



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:26 AM UTC

PDB ID : 6JTA / pdb_00006jta
Title : Crystal Structure of D464A L465A mutant of FGAM Synthetase
Authors : Sharma, N.; Ahalawat, N.; Sandhu, P.; Mondal, J.; Anand, R.
Deposited on : 2019-04-10
Resolution : 1.75 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

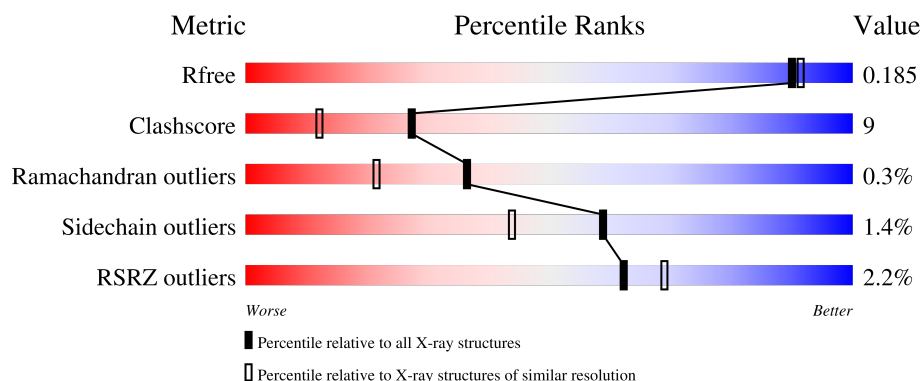
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

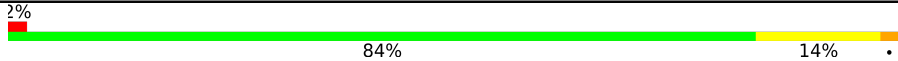
The reported resolution of this entry is 1.75 Å.

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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	1303	

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	EDO	A	1312	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	1319	-	-	X	-
5	EDO	A	1323	-	-	X	-
5	EDO	A	1325	-	-	X	-
5	EDO	A	1328	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11632 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	1298	Total	C	N	O	S	0	34	0
			10134	6368	1800	1916	50			

There are 10 discrepancies between the modelled and reference sequences:

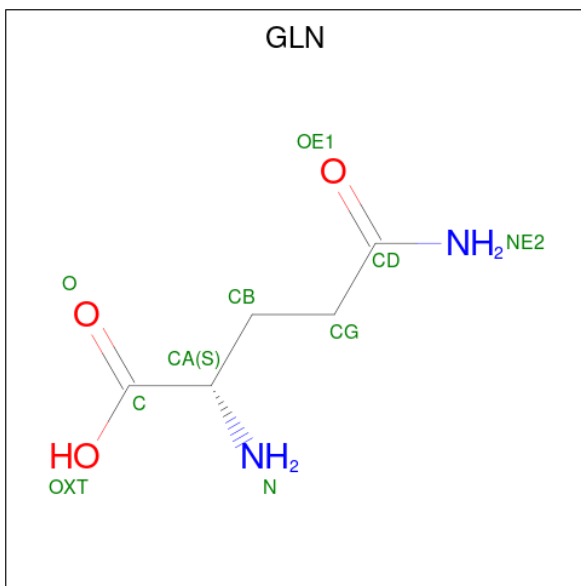
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-6	LEU	-	expression tag	UNP A0A0D6F9Y3
A	-5	VAL	-	expression tag	UNP A0A0D6F9Y3
A	-4	PRO	-	expression tag	UNP A0A0D6F9Y3
A	-3	ARG	-	expression tag	UNP A0A0D6F9Y3
A	-2	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-1	SER	-	expression tag	UNP A0A0D6F9Y3
A	0	HIS	-	expression tag	UNP A0A0D6F9Y3
A	464	ALA	ASP	engineered mutation	UNP A0A0D6F9Y3
A	465	ALA	LEU	engineered mutation	UNP A0A0D6F9Y3

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is GLUTAMINE (CCD ID: GLN) (formula: $\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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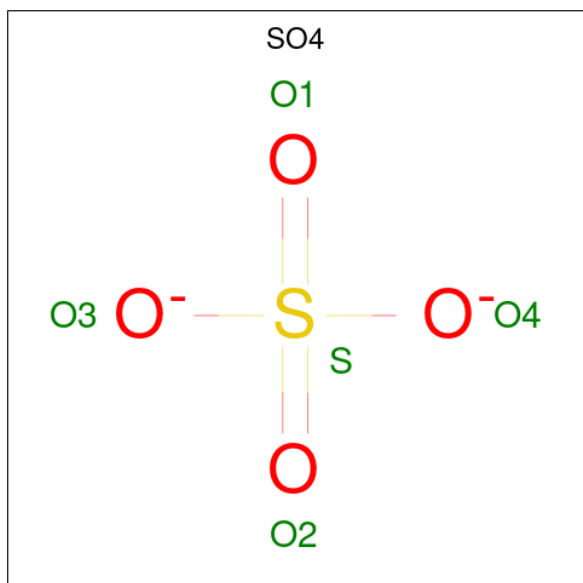
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0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

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

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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

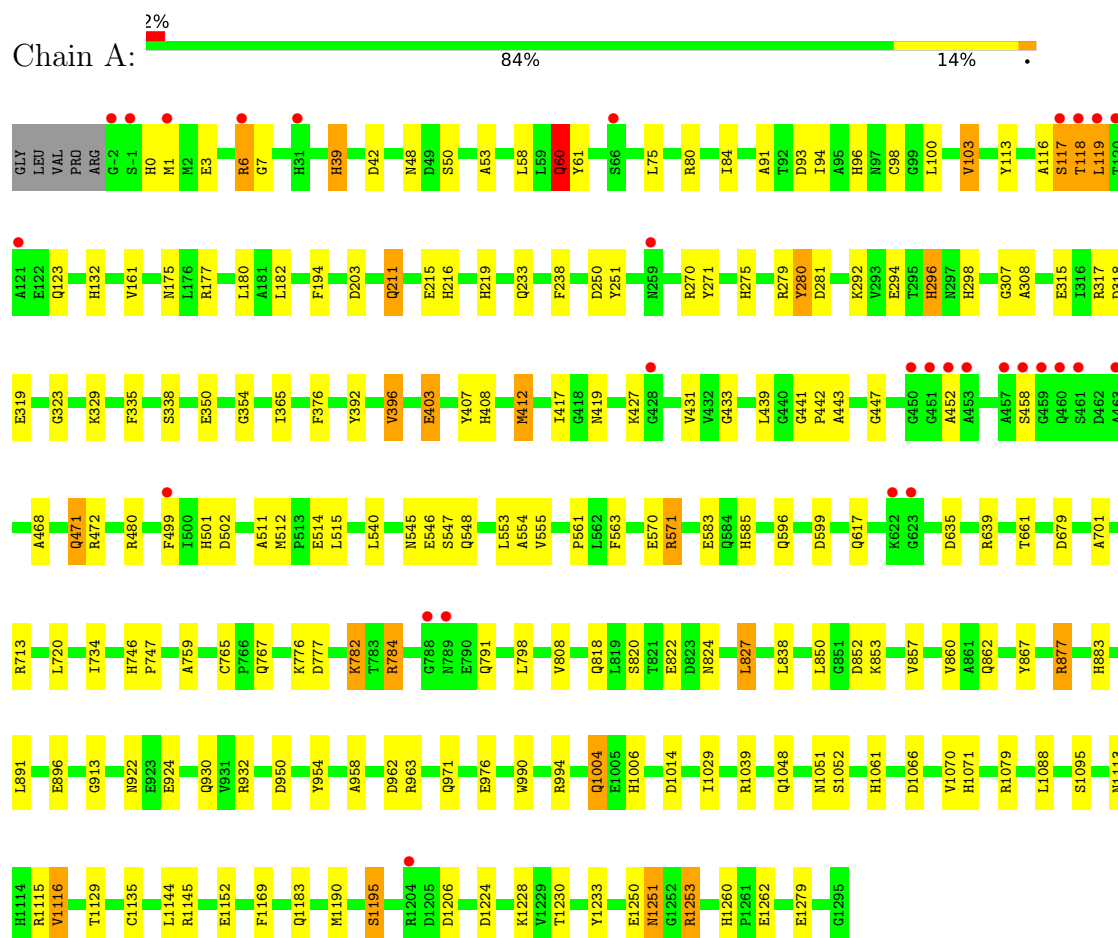
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1204	Total O 1204 1204	0	0

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	146.80Å 146.80Å 141.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.72 – 1.75 39.72 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.72-1.75) 99.8 (39.72-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.151 , 0.181 0.163 , 0.185	Depositor DCC
R_{free} test set	8643 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11632	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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

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: ADP, MG, EDO, GOL, SO4

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	1.56	77/10438 (0.7%)	1.26	31/14168 (0.2%)

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	571[A]	ARG	CA-C	10.54	1.66	1.53
1	A	571[B]	ARG	CA-C	10.54	1.66	1.53
1	A	412[A]	MET	CA-C	10.53	1.66	1.53
1	A	412[B]	MET	CA-C	10.53	1.66	1.53
1	A	784[A]	ARG	CA-C	10.48	1.65	1.52
1	A	784[B]	ARG	CA-C	10.48	1.65	1.52
1	A	281[A]	ASP	CA-C	9.15	1.64	1.52
1	A	281[B]	ASP	CA-C	9.15	1.64	1.52
1	A	765	CYS	C-O	-8.14	1.16	1.24
1	A	877[A]	ARG	CA-C	7.66	1.63	1.53
1	A	877[B]	ARG	CA-C	7.66	1.63	1.53
1	A	480	ARG	C-O	-7.40	1.15	1.24
1	A	392	TYR	C-O	-6.88	1.15	1.24
1	A	514	GLU	C-O	-6.77	1.16	1.24
1	A	971	GLN	CA-C	6.63	1.60	1.52
1	A	639	ARG	C-O	-6.56	1.16	1.24
1	A	1253[A]	ARG	CA-C	6.40	1.61	1.52
1	A	1253[B]	ARG	CA-C	6.40	1.61	1.52
1	A	103	VAL	C-O	6.21	1.30	1.23
1	A	194	PHE	CA-C	6.20	1.61	1.52
1	A	501	HIS	CA-C	-6.18	1.44	1.52
1	A	827	LEU	CA-C	-6.07	1.45	1.52
1	A	962	ASP	CA-C	-6.04	1.45	1.52
1	A	215	GLU	C-O	-6.01	1.17	1.24
1	A	853	LYS	C-O	-5.99	1.16	1.24
1	A	7	GLY	C-O	-5.95	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	561	PRO	CA-C	5.88	1.60	1.52
1	A	759	ALA	C-O	-5.87	1.17	1.24
1	A	113	TYR	C-O	5.84	1.30	1.24
1	A	100	LEU	N-CA	5.80	1.54	1.46
1	A	50	SER	CA-C	5.77	1.60	1.52
1	A	161	VAL	N-CA	-5.71	1.39	1.46
1	A	60	GLN	CA-C	-5.68	1.45	1.52
1	A	433	GLY	CA-C	5.66	1.59	1.51
1	A	990	TRP	N-CA	5.64	1.52	1.46
1	A	554	ALA	N-CA	5.62	1.52	1.46
1	A	365	ILE	CA-C	5.62	1.59	1.52
1	A	280	TYR	C-O	-5.60	1.17	1.23
1	A	417	ILE	N-CA	-5.59	1.39	1.46
1	A	84	ILE	N-CA	5.58	1.53	1.46
1	A	350	GLU	C-O	-5.57	1.17	1.24
1	A	501	HIS	C-O	5.56	1.30	1.23
1	A	439	LEU	N-CA	5.56	1.53	1.46
1	A	1071	HIS	CA-C	-5.54	1.45	1.52
1	A	808	VAL	CA-CB	5.52	1.60	1.54
1	A	838	LEU	N-CA	5.50	1.53	1.45
1	A	1144	LEU	CA-C	-5.46	1.45	1.52
1	A	1195	SER	C-O	-5.45	1.18	1.23
1	A	48	ASN	N-CA	5.45	1.53	1.45
1	A	818	GLN	CD-NE2	-5.42	1.21	1.33
1	A	58	LEU	C-O	5.38	1.30	1.24
1	A	1129	THR	N-CA	5.37	1.52	1.45
1	A	203	ASP	C-O	-5.36	1.18	1.24
1	A	701	ALA	CA-C	5.35	1.59	1.52
1	A	458	SER	C-O	5.34	1.30	1.23
1	A	1224	ASP	C-O	-5.34	1.16	1.23
1	A	720	LEU	C-O	-5.33	1.17	1.24
1	A	822	GLU	N-CA	5.29	1.53	1.46
1	A	1116	VAL	C-O	-5.25	1.17	1.24
1	A	323	GLY	C-O	-5.24	1.17	1.24
1	A	1250	GLU	C-O	-5.21	1.18	1.24
1	A	6	ARG	C-O	-5.20	1.17	1.23
1	A	932	ARG	C-O	-5.20	1.17	1.23
1	A	635	ASP	C-O	-5.19	1.18	1.24
1	A	1014	ASP	C-O	-5.19	1.17	1.24
1	A	1169	PHE	N-CA	-5.17	1.39	1.46
1	A	376	PHE	N-CA	-5.14	1.40	1.46
1	A	767[A]	GLN	C-O	-5.13	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767[B]	GLN	C-O	-5.13	1.18	1.24
1	A	1004	GLN	CD-NE2	-5.11	1.22	1.33
1	A	403	GLU	C-O	-5.11	1.17	1.23
1	A	39	HIS	N-CA	-5.08	1.39	1.45
1	A	407	TYR	C-O	-5.07	1.17	1.23
1	A	1079	ARG	N-CA	-5.07	1.39	1.46
1	A	1070	VAL	N-CA	-5.06	1.39	1.46
1	A	734	ILE	N-CA	5.04	1.52	1.46
1	A	867	TYR	N-CA	5.03	1.52	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	ALA	N-CA-C	7.91	121.22	110.55
1	A	1253[A]	ARG	N-CA-C	7.37	121.53	112.54
1	A	1253[B]	ARG	N-CA-C	7.37	121.53	112.54
1	A	1253[A]	ARG	CA-C-O	6.74	127.66	119.38
1	A	1253[B]	ARG	CA-C-O	6.74	127.66	119.38
1	A	511	ALA	N-CA-C	6.59	118.54	111.36
1	A	877[A]	ARG	CA-C-O	6.49	128.86	120.81
1	A	877[B]	ARG	CA-C-O	6.49	128.86	120.81
1	A	298	HIS	CA-C-N	-6.39	112.41	119.19
1	A	298	HIS	C-N-CA	-6.39	112.41	119.19
1	A	91	ALA	N-CA-C	-6.25	104.47	111.28
1	A	80	ARG	CB-CA-C	5.97	118.79	109.42
1	A	53	ALA	N-CA-C	-5.85	105.03	111.82
1	A	407	TYR	N-CA-C	5.85	117.45	110.44
1	A	60	GLN	CB-CA-C	-5.61	101.80	110.78
1	A	994	ARG	CG-CD-NE	-5.54	99.81	112.00
1	A	376	PHE	N-CA-C	5.37	116.94	111.14
1	A	233	GLN	CA-C-N	5.25	124.95	119.64
1	A	233	GLN	C-N-CA	5.25	124.95	119.64
1	A	617	GLN	N-CA-C	5.23	117.97	109.24
1	A	512	MET	CA-C-N	-5.18	113.70	119.19
1	A	512	MET	C-N-CA	-5.18	113.70	119.19
1	A	1144	LEU	CB-CA-C	-5.14	102.03	110.72
1	A	857	VAL	N-CA-CB	5.13	116.39	110.49
1	A	211	GLN	N-CA-C	-5.13	105.77	111.36
1	A	1228	LYS	CA-CB-CG	5.10	124.30	114.10
1	A	98	CYS	N-CA-C	-5.09	106.31	112.88
1	A	563	PHE	N-CA-C	5.07	116.81	111.28
1	A	571[A]	ARG	CA-C-O	5.04	127.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571[B]	ARG	CA-C-O	5.04	127.39	121.54
1	A	570	GLU	N-CA-C	5.00	119.23	113.18

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	10134	0	9961	163	0
2	A	27	0	12	0	0
3	A	10	0	7	4	0
4	A	72	0	94	21	0
5	A	92	0	138	57	0
6	A	3	0	0	0	0
7	A	90	0	0	0	0
8	A	1204	0	0	56	0
All	All	11632	0	10212	188	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 (188) 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)
5:A:1323:EDO:H21	5:A:1325:EDO:H12	1.34	1.09
1:A:1039:ARG:H	5:A:1337:EDO:H22	1.33	0.90
1:A:412[A]:MET:HE2	8:A:2219:HOH:O	1.72	0.89
1:A:292:LYS:HE3	8:A:1743:HOH:O	1.76	0.85
1:A:270[B]:ARG:HD3	8:A:1425:HOH:O	1.77	0.84
1:A:175:ASN:HD21	1:A:182:LEU:H	1.26	0.83
1:A:1279:GLU:HG3	8:A:1547:HOH:O	1.78	0.83
1:A:824:ASN:HD21	1:A:958:ALA:H	1.27	0.81
1:A:96:HIS:HE1	1:A:103:VAL:O	1.63	0.81
1:A:963:ARG:HH22	5:A:1328:EDO:H21	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:SER:H	1:A:930:GLN:HE22	1.30	0.78
1:A:219:HIS:HE1	5:A:1323:EDO:C2	1.97	0.77
1:A:782:LYS:NZ	1:A:784[A]:ARG:NH2	2.33	0.77
1:A:441:GLY:HA3	5:A:1312:EDO:H22	1.68	0.76
1:A:713:ARG:HH12	4:A:1335:GOL:H2	1.49	0.76
1:A:1135:CYS:SG	3:A:1302:GLN:CD	2.69	0.76
1:A:270[B]:ARG:CD	8:A:1425:HOH:O	2.33	0.76
1:A:545:ASN:HD22	1:A:547:SER:H	1.32	0.75
1:A:427:LYS:CD	8:A:1543:HOH:O	2.35	0.75
1:A:782:LYS:HZ3	1:A:784[A]:ARG:NH2	1.86	0.74
5:A:1312:EDO:H12	8:A:1868:HOH:O	1.87	0.73
1:A:963:ARG:HH12	5:A:1328:EDO:H21	1.53	0.73
1:A:132:HIS:NE2	5:A:1336:EDO:H12	2.03	0.73
1:A:335:PHE:CZ	1:A:412[B]:MET:HE1	2.24	0.73
1:A:499:PHE:CD2	1:A:515[B]:LEU:HD12	2.24	0.72
1:A:571[A]:ARG:NH2	8:A:1401:HOH:O	2.20	0.72
1:A:335:PHE:CE1	1:A:412[B]:MET:HE1	2.26	0.71
1:A:75:LEU:HD23	8:A:1878:HOH:O	1.90	0.71
5:A:1333:EDO:H21	8:A:2237:HOH:O	1.90	0.71
1:A:950:ASP:HB2	5:A:1319:EDO:H21	1.73	0.71
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.57	0.70
1:A:219:HIS:CE1	5:A:1323:EDO:H22	2.26	0.69
1:A:1152:GLU:CB	4:A:1307:GOL:H11	2.21	0.69
4:A:1310:GOL:H11	8:A:2271:HOH:O	1.93	0.69
1:A:427:LYS:HD3	8:A:1543:HOH:O	1.93	0.69
1:A:963:ARG:NH2	5:A:1328:EDO:H21	2.08	0.69
1:A:1039:ARG:N	5:A:1337:EDO:H22	2.07	0.69
1:A:431:VAL:HG13	8:A:1537:HOH:O	1.93	0.68
1:A:922:ASN:HD22	1:A:924:GLU:H	1.41	0.68
1:A:784[B]:ARG:NH1	5:A:1332:EDO:H11	2.09	0.67
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.77	0.67
1:A:177:ARG:NH1	8:A:1404:HOH:O	2.27	0.67
1:A:279:ARG:CZ	8:A:1826:HOH:O	2.42	0.67
1:A:116:ALA:HB1	1:A:119:LEU:HD13	1.77	0.67
5:A:1323:EDO:H21	8:A:1652:HOH:O	1.94	0.66
1:A:1052:SER:HB3	8:A:1541:HOH:O	1.95	0.66
1:A:292:LYS:CE	8:A:1743:HOH:O	2.38	0.66
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.79	0.65
1:A:219:HIS:HE1	5:A:1323:EDO:H22	1.62	0.64
1:A:583:GLU:H	5:A:1315:EDO:H22	1.62	0.64
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:HIS:HD2	1:A:42:ASP:OD1	1.81	0.63
1:A:132:HIS:NE2	5:A:1336:EDO:C1	2.62	0.62
1:A:1251:ASN:HD22	1:A:1253[A]:ARG:H	1.46	0.62
1:A:1251:ASN:HD22	1:A:1253[B]:ARG:H	1.46	0.62
1:A:499:PHE:HD2	1:A:515[B]:LEU:HD12	1.64	0.62
1:A:950:ASP:HB2	5:A:1319:EDO:C2	2.30	0.62
1:A:238:PHE:CZ	4:A:1309:GOL:H12	2.34	0.62
1:A:329:LYS:HG3	8:A:1476:HOH:O	1.99	0.62
5:A:1325:EDO:H12	8:A:1652:HOH:O	2.00	0.62
1:A:782:LYS:HE2	1:A:784[A]:ARG:NH2	2.15	0.61
1:A:963:ARG:HH12	5:A:1328:EDO:C2	2.13	0.61
1:A:776:LYS:CE	5:A:1325:EDO:H11	2.31	0.61
1:A:776:LYS:HE3	5:A:1325:EDO:H11	1.83	0.61
1:A:963:ARG:NH1	5:A:1328:EDO:H21	2.14	0.61
1:A:1039:ARG:H	5:A:1337:EDO:C2	2.11	0.61
5:A:1312:EDO:H11	8:A:1788:HOH:O	1.99	0.60
5:A:1323:EDO:H21	5:A:1325:EDO:C1	2.20	0.60
1:A:1113:ASN:HD22	1:A:1116:VAL:H	1.48	0.60
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.84	0.60
1:A:442:PRO:O	5:A:1312:EDO:H21	2.01	0.59
1:A:782:LYS:CE	1:A:784[A]:ARG:NH2	2.66	0.59
1:A:308:ALA:HA	1:A:412[A]:MET:HE3	1.85	0.58
1:A:427:LYS:HD2	8:A:1543:HOH:O	2.00	0.58
1:A:471:GLN:HE21	1:A:472:ARG:H	1.51	0.58
1:A:860:VAL:HB	4:A:1304:GOL:H2	1.85	0.58
4:A:1305:GOL:H32	8:A:1965:HOH:O	2.04	0.58
5:A:1324:EDO:H21	8:A:1679:HOH:O	2.03	0.57
1:A:776:LYS:HE3	5:A:1325:EDO:C1	2.34	0.57
5:A:1317:EDO:H12	8:A:2470:HOH:O	2.04	0.57
4:A:1331:GOL:H31	8:A:2281:HOH:O	2.04	0.57
1:A:412[A]:MET:CE	8:A:2219:HOH:O	2.43	0.56
1:A:219:HIS:HE1	5:A:1323:EDO:C1	2.18	0.56
4:A:1304:GOL:H12	8:A:1553:HOH:O	2.04	0.56
1:A:412[B]:MET:HE3	1:A:412[B]:MET:HA	1.88	0.56
1:A:1251:ASN:ND2	1:A:1253[A]:ARG:H	2.04	0.56
1:A:1251:ASN:ND2	1:A:1253[B]:ARG:H	2.04	0.56
4:A:1306:GOL:H12	8:A:1439:HOH:O	2.06	0.55
1:A:396[A]:VAL:HG13	1:A:850:LEU:HD22	1.89	0.55
5:A:1316:EDO:C1	8:A:1960:HOH:O	2.53	0.55
5:A:1323:EDO:C2	5:A:1325:EDO:H12	2.22	0.54
1:A:540:LEU:C	1:A:540:LEU:HD23	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:HIS:HD2	8:A:2498:HOH:O	1.90	0.54
5:A:1312:EDO:C1	8:A:1868:HOH:O	2.48	0.54
1:A:354:GLY:O	1:A:408:HIS:HE1	1.91	0.53
1:A:1230:THR:HA	4:A:1314:GOL:H31	1.90	0.53
1:A:216:HIS:HD2	8:A:1680:HOH:O	1.90	0.53
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.06	0.53
1:A:251:TYR:H	4:A:1308:GOL:H11	1.73	0.53
1:A:776:LYS:HD2	5:A:1325:EDO:H11	1.92	0.52
1:A:782:LYS:HZ3	1:A:784[A]:ARG:HH22	1.57	0.52
1:A:219:HIS:CE1	5:A:1323:EDO:H11	2.44	0.52
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.93	0.52
1:A:338:SER:OG	1:A:408:HIS:HD2	1.93	0.52
1:A:211:GLN:HE22	1:A:452:ALA:H	1.57	0.52
1:A:776:LYS:CD	5:A:1325:EDO:H11	2.40	0.52
1:A:75:LEU:CD2	8:A:1878:HOH:O	2.54	0.51
1:A:335:PHE:CE1	1:A:412[B]:MET:CE	2.92	0.51
1:A:950:ASP:CB	5:A:1319:EDO:H21	2.39	0.51
5:A:1324:EDO:H12	8:A:2425:HOH:O	2.10	0.51
1:A:219:HIS:CE1	5:A:1323:EDO:C2	2.82	0.51
3:A:1302:GLN:NE2	8:A:1417:HOH:O	2.41	0.50
4:A:1331:GOL:C3	8:A:2281:HOH:O	2.59	0.50
1:A:117:SER:OG	1:A:118:THR:N	2.43	0.50
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.58	0.50
1:A:219:HIS:HE1	5:A:1323:EDO:H11	1.74	0.50
1:A:296:HIS:HD2	1:A:307:GLY:O	1.95	0.49
1:A:963:ARG:CZ	5:A:1328:EDO:H21	2.42	0.49
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.96	0.49
1:A:335:PHE:CE1	1:A:412[B]:MET:SD	3.06	0.49
1:A:447:GLY:HA2	1:A:468:ALA:O	2.13	0.49
1:A:782:LYS:HE2	1:A:784[A]:ARG:CZ	2.43	0.49
1:A:1135:CYS:SG	3:A:1302:GLN:CG	3.00	0.49
4:A:1310:GOL:C1	8:A:2271:HOH:O	2.55	0.49
1:A:546:GLU:HB3	5:A:1333:EDO:H11	1.95	0.48
1:A:1006:HIS:HE1	8:A:1517:HOH:O	1.95	0.48
1:A:294[A]:GLU:OE1	1:A:318:ASP:OD1	2.31	0.48
1:A:862:GLN:HE22	5:A:1319:EDO:C2	2.27	0.48
1:A:60:GLN:NE2	8:A:1403:HOH:O	2.24	0.48
1:A:308:ALA:CA	1:A:412[A]:MET:HE3	2.43	0.48
1:A:784[A]:ARG:NH2	5:A:1330:EDO:O1	2.38	0.47
1:A:6:ARG:HD2	8:A:1715:HOH:O	2.15	0.47
1:A:119:LEU:HA	1:A:123:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:PRO:HA	4:A:1305:GOL:H12	1.96	0.47
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.23	0.47
5:A:1316:EDO:H11	8:A:1960:HOH:O	2.13	0.47
1:A:251:TYR:H	4:A:1308:GOL:C1	2.28	0.47
1:A:713:ARG:HH12	4:A:1335:GOL:C2	2.21	0.46
1:A:1145:ARG:HB2	8:A:1863:HOH:O	2.14	0.46
1:A:784[B]:ARG:HH11	5:A:1332:EDO:H11	1.78	0.46
1:A:585:HIS:HD2	8:A:2414:HOH:O	1.99	0.46
1:A:499:PHE:HA	8:A:1543:HOH:O	2.15	0.46
1:A:238:PHE:CE1	4:A:1309:GOL:H12	2.51	0.46
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.99	0.46
1:A:96:HIS:CE1	1:A:103:VAL:O	2.55	0.45
1:A:219:HIS:CE1	5:A:1323:EDO:C1	2.99	0.45
1:A:553[A]:LEU:HD12	1:A:555:VAL:HG23	1.98	0.45
1:A:318:ASP:OD2	1:A:502[B]:ASP:CG	2.59	0.45
1:A:396[A]:VAL:CG1	1:A:850:LEU:HD22	2.46	0.45
1:A:1:MET:HE3	1:A:1:MET:HB2	1.72	0.45
1:A:250:ASP:HA	4:A:1308:GOL:H11	2.00	0.44
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.52	0.44
1:A:877[B]:ARG:HG3	1:A:877[B]:ARG:HH21	1.82	0.44
1:A:976:GLU:OE1	5:A:1328:EDO:H22	2.18	0.44
1:A:1006:HIS:HD2	8:A:1969:HOH:O	2.01	0.44
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.17	0.43
1:A:798:LEU:HD13	8:A:1665:HOH:O	2.17	0.43
1:A:862:GLN:HE22	5:A:1319:EDO:H22	1.82	0.43
1:A:713:ARG:NH1	4:A:1335:GOL:H2	2.27	0.43
1:A:913:GLY:CA	4:A:1310:GOL:H2	2.48	0.43
1:A:1061:HIS:HD2	8:A:1970:HOH:O	2.01	0.43
1:A:1051:ASN:HB3	8:A:1416:HOH:O	2.18	0.43
1:A:39:HIS:HD2	8:A:1406:HOH:O	2.01	0.43
1:A:0:HIS:CD2	1:A:42:ASP:OD1	2.67	0.43
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.17	0.42
5:A:1312:EDO:H22	8:A:1788:HOH:O	2.18	0.42
1:A:784[B]:ARG:NH1	5:A:1332:EDO:C1	2.82	0.42
1:A:175:ASN:ND2	1:A:182:LEU:H	2.04	0.42
5:A:1323:EDO:H12	8:A:1603:HOH:O	2.18	0.42
1:A:553[A]:LEU:CD1	1:A:555:VAL:HG23	2.49	0.42
1:A:1183:GLN:HG3	8:A:2548:HOH:O	2.19	0.42
1:A:950:ASP:CA	5:A:1319:EDO:H21	2.50	0.42
1:A:891:LEU:C	1:A:891:LEU:HD13	2.45	0.42
1:A:827:LEU:HD23	1:A:954:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:CYS:SG	3:A:1302:GLN:OE1	2.77	0.41
1:A:93[A]:ASP:O	1:A:94:ILE:C	2.64	0.41
1:A:1113:ASN:HD21	1:A:1115:ARG:HB3	1.85	0.41
1:A:441:GLY:C	5:A:1312:EDO:C2	2.93	0.41
1:A:1048:GLN:O	1:A:1095:SER:HA	2.20	0.41
1:A:1066:ASP:OD1	8:A:1402:HOH:O	2.22	0.41
1:A:913:GLY:HA3	8:A:1621:HOH:O	2.21	0.40
1:A:441:GLY:CA	5:A:1312:EDO:H22	2.46	0.40
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.40	0.40
4:A:1306:GOL:C1	8:A:1439:HOH:O	2.67	0.40
1:A:219:HIS:CD2	1:A:777:ASP:OD1	2.73	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	1330/1303 (102%)	1293 (97%)	33 (2%)	4 (0%)	36 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	117	SER
1	A	119	LEU
1	A	661	THR

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1060/1039 (102%)	1045 (99%)	15 (1%)	59 44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	60	GLN
1	A	296	HIS
1	A	396[A]	VAL
1	A	396[B]	VAL
1	A	471	GLN
1	A	596	GLN
1	A	782	LYS
1	A	791	GLN
1	A	1029	ILE
1	A	1088	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1206	ASP
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	31	HIS
1	A	39	HIS
1	A	96	HIS
1	A	123	GLN
1	A	169	GLN
1	A	175	ASN
1	A	211	GLN
1	A	216	HIS
1	A	219	HIS
1	A	275	HIS
1	A	276	ASN
1	A	284	GLN
1	A	298	HIS

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Mol	Chain	Res	Type
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	585	HIS
1	A	739	ASN
1	A	746	HIS
1	A	824	ASN
1	A	862	GLN
1	A	883	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1061	HIS
1	A	1113	ASN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS

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 58 ligands modelled in this entry, 3 are monoatomic - leaving 55 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	1308	-	5,5,5	0.56	0	5,5,5	1.18	0
5	EDO	A	1330	-	3,3,3	0.24	0	2,2,2	0.31	0
7	SO4	A	1351	-	4,4,4	0.84	0	6,6,6	1.13	1 (16%)
5	EDO	A	1321	-	3,3,3	0.43	0	2,2,2	1.04	0
5	EDO	A	1317	-	3,3,3	0.59	0	2,2,2	0.14	0
7	SO4	A	1346	-	4,4,4	0.74	0	6,6,6	1.17	0
4	GOL	A	1331	-	5,5,5	1.17	1 (20%)	5,5,5	0.98	0
5	EDO	A	1312	-	3,3,3	0.28	0	2,2,2	0.18	0
5	EDO	A	1325	-	3,3,3	0.38	0	2,2,2	0.29	0
4	GOL	A	1314	-	5,5,5	0.50	0	5,5,5	0.78	0
5	EDO	A	1319	-	3,3,3	0.68	0	2,2,2	1.75	1 (50%)
5	EDO	A	1329	-	3,3,3	0.21	0	2,2,2	0.71	0
7	SO4	A	1343	-	4,4,4	0.78	0	6,6,6	1.42	1 (16%)
7	SO4	A	1347	-	4,4,4	0.44	0	6,6,6	1.06	0
7	SO4	A	1356	-	4,4,4	0.48	0	6,6,6	0.40	0
7	SO4	A	1357	-	4,4,4	0.76	0	6,6,6	0.38	0
5	EDO	A	1318	-	3,3,3	0.70	0	2,2,2	1.07	0
5	EDO	A	1328	-	3,3,3	0.39	0	2,2,2	0.53	0
5	EDO	A	1322	-	3,3,3	0.27	0	2,2,2	1.09	0
5	EDO	A	1313	-	3,3,3	0.42	0	2,2,2	0.42	0
4	GOL	A	1335	-	5,5,5	0.61	0	5,5,5	1.25	1 (20%)
4	GOL	A	1303	-	5,5,5	0.62	0	5,5,5	1.15	0
4	GOL	A	1307	-	5,5,5	0.48	0	5,5,5	1.31	0
7	SO4	A	1342	-	4,4,4	0.54	0	6,6,6	0.55	0
7	SO4	A	1358	-	4,4,4	0.48	0	6,6,6	0.63	0
2	ADP	A	1301	6	28,29,29	1.29	2 (7%)	43,45,45	1.50	6 (13%)
4	GOL	A	1311	-	5,5,5	0.83	0	5,5,5	1.31	1 (20%)
7	SO4	A	1344	-	4,4,4	0.48	0	6,6,6	1.09	1 (16%)
5	EDO	A	1327	-	3,3,3	0.28	0	2,2,2	0.81	0
7	SO4	A	1345	-	4,4,4	0.43	0	6,6,6	0.73	0
5	EDO	A	1323	-	3,3,3	0.24	0	2,2,2	0.23	0
5	EDO	A	1315	-	3,3,3	0.85	0	2,2,2	0.26	0
7	SO4	A	1355	-	4,4,4	0.40	0	6,6,6	0.58	0
5	EDO	A	1324	-	3,3,3	0.73	0	2,2,2	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	1305	-	5,5,5	1.27	1 (20%)	5,5,5	1.56	1 (20%)
5	EDO	A	1326	-	3,3,3	0.59	0	2,2,2	0.16	0
7	SO4	A	1353	-	4,4,4	0.36	0	6,6,6	0.65	0
4	GOL	A	1304	-	5,5,5	1.16	0	5,5,5	1.05	0
5	EDO	A	1334	-	3,3,3	0.30	0	2,2,2	0.13	0
5	EDO	A	1316	-	3,3,3	0.63	0	2,2,2	0.30	0
4	GOL	A	1306	-	5,5,5	0.84	0	5,5,5	3.03	3 (60%)
7	SO4	A	1352	-	4,4,4	0.92	0	6,6,6	0.49	0
4	GOL	A	1309	-	5,5,5	0.54	0	5,5,5	0.66	0
7	SO4	A	1348	-	4,4,4	1.00	0	6,6,6	1.00	0
5	EDO	A	1336	-	3,3,3	0.34	0	2,2,2	0.41	0
7	SO4	A	1341	-	4,4,4	0.94	0	6,6,6	0.80	0
7	SO4	A	1350	-	4,4,4	1.12	1 (25%)	6,6,6	1.40	1 (16%)
5	EDO	A	1333	-	3,3,3	0.34	0	2,2,2	0.42	0
3	GLN	A	1302	-	8,9,9	1.38	1 (12%)	8,11,11	0.65	0
4	GOL	A	1310	-	5,5,5	0.45	0	5,5,5	0.88	0
7	SO4	A	1349	-	4,4,4	0.59	0	6,6,6	0.59	0
5	EDO	A	1337	-	3,3,3	0.20	0	2,2,2	0.28	0
7	SO4	A	1354	-	4,4,4	0.59	0	6,6,6	0.66	0
5	EDO	A	1332	-	3,3,3	0.26	0	2,2,2	0.92	0
5	EDO	A	1320	-	3,3,3	0.63	0	2,2,2	0.27	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
4	GOL	A	1308	-	-	0/4/4/4	-
5	EDO	A	1330	-	-	1/1/1/1	-
5	EDO	A	1321	-	-	1/1/1/1	-
5	EDO	A	1317	-	-	1/1/1/1	-
4	GOL	A	1331	-	-	2/4/4/4	-
5	EDO	A	1312	-	-	1/1/1/1	-
5	EDO	A	1325	-	-	1/1/1/1	-
4	GOL	A	1314	-	-	2/4/4/4	-
5	EDO	A	1319	-	-	0/1/1/1	-
5	EDO	A	1329	-	-	0/1/1/1	-
5	EDO	A	1318	-	-	0/1/1/1	-
5	EDO	A	1328	-	-	0/1/1/1	-
5	EDO	A	1322	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1313	-	-	1/1/1/1	-
4	GOL	A	1335	-	-	2/4/4/4	-
4	GOL	A	1303	-	-	0/4/4/4	-
4	GOL	A	1307	-	-	1/4/4/4	-
2	ADP	A	1301	6	-	2/16/32/32	0/3/3/3
4	GOL	A	1311	-	-	4/4/4/4	-
5	EDO	A	1327	-	-	0/1/1/1	-
5	EDO	A	1323	-	-	0/1/1/1	-
5	EDO	A	1315	-	-	1/1/1/1	-
5	EDO	A	1324	-	-	1/1/1/1	-
4	GOL	A	1305	-	-	2/4/4/4	-
5	EDO	A	1326	-	-	1/1/1/1	-
4	GOL	A	1304	-	-	2/4/4/4	-
5	EDO	A	1334	-	-	1/1/1/1	-
5	EDO	A	1316	-	-	1/1/1/1	-
4	GOL	A	1306	-	-	0/4/4/4	-
4	GOL	A	1309	-	-	3/4/4/4	-
5	EDO	A	1336	-	-	1/1/1/1	-
5	EDO	A	1333	-	-	0/1/1/1	-
3	GLN	A	1302	-	-	1/9/9/9	-
4	GOL	A	1310	-	-	2/4/4/4	-
5	EDO	A	1337	-	-	1/1/1/1	-
5	EDO	A	1332	-	-	1/1/1/1	-
5	EDO	A	1320	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	C4-N9	-4.07	1.29	1.37
3	A	1302	GLN	OXT-C	-3.36	1.19	1.30
4	A	1305	GOL	O2-C2	-2.57	1.35	1.43
2	A	1301	ADP	PA-O1A	-2.23	1.43	1.50
4	A	1331	GOL	O2-C2	-2.16	1.37	1.43
7	A	1350	SO4	O2-S	2.05	1.57	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1306	GOL	O2-C2-C3	-5.20	87.65	109.18
2	A	1301	ADP	C4-N9-C8	4.77	110.75	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ADP	O4'-C1'-N9	4.37	116.48	108.09
4	A	1306	GOL	O3-C3-C2	-3.51	94.58	110.38
2	A	1301	ADP	C4'-O4'-C1'	2.62	115.26	109.47
7	A	1343	SO4	O3-S-O1	2.52	122.71	109.56
5	A	1319	EDO	O1-C1-C2	2.40	130.70	112.39
4	A	1335	GOL	O1-C1-C2	2.39	121.13	110.38
2	A	1301	ADP	O3B-PB-O2B	2.35	116.60	107.80
4	A	1305	GOL	C3-C2-C1	2.33	120.33	111.80
7	A	1350	SO4	O4-S-O1	2.31	121.63	109.56
7	A	1351	SO4	O4-S-O2	2.25	121.35	109.56
4	A	1306	GOL	C3-C2-C1	2.24	120.02	111.80
2	A	1301	ADP	C1'-N9-C8	-2.18	122.25	127.09
4	A	1311	GOL	O1-C1-C2	-2.17	100.61	110.38
7	A	1344	SO4	O4-S-O2	2.11	120.60	109.56
2	A	1301	ADP	O4'-C1'-C2'	-2.10	102.13	106.62

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O2B
4	A	1304	GOL	C1-C2-C3-O3
4	A	1304	GOL	O2-C2-C3-O3
4	A	1305	GOL	C1-C2-C3-O3
4	A	1309	GOL	C1-C2-C3-O3
4	A	1310	GOL	O1-C1-C2-C3
4	A	1311	GOL	O1-C1-C2-C3
4	A	1331	GOL	O2-C2-C3-O3
4	A	1335	GOL	O1-C1-C2-C3
4	A	1307	GOL	O1-C1-C2-C3
4	A	1309	GOL	O1-C1-C2-C3
4	A	1311	GOL	C1-C2-C3-O3
4	A	1331	GOL	C1-C2-C3-O3
4	A	1305	GOL	O2-C2-C3-O3
4	A	1310	GOL	O1-C1-C2-O2
4	A	1311	GOL	O1-C1-C2-O2
4	A	1335	GOL	O1-C1-C2-O2
5	A	1313	EDO	O1-C1-C2-O2
5	A	1315	EDO	O1-C1-C2-O2
5	A	1325	EDO	O1-C1-C2-O2
5	A	1312	EDO	O1-C1-C2-O2
5	A	1316	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1321	EDO	O1-C1-C2-O2
5	A	1322	EDO	O1-C1-C2-O2
5	A	1337	EDO	O1-C1-C2-O2
4	A	1309	GOL	O2-C2-C3-O3
5	A	1317	EDO	O1-C1-C2-O2
3	A	1302	GLN	CA-CB-CG-CD
4	A	1314	GOL	O2-C2-C3-O3
5	A	1320	EDO	O1-C1-C2-O2
5	A	1324	EDO	O1-C1-C2-O2
4	A	1314	GOL	O1-C1-C2-C3
4	A	1311	GOL	O2-C2-C3-O3
5	A	1326	EDO	O1-C1-C2-O2
5	A	1332	EDO	O1-C1-C2-O2
5	A	1336	EDO	O1-C1-C2-O2
2	A	1301	ADP	PA-O3A-PB-O3B
5	A	1330	EDO	O1-C1-C2-O2
5	A	1334	EDO	O1-C1-C2-O2

There are no ring outliers.

25 monomers are involved in 82 short contacts:

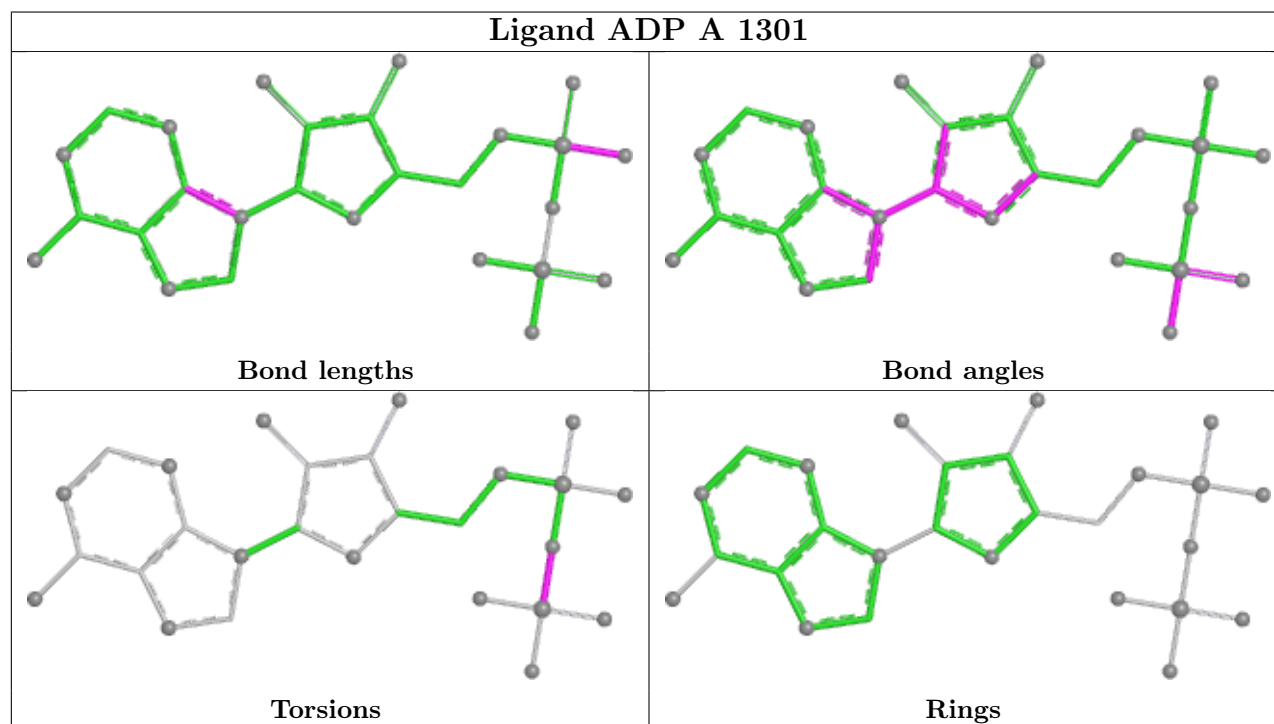
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1308	GOL	3	0
5	A	1330	EDO	1	0
5	A	1317	EDO	1	0
4	A	1331	GOL	2	0
5	A	1312	EDO	8	0
5	A	1325	EDO	9	0
4	A	1314	GOL	1	0
5	A	1319	EDO	6	0
5	A	1328	EDO	7	0
4	A	1335	GOL	3	0
4	A	1307	GOL	1	0
5	A	1323	EDO	13	0
5	A	1315	EDO	1	0
5	A	1324	EDO	2	0
4	A	1305	GOL	2	0
4	A	1304	GOL	2	0
5	A	1316	EDO	2	0
4	A	1306	GOL	2	0
4	A	1309	GOL	2	0
5	A	1336	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1333	EDO	2	0
3	A	1302	GLN	4	0
4	A	1310	GOL	3	0
5	A	1337	EDO	3	0
5	A	1332	EDO	3	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 ⓘ

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	1298/1303 (99%)	-0.25	29 (2%) 62 69	10, 20, 42, 72	34 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	ASN	4.0
1	A	459	GLY	3.9
1	A	457	ALA	3.7
1	A	789	ASN	3.4
1	A	453	ALA	3.3
1	A	622	LYS	3.2
1	A	1204	ARG	3.0
1	A	31	HIS	3.0
1	A	-2	GLY	2.9
1	A	66	SER	2.9
1	A	461	SER	2.8
1	A	118	THR	2.8
1	A	428	GLY	2.7
1	A	460	GLN	2.6
1	A	623	GLY	2.6
1	A	450	GLY	2.5
1	A	119	LEU	2.5
1	A	117	SER	2.4
1	A	458	SER	2.4
1	A	463	ALA	2.4
1	A	452	ALA	2.4
1	A	451	GLY	2.3
1	A	788	GLY	2.3
1	A	6	ARG	2.3
1	A	121	ALA	2.3
1	A	1	MET	2.2
1	A	499	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	THR	2.2
1	A	-1	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	EDO	A	1327	4/4	0.68	0.24	56,68,71,76	0
5	EDO	A	1320	4/4	0.71	0.23	57,58,61,62	0
5	EDO	A	1329	4/4	0.73	0.21	61,62,64,67	0
5	EDO	A	1336	4/4	0.73	0.23	51,62,62,66	0
5	EDO	A	1332	4/4	0.75	0.21	48,50,59,65	0
5	EDO	A	1325	4/4	0.75	0.23	42,55,61,63	0
5	EDO	A	1334	4/4	0.76	0.19	58,59,61,63	0
5	EDO	A	1321	4/4	0.76	0.18	44,49,50,50	0
5	EDO	A	1337	4/4	0.76	0.24	60,67,68,73	0
5	EDO	A	1322	4/4	0.77	0.22	48,55,57,58	0
5	EDO	A	1328	4/4	0.78	0.19	38,52,54,56	0
5	EDO	A	1326	4/4	0.78	0.18	47,58,58,66	0
4	GOL	A	1309	6/6	0.78	0.21	40,65,69,75	0
4	GOL	A	1310	6/6	0.79	0.17	38,61,63,64	0
5	EDO	A	1330	4/4	0.79	0.23	60,61,64,65	0
5	EDO	A	1333	4/4	0.81	0.25	45,56,60,73	0
7	SO4	A	1355	5/5	0.81	0.16	59,84,93,100	0
5	EDO	A	1313	4/4	0.82	0.21	37,47,47,60	0
4	GOL	A	1307	6/6	0.82	0.19	34,47,57,61	0
5	EDO	A	1324	4/4	0.82	0.16	47,49,53,59	0
7	SO4	A	1354	5/5	0.83	0.11	68,68,73,76	0

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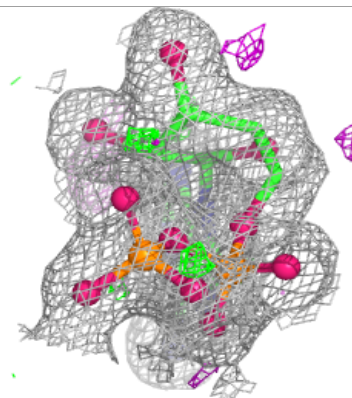
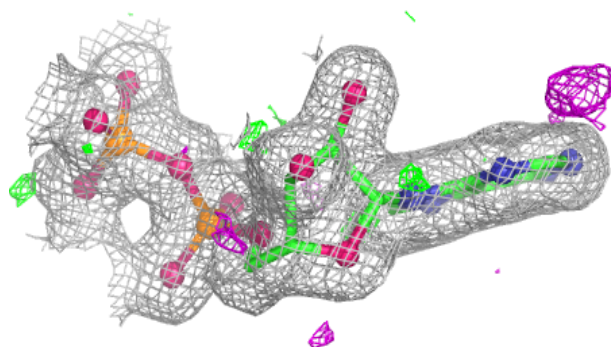
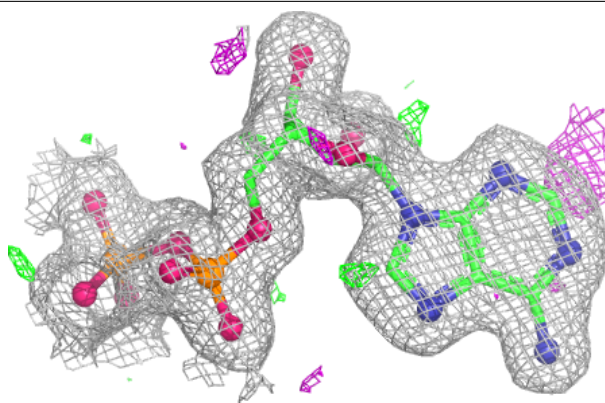
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1323	4/4	0.83	0.18	44,52,53,71	0
7	SO4	A	1358	5/5	0.84	0.12	66,79,86,95	0
4	GOL	A	1308	6/6	0.85	0.16	40,46,54,55	0
5	EDO	A	1316	4/4	0.85	0.15	39,42,42,44	0
7	SO4	A	1356	5/5	0.85	0.09	68,74,80,93	0
4	GOL	A	1311	6/6	0.85	0.15	36,42,54,57	0
7	SO4	A	1357	5/5	0.86	0.10	64,73,79,81	0
4	GOL	A	1335	6/6	0.86	0.15	33,48,52,53	0
5	EDO	A	1317	4/4	0.87	0.14	44,51,54,55	0
5	EDO	A	1312	4/4	0.88	0.16	42,44,45,65	0
4	GOL	A	1304	6/6	0.88	0.15	27,45,54,65	0
5	EDO	A	1318	4/4	0.88	0.12	39,39,45,53	0
5	EDO	A	1315	4/4	0.88	0.12	35,36,37,52	0
4	GOL	A	1314	6/6	0.89	0.13	25,36,39,42	0
4	GOL	A	1305	6/6	0.90	0.12	29,37,44,53	0
4	GOL	A	1306	6/6	0.90	0.11	30,39,45,47	0
7	SO4	A	1353	5/5	0.91	0.09	54,62,72,74	0
4	GOL	A	1303	6/6	0.91	0.11	23,24,38,41	0
7	SO4	A	1352	5/5	0.92	0.08	39,49,53,56	0
5	EDO	A	1319	4/4	0.93	0.12	36,38,41,42	0
7	SO4	A	1350	5/5	0.94	0.08	35,35,45,47	0
3	GLN	A	1302	10/10	0.95	0.07	13,16,18,19	2
7	SO4	A	1351	5/5	0.95	0.07	29,37,41,43	0
4	GOL	A	1331	6/6	0.95	0.12	20,28,33,36	0
7	SO4	A	1346	5/5	0.96	0.08	33,34,46,58	0
7	SO4	A	1348	5/5	0.96	0.13	25,32,38,39	0
7	SO4	A	1349	5/5	0.96	0.06	40,44,49,54	0
7	SO4	A	1344	5/5	0.96	0.07	27,36,40,47	0
7	SO4	A	1347	5/5	0.97	0.06	30,38,44,44	0
7	SO4	A	1345	5/5	0.97	0.05	38,39,47,52	0
7	SO4	A	1343	5/5	0.97	0.12	32,36,38,44	0
6	MG	A	1340	1/1	0.98	0.02	15,15,15,15	0
6	MG	A	1339	1/1	0.99	0.02	15,15,15,15	0
2	ADP	A	1301	27/27	0.99	0.03	12,14,15,16	0
7	SO4	A	1341	5/5	0.99	0.05	21,21,24,25	0
7	SO4	A	1342	5/5	0.99	0.05	21,26,27,31	0
6	MG	A	1338	1/1	0.99	0.03	14,14,14,14	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 1301:

$2mF_o-DF_c$ (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.