164:ARG:HH22	5:A:1331:GOL:C1	1.88	0.86
5:A:1333:GOL:C1	7:A:2317:HOH:O	2.22	0.86
1:A:1152:GLU:HG3	5:A:1333:GOL:H12	1.56	0.85
1:A:1052:SER:HB3	7:A:1594:HOH:O	1.76	0.85
5:A:1333:GOL:H11	7:A:2317:HOH:O	1.76	0.83
1:A:747:PRO:HA	5:A:1337:GOL:H12	1.61	0.82
1:A:215:GLU:HA	7:A:1427:HOH:O	1.82	0.80
1:A:175:ASN:HD21	1:A:182:LEU:H	1.27	0.79
1:A:515[A]:LEU:C	1:A:515[A]:LEU:HD23	2.07	0.79
1:A:176[B]:LEU:N	1:A:176[B]:LEU:HD22	1.97	0.79
1:A:820:SER:H	1:A:930:GLN:HE22	1.28	0.79
5:A:1342:GOL:H31	7:A:1709:HOH:O	1.83	0.77
1:A:916:HIS:NE2	5:A:1343:GOL:H31	2.00	0.75
1:A:176[B]:LEU:CD2	7:A:2372:HOH:O	2.31	0.74
1:A:96:HIS:HE1	1:A:103:VAL:O	1.70	0.74
1:A:1117[B]:ARG:NH1	7:A:1402:HOH:O	2.22	0.72
1:A:916:HIS:CE1	5:A:1343:GOL:H12	2.25	0.72
1:A:1164:ARG:NH2	5:A:1331:GOL:H12	2.04	0.71
1:A:782:LYS:CE	1:A:793:GLU:OE2	2.39	0.71
1:A:251:TYR:H	5:A:1335:GOL:C3	2.03	0.70
1:A:746:HIS:CD2	5:A:1347:GOL:H11	2.25	0.70
1:A:782:LYS:HE2	1:A:793:GLU:OE2	1.92	0.70
1:A:545:ASN:HD22	1:A:547:SER:H	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.57	0.69
1:A:873:LEU:HD21	1:A:942[B]:LEU:HD23	1.76	0.68
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.77	0.67
1:A:1226:PHE:HZ	7:A:1458:HOH:O	1.77	0.67
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.78	0.67
5:A:1337:GOL:H11	7:A:2600:HOH:O	1.93	0.67
1:A:553[B]:LEU:HD12	1:A:553[B]:LEU:C	2.20	0.67
1:A:335:PHE:CE1	1:A:412[B]:MET:SD	2.88	0.66
1:A:251:TYR:H	5:A:1335:GOL:H32	1.60	0.66
1:A:922:ASN:HD22	1:A:924:GLU:H	1.40	0.66
5:A:1336:GOL:H12	7:A:2227:HOH:O	1.94	0.65
1:A:746:HIS:HD2	5:A:1347:GOL:H32	1.61	0.65
1:A:499:PHE:CD2	1:A:515[B]:LEU:HD12	2.31	0.65
1:A:793:GLU:OE2	5:A:1347:GOL:H31	1.97	0.65
1:A:108:ARG:HH21	5:A:1332:GOL:H12	1.62	0.65
1:A:782:LYS:HZ3	5:A:1347:GOL:C3	2.10	0.64
1:A:782:LYS:HE2	5:A:1347:GOL:H31	1.78	0.64
1:A:1045[B]:LEU:HD21	1:A:1088[B]:LEU:HD12	1.80	0.63
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.80	0.63
1:A:1088[A]:LEU:HD23	1:A:1088[A]:LEU:C	2.23	0.63
5:A:1336:GOL:H31	7:A:1732:HOH:O	1.99	0.63
1:A:471:GLN:HE21	1:A:472:ARG:H	1.45	0.63
5:A:1342:GOL:C3	7:A:1709:HOH:O	2.42	0.63
1:A:873:LEU:CD2	1:A:942[B]:LEU:HD23	2.30	0.62
1:A:784:ARG:NH2	5:A:1347:GOL:H2	2.15	0.62
5:A:1345:GOL:H11	7:A:1583:HOH:O	2.00	0.61
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.84	0.61
2:A:1302:EDO:H22	7:A:1788:HOH:O	2.01	0.61
1:A:275:HIS:HD2	7:A:2623:HOH:O	1.83	0.60
1:A:860:VAL:HB	5:A:1342:GOL:H2	1.83	0.60
1:A:101[A]:GLN:NE2	7:A:1415:HOH:O	2.33	0.59
1:A:329[A]:LYS:NZ	1:A:419:ASN:HD21	2.01	0.59
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.85	0.59
1:A:746:HIS:CD2	5:A:1347:GOL:H32	2.36	0.59
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.49	0.58
1:A:329[B]:LYS:HG3	7:A:1705:HOH:O	2.03	0.58
1:A:75:LEU:HD23	7:A:1419:HOH:O	2.03	0.58
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.86	0.57
1:A:1251:ASN:ND2	1:A:1253:ARG:H	2.02	0.57
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.52	0.57
1:A:680:CYS:SG	1:A:726[B]:THR:HG21	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:HIS:HE1	5:A:1343:GOL:H12	1.71	0.56
1:A:623:GLY:HA3	1:A:852[B]:ASP:HA	1.88	0.56
1:A:1045[B]:LEU:HD21	1:A:1088[B]:LEU:CD1	2.35	0.56
1:A:176[B]:LEU:HD21	7:A:2697:HOH:O	2.05	0.55
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.14	0.55
1:A:176[B]:LEU:N	1:A:176[B]:LEU:CD2	2.68	0.55
1:A:1135:CYG:CD1	7:A:1719:HOH:O	2.54	0.55
1:A:329[B]:LYS:CG	7:A:1705:HOH:O	2.55	0.55
1:A:75:LEU:CD2	7:A:1419:HOH:O	2.57	0.53
1:A:776:LYS:HE3	7:A:2484:HOH:O	2.07	0.53
1:A:1145:ARG:HB2	7:A:1971:HOH:O	2.07	0.53
1:A:338:SER:OG	1:A:408:HIS:HD2	1.91	0.53
1:A:1117[B]:ARG:NH2	7:A:1410:HOH:O	2.34	0.53
1:A:767[A]:GLN:CD	7:A:1471:HOH:O	2.51	0.53
1:A:1045[B]:LEU:CG	1:A:1088[B]:LEU:HD11	2.38	0.53
1:A:219:HIS:N	7:A:1427:HOH:O	2.42	0.52
1:A:540:LEU:C	1:A:540:LEU:HD23	2.33	0.52
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.08	0.52
1:A:916:HIS:NE2	5:A:1343:GOL:C3	2.72	0.52
1:A:552:VAL:C	1:A:553[A]:LEU:HD23	2.35	0.52
1:A:1011:ASN:C	1:A:1011:ASN:HD22	2.19	0.51
1:A:296[B]:HIS:HD2	1:A:307:GLY:O	1.93	0.51
1:A:1152:GLU:CG	5:A:1333:GOL:H12	2.35	0.51
1:A:553[A]:LEU:HD23	1:A:553[A]:LEU:N	2.25	0.51
1:A:354:GLY:O	1:A:408:HIS:HE1	1.94	0.50
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:CD1	2.76	0.50
1:A:1226:PHE:CZ	7:A:1458:HOH:O	2.55	0.50
1:A:969:ASN:N	7:A:1409:HOH:O	2.41	0.49
1:A:274:ASP:HB2	7:A:1606:HOH:O	2.12	0.49
1:A:120:THR:H	1:A:123:GLN:HE21	1.60	0.49
1:A:1006:HIS:HD2	7:A:1950:HOH:O	1.95	0.49
1:A:217[B]:CYS:C	7:A:1407:HOH:O	2.56	0.49
1:A:782:LYS:CE	5:A:1347:GOL:H31	2.43	0.48
1:A:1260:HIS:HE1	7:A:1719:HOH:O	1.96	0.48
1:A:1045[B]:LEU:CG	1:A:1088[B]:LEU:CD1	2.92	0.48
1:A:852[B]:ASP:OD1	7:A:1401:HOH:O	2.20	0.48
1:A:767[A]:GLN:CG	7:A:1471:HOH:O	2.61	0.48
1:A:782:LYS:HZ3	5:A:1347:GOL:H32	1.79	0.47
2:A:1302:EDO:C2	7:A:1788:HOH:O	2.60	0.47
1:A:444[A]:MET:HG2	1:A:534[A]:GLU:HG2	1.96	0.47
1:A:942[A]:LEU:O	1:A:945:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:ASP:HB2	7:A:2447:HOH:O	2.15	0.47
1:A:329[B]:LYS:O	1:A:383:PRO:HD2	2.14	0.47
1:A:782:LYS:NZ	5:A:1347:GOL:C3	2.76	0.47
1:A:-3:ARG:NH1	7:A:1447:HOH:O	2.48	0.46
1:A:510[A]:ASN:ND2	1:A:514:GLU:OE1	2.48	0.46
1:A:969:ASN:CA	7:A:1409:HOH:O	2.63	0.46
1:A:1006:HIS:HE1	7:A:1661:HOH:O	1.97	0.46
1:A:1011:ASN:ND2	1:A:1013:THR:H	2.14	0.46
1:A:175:ASN:ND2	1:A:182:LEU:H	2.05	0.46
1:A:279:ARG:CZ	7:A:1818:HOH:O	2.62	0.46
1:A:782:LYS:HE3	1:A:793:GLU:OE2	2.14	0.46
1:A:217[A]:CYS:C	7:A:1407:HOH:O	2.59	0.46
1:A:216:HIS:C	7:A:1407:HOH:O	2.60	0.45
1:A:329[A]:LYS:HZ2	1:A:419:ASN:HD21	1.63	0.45
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.50	0.45
1:A:657[B]:ASP:OD2	1:A:660:VAL:HG12	2.16	0.45
1:A:1151:SER:H	5:A:1333:GOL:H11	1.81	0.45
1:A:969:ASN:ND2	5:A:1343:GOL:O2	2.49	0.45
1:A:219:HIS:N	7:A:1407:HOH:O	2.42	0.45
1:A:723:ILE:O	1:A:726[B]:THR:HG23	2.17	0.45
1:A:152:HIS:CD2	4:A:1326:SO4:O4	2.70	0.45
1:A:1048:GLN:O	1:A:1095:SER:HA	2.17	0.45
1:A:553[B]:LEU:C	1:A:553[B]:LEU:CD1	2.89	0.44
1:A:-7:GLY:O	1:A:3:GLU:HA	2.17	0.44
1:A:22:ARG:NE	7:A:1462:HOH:O	2.51	0.44
1:A:515[A]:LEU:HD23	1:A:515[A]:LEU:O	2.16	0.44
1:A:595:ASN:HD22	2:A:1306:EDO:H12	1.83	0.44
1:A:435:LYS:HG3	1:A:560:LEU:HD22	1.98	0.44
1:A:412[A]:MET:SD	7:A:2399:HOH:O	2.61	0.43
1:A:545:ASN:ND2	1:A:547:SER:H	2.13	0.43
2:A:1308:EDO:C1	7:A:2542:HOH:O	2.66	0.43
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.16	0.43
1:A:96:HIS:CE1	1:A:103:VAL:O	2.61	0.43
1:A:1011:ASN:CG	7:A:1458:HOH:O	2.61	0.43
1:A:-3:ARG:NH2	7:A:1447:HOH:O	2.51	0.43
1:A:877[B]:ARG:HG3	1:A:877[B]:ARG:HH21	1.83	0.43
1:A:969:ASN:HA	7:A:1409:HOH:O	2.18	0.43
1:A:211:GLN:HB2	7:A:1928:HOH:O	2.18	0.42
1:A:443:ALA:HB3	7:A:2163:HOH:O	2.19	0.42
1:A:668:GLN:HG2	3:A:1312:ADP:H1'	2.00	0.42
1:A:787:GLU:HB3	1:A:792:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1345:GOL:C1	7:A:1583:HOH:O	2.65	0.42
1:A:1051:ASN:HB2	2:A:1302:EDO:O1	2.20	0.42
1:A:515[A]:LEU:C	1:A:515[A]:LEU:CD2	2.78	0.42
1:A:827:LEU:HD23	1:A:954:TYR:HA	2.01	0.41
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.85	0.41
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.38	0.41
1:A:782:LYS:NZ	5:A:1347:GOL:H31	2.35	0.41
1:A:1088[A]:LEU:C	1:A:1088[A]:LEU:CD2	2.91	0.41
1:A:275:HIS:HE1	7:A:2566:HOH:O	2.02	0.41
1:A:901:GLY:HA2	2:A:1308:EDO:H22	2.01	0.41
1:A:80:ARG:HD3	7:A:1459:HOH:O	2.20	0.41
1:A:144[A]:THR:HG21	7:A:2049:HOH:O	2.19	0.41
1:A:360:VAL:HB	1:A:364[B]:ASP:CB	2.50	0.41
1:A:1183:GLN:HG3	7:A:2719:HOH:O	2.20	0.41
1:A:305:TRP:HB3	1:A:306:PRO:HD3	2.03	0.41
1:A:553[B]:LEU:HD13	1:A:555:VAL:HG23	2.01	0.41
1:A:259:ASN:HB2	7:A:1987:HOH:O	2.21	0.41
1:A:585:HIS:HD2	7:A:2392:HOH:O	2.04	0.41
1:A:1088[A]:LEU:HD23	1:A:1089:VAL:N	2.35	0.41
1:A:515[A]:LEU:HD23	1:A:516:VAL:N	2.36	0.40
1:A:610:PRO:HG2	7:A:1902:HOH:O	2.22	0.40
1:A:177:ARG:NH2	7:A:1416:HOH:O	2.33	0.40
1:A:1117[B]:ARG:NE	7:A:1410:HOH:O	2.28	0.40
1:A:1279[A]:GLU:O	1:A:1279[A]:GLU:HG3	2.12	0.40
1:A:144[A]:THR:CG2	7:A:2049:HOH:O	2.69	0.40
1:A:907[B]:VAL:CG2	1:A:966:ILE:HD13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1327/1301 (102%)	1287 (97%)	38 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	661	THR
1	A	886	SER

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	1072/1040 (103%)	1038 (97%)	34 (3%)	34	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	22	ARG
1	A	24	GLN
1	A	27	ASN
1	A	104	ASP
1	A	119	LEU
1	A	125	ARG
1	A	144[A]	THR
1	A	144[B]	THR
1	A	296[A]	HIS
1	A	296[B]	HIS
1	A	445	ASN
1	A	465	LEU
1	A	471	GLN
1	A	515[A]	LEU
1	A	515[B]	LEU
1	A	553[A]	LEU
1	A	553[B]	LEU
1	A	560	LEU

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Mol	Chain	Res	Type
1	A	596	GLN
1	A	622	LYS
1	A	782	LYS
1	A	815	LEU
1	A	942[A]	LEU
1	A	942[B]	LEU
1	A	945	GLN
1	A	1144	LEU
1	A	1190[A]	MET
1	A	1190[B]	MET
1	A	1195	SER
1	A	1251	ASN
1	A	1275	GLU
1	A	1279[A]	GLU
1	A	1279[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	96	HIS
1	A	123	GLN
1	A	175	ASN
1	A	211	GLN
1	A	219	HIS
1	A	275	HIS
1	A	298	HIS
1	A	339	ASN
1	A	408	HIS
1	A	419	ASN
1	A	445	ASN
1	A	471	GLN
1	A	545	ASN
1	A	548	GLN
1	A	559	GLN
1	A	585	HIS
1	A	595	ASN
1	A	617	GLN
1	A	739	ASN
1	A	746	HIS
1	A	824	ASN
1	A	836	ASN

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Mol	Chain	Res	Type
1	A	883	HIS
1	A	922	ASN
1	A	930	GLN
1	A	969	ASN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1011	ASN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
1	CYG	A	1135	1	12,14,15	2.09	2 (16%)	10,17,19	4.92	5 (50%)

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
1	CYG	A	1135	1	-	1/14/16/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	5.60	1.56	1.50
1	A	1135	CYG	CD1-SG	3.09	1.83	1.76

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-CG1	-11.20	111.06	123.98
1	A	1135	CYG	CG1-CD1-SG	7.70	122.58	113.40
1	A	1135	CYG	CB1-CG1-CD1	-6.03	98.95	112.27
1	A	1135	CYG	OE2-CD1-SG	2.67	126.08	122.68
1	A	1135	CYG	CB-CA-C	2.64	117.98	110.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1135	CYG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 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
4	SO4	A	1320	-	4,4,4	1.39	1 (25%)	6,6,6	1.03	0
3	ADP	A	1312	6	28,29,29	1.56	4 (14%)	43,45,45	1.37	6 (13%)
2	EDO	A	1301	-	3,3,3	0.32	0	2,2,2	0.57	0
5	GOL	A	1334	-	5,5,5	0.59	0	5,5,5	0.68	0
4	SO4	A	1319	-	4,4,4	0.39	0	6,6,6	0.47	0
5	GOL	A	1342	-	5,5,5	1.84	2 (40%)	5,5,5	2.44	3 (60%)
2	EDO	A	1302	-	3,3,3	0.33	0	2,2,2	0.66	0
4	SO4	A	1315	-	4,4,4	0.46	0	6,6,6	1.15	0
5	GOL	A	1343	-	5,5,5	0.37	0	5,5,5	0.40	0
4	SO4	A	1317	-	4,4,4	0.51	0	6,6,6	1.01	0
2	EDO	A	1307	-	3,3,3	0.64	0	2,2,2	0.24	0
2	EDO	A	1308	-	3,3,3	0.70	0	2,2,2	0.47	0
2	EDO	A	1310	-	3,3,3	0.48	0	2,2,2	0.93	0
4	SO4	A	1318	-	4,4,4	0.90	0	6,6,6	0.99	0
5	GOL	A	1336	-	5,5,5	1.09	1 (20%)	5,5,5	0.72	0
5	GOL	A	1335	-	5,5,5	0.60	0	5,5,5	0.41	0
4	SO4	A	1324	-	4,4,4	0.61	0	6,6,6	0.97	0
4	SO4	A	1314	-	4,4,4	0.43	0	6,6,6	0.43	0
5	GOL	A	1345	-	5,5,5	0.40	0	5,5,5	1.17	1 (20%)
4	SO4	A	1329	-	4,4,4	0.69	0	6,6,6	0.90	0
5	GOL	A	1331	-	5,5,5	0.51	0	5,5,5	1.29	0
5	GOL	A	1333	-	5,5,5	1.10	1 (20%)	5,5,5	0.96	0
2	EDO	A	1304	-	3,3,3	0.75	0	2,2,2	0.63	0
4	SO4	A	1328	-	4,4,4	0.81	0	6,6,6	0.27	0
4	SO4	A	1322	-	4,4,4	0.98	0	6,6,6	0.76	0
2	EDO	A	1303	-	3,3,3	0.45	0	2,2,2	0.53	0
4	SO4	A	1316	-	4,4,4	0.48	0	6,6,6	1.20	0
2	EDO	A	1309	-	3,3,3	0.46	0	2,2,2	0.93	0
5	GOL	A	1340	-	5,5,5	0.78	0	5,5,5	1.32	1 (20%)
5	GOL	A	1341	-	5,5,5	0.28	0	5,5,5	0.63	0
2	EDO	A	1311	-	3,3,3	0.35	0	2,2,2	0.74	0
5	GOL	A	1332	-	5,5,5	0.84	0	5,5,5	0.66	0
5	GOL	A	1344	-	5,5,5	1.01	0	5,5,5	1.50	1 (20%)
5	GOL	A	1347	-	5,5,5	0.38	0	5,5,5	1.09	0
2	EDO	A	1306	-	3,3,3	0.57	0	2,2,2	0.57	0
2	EDO	A	1305	-	3,3,3	0.27	0	2,2,2	1.34	0
5	GOL	A	1337	-	5,5,5	0.71	0	5,5,5	0.57	0
4	SO4	A	1323	-	4,4,4	0.98	0	6,6,6	0.80	0
5	GOL	A	1330	-	5,5,5	0.78	0	5,5,5	1.35	0
4	SO4	A	1321	-	4,4,4	0.86	0	6,6,6	1.02	1 (16%)
4	SO4	A	1327	-	4,4,4	0.75	0	6,6,6	1.21	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1326	-	4,4,4	0.46	0	6,6,6	0.42	0
5	GOL	A	1339	-	5,5,5	0.39	0	5,5,5	0.99	0
5	GOL	A	1338	-	5,5,5	0.40	0	5,5,5	0.83	0
5	GOL	A	1346	-	5,5,5	0.24	0	5,5,5	1.20	0
4	SO4	A	1313	-	4,4,4	1.01	0	6,6,6	1.43	1 (16%)
4	SO4	A	1325	-	4,4,4	0.72	0	6,6,6	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1312	6	-	1/16/32/32	0/3/3/3
2	EDO	A	1301	-	-	0/1/1/1	-
5	GOL	A	1334	-	-	0/4/4/4	-
5	GOL	A	1342	-	-	4/4/4/4	-
2	EDO	A	1302	-	-	1/1/1/1	-
5	GOL	A	1343	-	-	2/4/4/4	-
2	EDO	A	1307	-	-	1/1/1/1	-
2	EDO	A	1308	-	-	1/1/1/1	-
2	EDO	A	1310	-	-	1/1/1/1	-
5	GOL	A	1336	-	-	0/4/4/4	-
5	GOL	A	1335	-	-	0/4/4/4	-
5	GOL	A	1345	-	-	2/4/4/4	-
5	GOL	A	1331	-	-	4/4/4/4	-
5	GOL	A	1333	-	-	4/4/4/4	-
2	EDO	A	1304	-	-	1/1/1/1	-
2	EDO	A	1303	-	-	1/1/1/1	-
2	EDO	A	1309	-	-	0/1/1/1	-
5	GOL	A	1340	-	-	2/4/4/4	-
5	GOL	A	1341	-	-	4/4/4/4	-
2	EDO	A	1311	-	-	1/1/1/1	-
5	GOL	A	1332	-	-	3/4/4/4	-
5	GOL	A	1344	-	-	2/4/4/4	-
5	GOL	A	1347	-	-	3/4/4/4	-
2	EDO	A	1306	-	-	1/1/1/1	-
2	EDO	A	1305	-	-	0/1/1/1	-
5	GOL	A	1337	-	-	2/4/4/4	-
5	GOL	A	1330	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1339	-	-	4/4/4/4	-
5	GOL	A	1338	-	-	4/4/4/4	-
5	GOL	A	1346	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1312	ADP	C5-C4	4.05	1.46	1.39
3	A	1312	ADP	C4-N9	-3.55	1.30	1.37
3	A	1312	ADP	PA-O3A	3.20	1.63	1.59
5	A	1342	GOL	O3-C3	-2.61	1.31	1.42
5	A	1336	GOL	O2-C2	-2.35	1.36	1.43
5	A	1342	GOL	O1-C1	-2.25	1.33	1.42
3	A	1312	ADP	C2-N1	2.14	1.37	1.33
4	A	1320	SO4	O2-S	2.08	1.57	1.44
5	A	1333	GOL	O2-C2	-2.04	1.37	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1312	ADP	C4-N9-C8	3.34	109.24	105.74
5	A	1342	GOL	O3-C3-C2	-3.13	96.30	110.38
3	A	1312	ADP	N3-C4-N9	2.99	132.25	127.17
3	A	1312	ADP	C5-C4-N3	-2.98	122.61	126.72
3	A	1312	ADP	C4-C5-N7	-2.95	107.21	110.58
5	A	1342	GOL	C3-C2-C1	-2.87	101.28	111.80
5	A	1342	GOL	O1-C1-C2	-2.84	97.58	110.38
4	A	1313	SO4	O4-S-O1	2.73	123.83	109.56
5	A	1344	GOL	C3-C2-C1	2.61	121.38	111.80
4	A	1327	SO4	O4-S-O2	2.39	122.08	109.56
5	A	1340	GOL	O2-C2-C1	2.25	118.51	109.18
3	A	1312	ADP	O2A-PA-O1A	2.13	122.36	112.44
5	A	1345	GOL	O1-C1-C2	-2.09	100.95	110.38
3	A	1312	ADP	N3-C2-N1	-2.04	125.49	128.58
4	A	1321	SO4	O4-S-O3	-2.01	97.45	108.54

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1331	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1331	GOL	O1-C1-C2-C3
5	A	1331	GOL	C1-C2-C3-O3
5	A	1333	GOL	O1-C1-C2-C3
5	A	1337	GOL	C1-C2-C3-O3
5	A	1337	GOL	O2-C2-C3-O3
5	A	1338	GOL	O1-C1-C2-O2
5	A	1338	GOL	O1-C1-C2-C3
5	A	1338	GOL	C1-C2-C3-O3
5	A	1339	GOL	C1-C2-C3-O3
5	A	1340	GOL	O1-C1-C2-C3
5	A	1342	GOL	O1-C1-C2-C3
5	A	1342	GOL	C1-C2-C3-O3
5	A	1343	GOL	O1-C1-C2-C3
5	A	1344	GOL	O1-C1-C2-C3
5	A	1345	GOL	O1-C1-C2-O2
5	A	1345	GOL	O1-C1-C2-C3
5	A	1346	GOL	O1-C1-C2-C3
5	A	1346	GOL	C1-C2-C3-O3
5	A	1346	GOL	O2-C2-C3-O3
5	A	1339	GOL	O2-C2-C3-O3
5	A	1332	GOL	O1-C1-C2-C3
5	A	1333	GOL	C1-C2-C3-O3
5	A	1339	GOL	O1-C1-C2-C3
5	A	1341	GOL	O1-C1-C2-C3
5	A	1341	GOL	C1-C2-C3-O3
5	A	1347	GOL	O1-C1-C2-C3
5	A	1331	GOL	O2-C2-C3-O3
5	A	1333	GOL	O1-C1-C2-O2
5	A	1342	GOL	O1-C1-C2-O2
5	A	1342	GOL	O2-C2-C3-O3
5	A	1344	GOL	O1-C1-C2-O2
5	A	1346	GOL	O1-C1-C2-O2
5	A	1347	GOL	O1-C1-C2-O2
2	A	1303	EDO	O1-C1-C2-O2
2	A	1307	EDO	O1-C1-C2-O2
2	A	1310	EDO	O1-C1-C2-O2
5	A	1340	GOL	O1-C1-C2-O2
5	A	1343	GOL	O1-C1-C2-O2
2	A	1302	EDO	O1-C1-C2-O2
2	A	1304	EDO	O1-C1-C2-O2
2	A	1311	EDO	O1-C1-C2-O2
3	A	1312	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	1308	EDO	O1-C1-C2-O2
5	A	1338	GOL	O2-C2-C3-O3
5	A	1347	GOL	O2-C2-C3-O3
2	A	1306	EDO	O1-C1-C2-O2
5	A	1332	GOL	O1-C1-C2-O2
5	A	1332	GOL	O2-C2-C3-O3
5	A	1333	GOL	O2-C2-C3-O3
5	A	1341	GOL	O2-C2-C3-O3
5	A	1341	GOL	O1-C1-C2-O2
5	A	1339	GOL	O1-C1-C2-O2

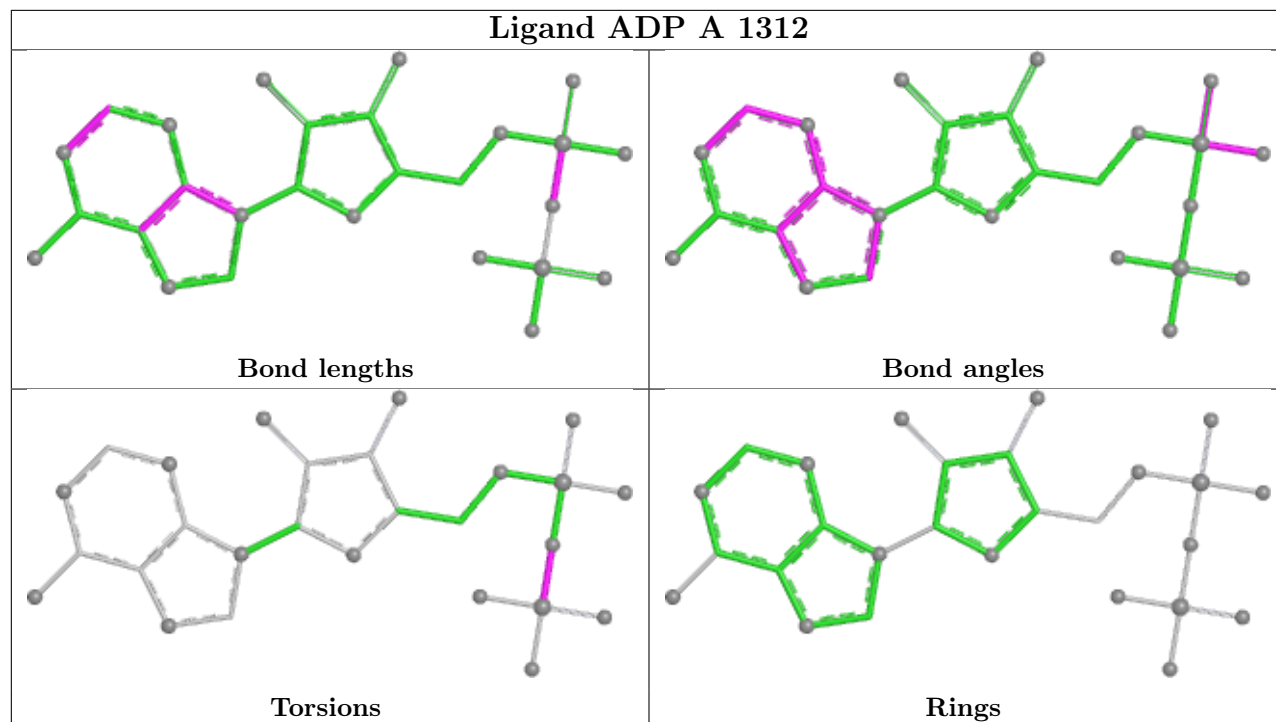
There are no ring outliers.

15 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1312	ADP	1	0
5	A	1342	GOL	3	0
2	A	1302	EDO	3	0
5	A	1343	GOL	5	0
2	A	1308	EDO	2	0
5	A	1336	GOL	2	0
5	A	1335	GOL	2	0
5	A	1345	GOL	2	0
5	A	1331	GOL	3	0
5	A	1333	GOL	5	0
5	A	1332	GOL	1	0
5	A	1347	GOL	11	0
2	A	1306	EDO	1	0
5	A	1337	GOL	3	0
4	A	1326	SO4	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 [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	1287/1301 (98%)	-0.51	16 (1%) 76 79	6, 15, 37, 67	45 (3%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-7	GLY	6.1
1	A	-5	VAL	5.2
1	A	-4	PRO	4.9
1	A	465	LEU	4.0
1	A	-6	LEU	3.8
1	A	789	ASN	3.7
1	A	-3	ARG	2.9
1	A	449	GLY	2.6
1	A	608	LYS	2.4
1	A	118	THR	2.4
1	A	119	LEU	2.3
1	A	-2	GLY	2.3
1	A	448	LEU	2.3
1	A	152	HIS	2.1
1	A	120	THR	2.1
1	A	-1	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CYG	A	1135	15/16	0.98	0.05	10,11,13,18	0

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($\text{\AA}^2$)	Q<0.9
4	SO4	A	1326	5/5	0.52	0.17	119,122,133,139	0
5	GOL	A	1345	6/6	0.73	0.20	51,59,64,67	0
5	GOL	A	1347	6/6	0.74	0.20	42,49,53,62	0
2	EDO	A	1306	4/4	0.75	0.20	53,55,60,61	0
5	GOL	A	1341	6/6	0.77	0.18	35,44,47,50	0
2	EDO	A	1309	4/4	0.77	0.17	44,50,55,55	0
5	GOL	A	1339	6/6	0.77	0.20	52,54,54,60	0
4	SO4	A	1325	5/5	0.79	0.12	57,58,72,80	0
2	EDO	A	1304	4/4	0.79	0.18	39,39,53,56	0
5	GOL	A	1346	6/6	0.80	0.17	52,57,57,67	0
5	GOL	A	1343	6/6	0.81	0.16	45,49,51,54	0
5	GOL	A	1331	6/6	0.84	0.16	40,42,50,52	0
5	GOL	A	1332	6/6	0.84	0.14	33,39,39,43	0
2	EDO	A	1303	4/4	0.84	0.18	42,57,58,71	0
2	EDO	A	1310	4/4	0.84	0.15	40,47,48,49	0
4	SO4	A	1324	5/5	0.85	0.10	54,55,70,79	0
5	GOL	A	1338	6/6	0.85	0.15	27,45,51,53	0
5	GOL	A	1336	6/6	0.86	0.17	24,35,39,41	1
2	EDO	A	1311	4/4	0.87	0.18	34,46,54,62	0
5	GOL	A	1334	6/6	0.88	0.12	28,36,38,38	0
5	GOL	A	1335	6/6	0.88	0.13	33,34,43,44	0
2	EDO	A	1305	4/4	0.88	0.17	41,47,52,62	0
4	SO4	A	1328	5/5	0.88	0.11	56,65,71,72	0
5	GOL	A	1333	6/6	0.88	0.13	32,37,42,56	0
5	GOL	A	1344	6/6	0.89	0.13	23,28,35,38	0
2	EDO	A	1307	4/4	0.89	0.17	31,46,55,59	0
5	GOL	A	1342	6/6	0.89	0.17	20,35,44,53	0
5	GOL	A	1337	6/6	0.89	0.16	23,38,40,50	0
2	EDO	A	1308	4/4	0.90	0.23	36,37,38,52	0
2	EDO	A	1302	4/4	0.90	0.43	45,50,51,68	0
2	EDO	A	1301	4/4	0.90	0.11	33,35,36,37	0
4	SO4	A	1323	5/5	0.91	0.16	37,45,51,55	0

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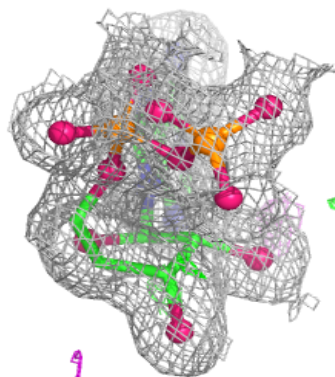
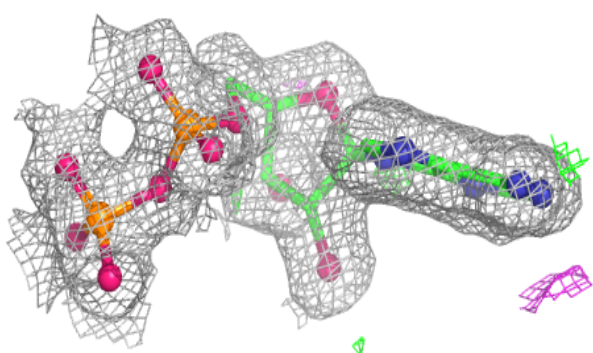
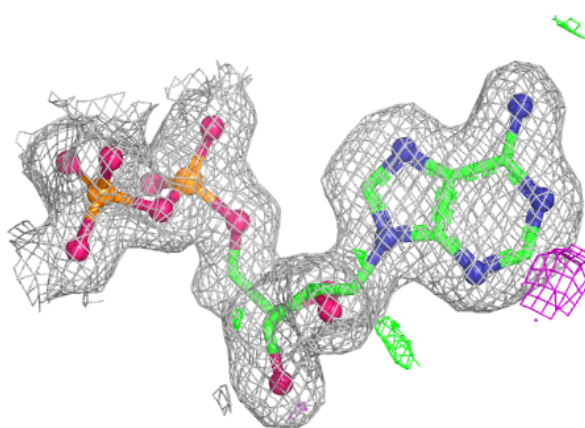
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1322	5/5	0.93	0.18	34,41,46,48	0
5	GOL	A	1340	6/6	0.94	0.10	14,21,24,35	0
4	SO4	A	1329	5/5	0.94	0.12	31,41,46,47	0
4	SO4	A	1313	5/5	0.95	0.09	18,22,29,33	0
4	SO4	A	1315	5/5	0.96	0.10	28,33,42,44	0
4	SO4	A	1316	5/5	0.96	0.13	31,33,37,44	0
4	SO4	A	1318	5/5	0.96	0.10	25,29,34,36	0
4	SO4	A	1320	5/5	0.96	0.12	20,28,35,36	0
5	GOL	A	1330	6/6	0.97	0.07	17,21,26,28	0
4	SO4	A	1321	5/5	0.97	0.14	40,42,50,51	0
4	SO4	A	1319	5/5	0.97	0.12	33,33,41,46	0
4	SO4	A	1317	5/5	0.98	0.11	24,33,36,42	0
4	SO4	A	1327	5/5	0.98	0.08	26,26,33,37	0
4	SO4	A	1314	5/5	0.99	0.05	17,21,22,24	0
3	ADP	A	1312	27/27	0.99	0.03	8,10,11,11	0
6	MG	A	1350	1/1	0.99	0.02	10,10,10,10	0
6	MG	A	1349	1/1	1.00	0.02	10,10,10,10	0
6	MG	A	1348	1/1	1.00	0.03	9,9,9,9	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 ADP A 1312:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.