



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:40 PM EDT

PDB ID : 6LYK / pdb_00006lyk
Title : Crystal Structure of R1263A mutant of Formylglycinamidase Synthetase
Authors : Sharma, N.; Tanwar, A.S.; Anand, R.
Deposited on : 2020-02-14
Resolution : 1.70 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

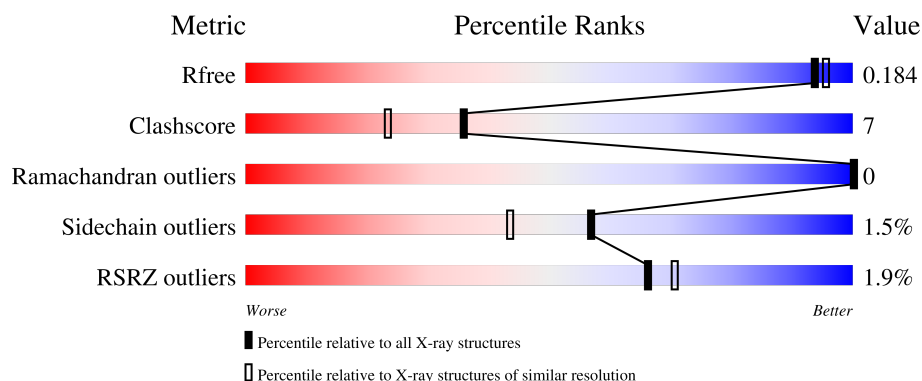
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

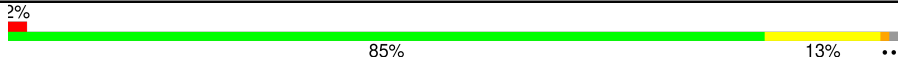
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	1305	

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
2	EDO	A	1602	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	1647	-	-	X	-
8	GOL	A	1651	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12144 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.

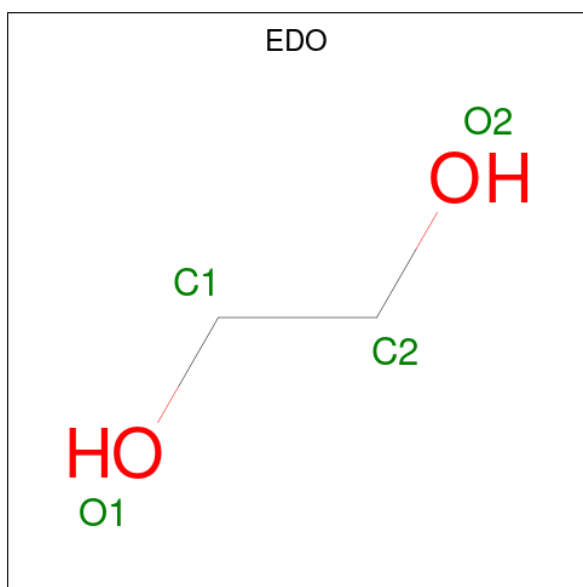
- Molecule 1 is a protein called Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1293	Total	C	N	O	S	0	75	0
			10360	6544	1822	1938	56			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P74881
A	-8	SER	-	expression tag	UNP P74881
A	-7	GLY	-	expression tag	UNP P74881
A	-6	LEU	-	expression tag	UNP P74881
A	-5	VAL	-	expression tag	UNP P74881
A	-4	PRO	-	expression tag	UNP P74881
A	-3	ARG	-	expression tag	UNP P74881
A	-2	GLY	-	expression tag	UNP P74881
A	-1	SER	-	expression tag	UNP P74881
A	0	HIS	-	expression tag	UNP P74881
A	1263	ALA	ARG	engineered mutation	UNP P74881

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



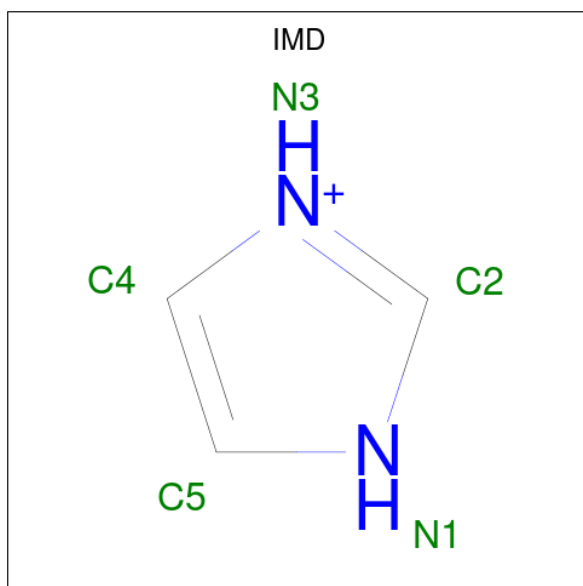
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total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

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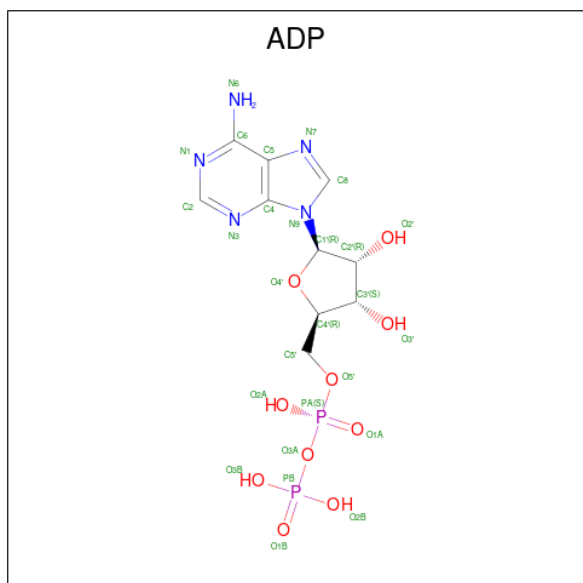
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



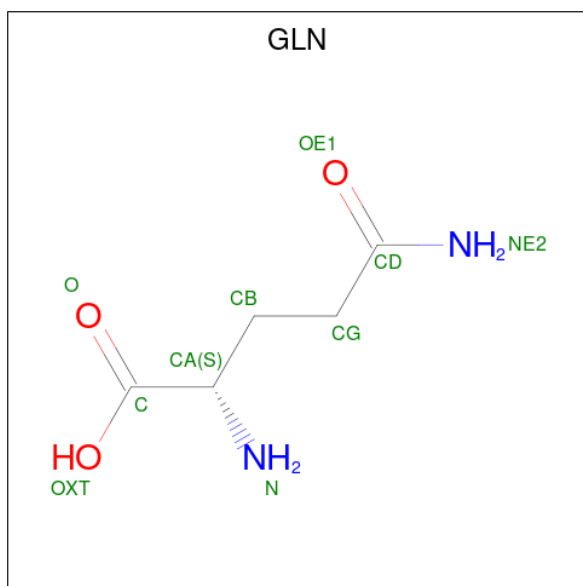
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).

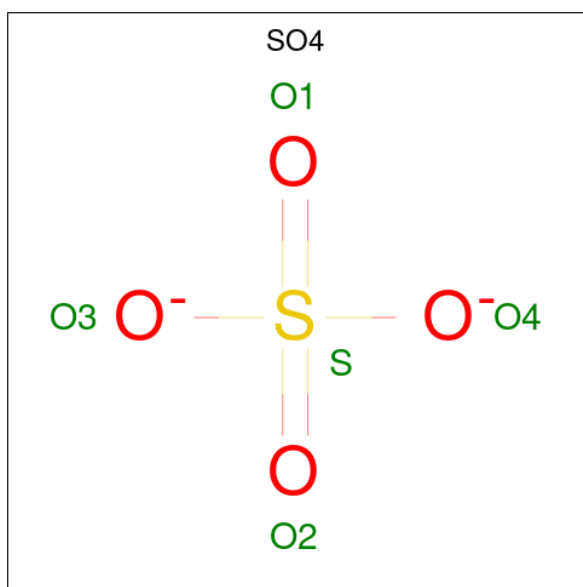


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	5	2	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Mg	0	0
			4	4		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



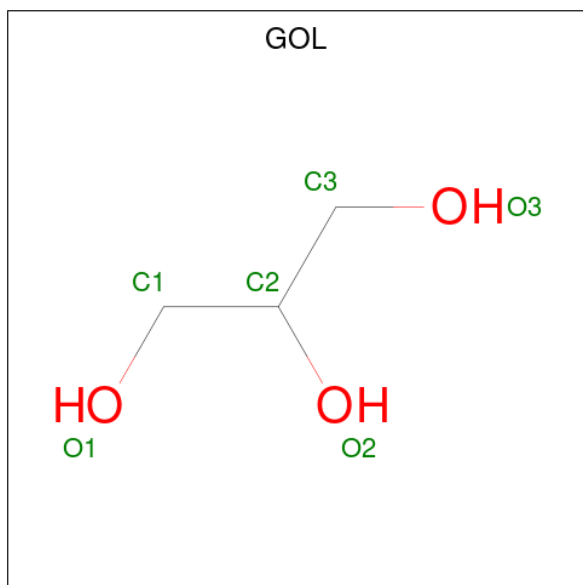
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	1
			10	8	2		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	1
			12	6	6		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	1
			12	6	6		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

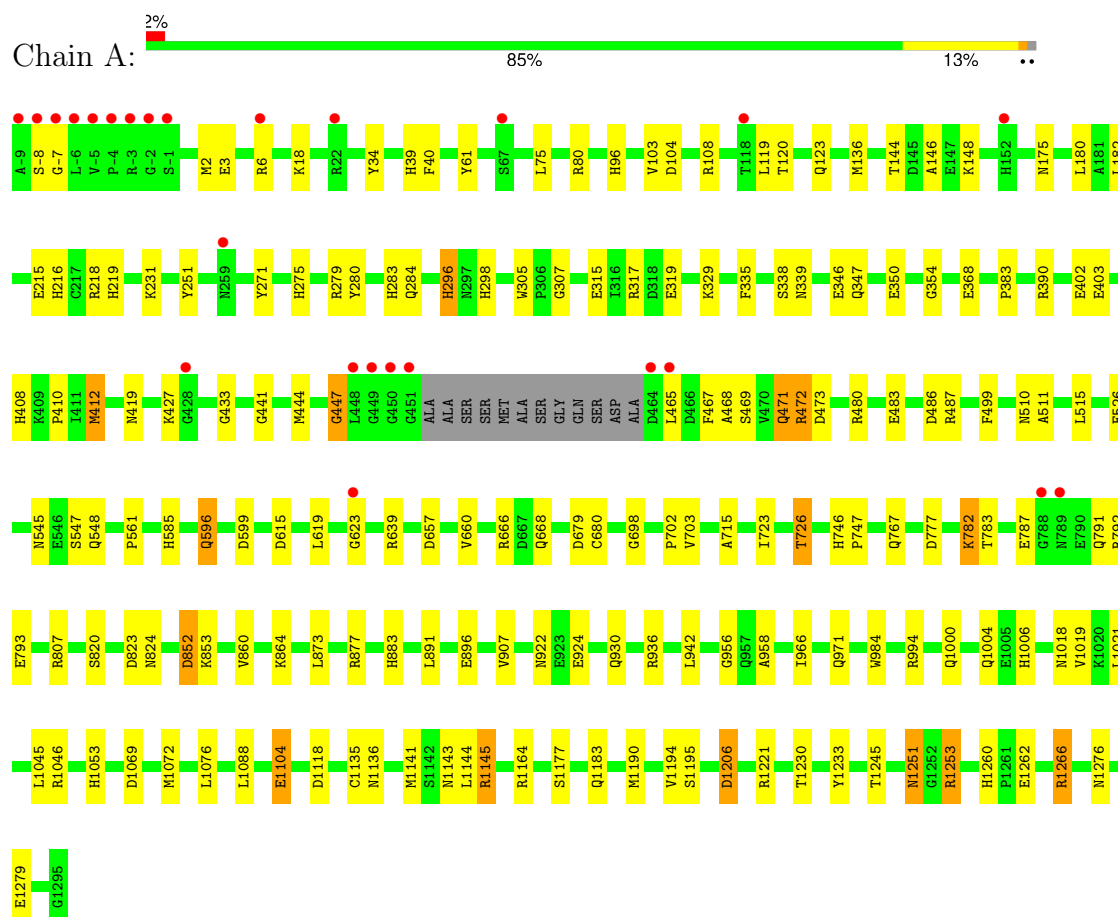
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1474	Total	O	0	0
			1474	1474		

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	146.90Å 146.90Å 141.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.74 – 1.70 39.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.74-1.70) 99.8 (39.74-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.152 , 0.177 0.164 , 0.184	Depositor DCC
R_{free} test set	9442 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12144	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: MG, ADP, EDO, IMD, SO4, GOL

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	1.38	53/10766 (0.5%)	1.18	28/14603 (0.2%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1266[A]	ARG	CA-C	10.96	1.66	1.52
1	A	1266[B]	ARG	CA-C	10.96	1.66	1.52
1	A	412[A]	MET	CA-C	10.51	1.66	1.53
1	A	412[B]	MET	CA-C	10.51	1.66	1.53
1	A	148[A]	LYS	CA-C	8.18	1.64	1.52
1	A	148[B]	LYS	CA-C	8.18	1.64	1.52
1	A	390	ARG	C-O	-7.29	1.14	1.24
1	A	347	GLN	C-O	-6.87	1.16	1.23
1	A	486	ASP	C-O	-6.84	1.16	1.24
1	A	639	ARG	C-O	-6.54	1.16	1.24
1	A	823[A]	ASP	CA-C	6.41	1.61	1.52
1	A	823[B]	ASP	CA-C	6.41	1.61	1.52
1	A	1253[A]	ARG	CA-C	6.35	1.61	1.52
1	A	1253[B]	ARG	CA-C	6.35	1.61	1.52
1	A	231	LYS	CA-C	-6.30	1.45	1.52
1	A	1046	ARG	C-O	-6.22	1.17	1.23
1	A	852[A]	ASP	CA-C	6.20	1.60	1.53
1	A	852[B]	ASP	CA-C	6.20	1.60	1.53
1	A	956	GLY	C-O	-5.86	1.19	1.23
1	A	715	ALA	N-CA	5.75	1.53	1.46
1	A	441	GLY	C-O	-5.74	1.16	1.24
1	A	666	ARG	C-O	-5.71	1.17	1.24
1	A	1145[A]	ARG	CA-C	5.65	1.60	1.52
1	A	1145[B]	ARG	CA-C	5.65	1.60	1.52
1	A	1141	MET	SD-CE	-5.62	1.65	1.79
1	A	1279	GLU	C-O	-5.60	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	ASP	C-O	-5.58	1.17	1.24
1	A	1206	ASP	C-O	-5.49	1.17	1.24
1	A	698	GLY	CA-C	5.49	1.56	1.51
1	A	1245	THR	C-O	-5.47	1.16	1.24
1	A	1183	GLN	C-O	5.45	1.30	1.23
1	A	1118	ASP	C-O	-5.39	1.17	1.24
1	A	615	ASP	CA-C	-5.38	1.46	1.52
1	A	472	ARG	C-O	-5.37	1.17	1.23
1	A	483	GLU	C-O	-5.28	1.18	1.24
1	A	984	TRP	N-CA	-5.27	1.40	1.46
1	A	433	GLY	CA-C	5.24	1.59	1.51
1	A	703	VAL	C-O	5.23	1.30	1.24
1	A	510[A]	ASN	CA-C	5.22	1.59	1.52
1	A	510[B]	ASN	CA-C	5.22	1.59	1.52
1	A	410	PRO	N-CA	-5.22	1.41	1.47
1	A	561	PRO	CA-C	5.18	1.59	1.52
1	A	473	ASP	C-O	-5.18	1.17	1.24
1	A	1177	SER	CA-C	5.17	1.57	1.52
1	A	447	GLY	CA-C	-5.16	1.45	1.51
1	A	807	ARG	C-O	-5.16	1.17	1.23
1	A	1164	ARG	C-O	-5.15	1.17	1.23
1	A	853	LYS	C-O	-5.14	1.17	1.24
1	A	480	ARG	C-O	-5.11	1.18	1.24
1	A	6	ARG	C-O	-5.04	1.17	1.23
1	A	971	GLN	CA-C	5.03	1.58	1.52
1	A	526	GLU	C-O	-5.02	1.18	1.24
1	A	702	PRO	CA-CB	-5.01	1.46	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-8	SER	N-CA-C	9.05	123.87	110.48
1	A	1253[A]	ARG	CA-C-O	7.88	129.08	119.31
1	A	1253[B]	ARG	CA-C-O	7.88	129.08	119.31
1	A	148[A]	LYS	CA-C-O	7.75	128.88	120.20
1	A	148[B]	LYS	CA-C-O	7.75	128.88	120.20
1	A	1145[A]	ARG	N-CA-C	7.08	121.02	112.38
1	A	1145[B]	ARG	N-CA-C	7.08	121.02	112.38
1	A	1253[A]	ARG	N-CA-C	6.91	121.45	112.89
1	A	1253[B]	ARG	N-CA-C	6.91	121.45	112.89
1	A	1104[A]	GLU	N-CA-C	6.61	118.56	111.36
1	A	1104[B]	GLU	N-CA-C	6.61	118.56	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852[A]	ASP	CA-C-O	6.39	128.29	120.56
1	A	852[B]	ASP	CA-C-O	6.39	128.29	120.56
1	A	511	ALA	N-CA-C	6.09	118.00	111.36
1	A	1145[A]	ARG	CA-C-O	5.95	126.69	119.49
1	A	1145[B]	ARG	CA-C-O	5.95	126.69	119.49
1	A	1104[A]	GLU	CA-C-O	5.93	126.70	120.42
1	A	1104[B]	GLU	CA-C-O	5.93	126.70	120.42
1	A	994	ARG	CG-CD-NE	-5.89	99.04	112.00
1	A	1053	HIS	N-CA-C	5.72	117.52	111.28
1	A	510[A]	ASN	CA-C-O	5.63	126.87	120.00
1	A	510[B]	ASN	CA-C-O	5.63	126.87	120.00
1	A	80	ARG	CB-CA-C	-5.42	100.96	109.52
1	A	1230	THR	N-CA-C	5.35	117.52	109.23
1	A	148[A]	LYS	N-CA-C	5.17	118.36	111.75
1	A	148[B]	LYS	N-CA-C	5.17	118.36	111.75
1	A	487	ARG	O-C-N	5.17	127.59	122.12
1	A	427	LYS	CB-CA-C	5.05	118.11	109.72

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	10360	0	10329	142	0
2	A	60	0	90	8	0
3	A	5	0	5	0	0
4	A	27	0	12	1	0
5	A	10	0	7	2	0
6	A	4	0	0	0	0
7	A	90	0	0	1	0
8	A	114	0	151	22	0
9	A	1474	0	0	56	0
All	All	12144	0	10594	155	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 7.

All (155) 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)
2:A:1608:EDO:H11	9:A:2845:HOH:O	1.74	0.84
1:A:75:LEU:HD23	9:A:1736:HOH:O	1.77	0.84
1:A:747:PRO:HA	8:A:1644:GOL:H31	1.58	0.82
1:A:296[B]:HIS:CE1	9:A:1854:HOH:O	2.33	0.82
1:A:820:SER:H	1:A:930:GLN:HE22	1.29	0.80
1:A:108:ARG:HE	8:A:1647:GOL:C3	1.95	0.80
1:A:175:ASN:HD21	1:A:182:LEU:H	1.28	0.80
1:A:144[A]:THR:HG23	9:A:1788:HOH:O	1.81	0.78
1:A:329[B]:LYS:HG3	9:A:1999:HOH:O	1.83	0.77
1:A:545:ASN:HD22	1:A:547:SER:H	1.33	0.77
1:A:108:ARG:HE	8:A:1647:GOL:H31	1.49	0.76
1:A:368:GLU:HG3	2:A:1610:EDO:H22	1.65	0.76
1:A:907[B]:VAL:CG1	1:A:966[B]:ILE:HD13	2.16	0.76
1:A:215:GLU:HA	9:A:1723:HOH:O	1.86	0.75
1:A:907[B]:VAL:HG13	1:A:966[B]:ILE:HD13	1.67	0.75
1:A:346:GLU:HG2	9:A:3050:HOH:O	1.87	0.75
1:A:824:ASN:HD21	1:A:958:ALA:H	1.33	0.74
1:A:75:LEU:CD2	9:A:1736:HOH:O	2.34	0.73
1:A:275:HIS:HD2	9:A:2961:HOH:O	1.69	0.73
1:A:922:ASN:HD22	1:A:924:GLU:H	1.35	0.72
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.54	0.72
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.73	0.71
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.71	0.71
1:A:723:ILE:O	1:A:726[A]:THR:HG23	1.92	0.70
1:A:96:HIS:HE1	1:A:103:VAL:O	1.75	0.69
1:A:215:GLU:H	8:A:1656:GOL:H2	1.58	0.69
1:A:783[B]:THR:HG21	9:A:2789:HOH:O	1.92	0.69
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.76	0.69
1:A:791:GLN:NE2	9:A:1704:HOH:O	2.25	0.69
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.40	0.69
1:A:1266[A]:ARG:NE	9:A:1706:HOH:O	2.26	0.68
1:A:329[B]:LYS:CG	9:A:1999:HOH:O	2.40	0.68
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.78	0.67
1:A:1251:ASN:HD22	1:A:1253[A]:ARG:H	1.41	0.66
1:A:907[B]:VAL:CG1	1:A:966[B]:ILE:CD1	2.73	0.66
1:A:1251:ASN:HD22	1:A:1253[B]:ARG:H	1.41	0.66
1:A:471:GLN:HE21	1:A:472:ARG:H	1.42	0.64
2:A:1602:EDO:C2	9:A:2879:HOH:O	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:CYS:SG	5:A:1618:GLN:CD	2.81	0.64
1:A:1072[B]:MET:HE2	9:A:2829:HOH:O	1.97	0.63
1:A:860:VAL:HB	8:A:1642:GOL:H12	1.81	0.62
1:A:1221:ARG:HH21	8:A:1651:GOL:C1	2.13	0.62
1:A:1145[B]:ARG:HG2	9:A:1744:HOH:O	1.99	0.62
1:A:907[B]:VAL:HG13	1:A:966[B]:ILE:CD1	2.30	0.61
1:A:1251:ASN:ND2	1:A:1253[A]:ARG:H	1.97	0.61
1:A:1251:ASN:ND2	1:A:1253[B]:ARG:H	1.97	0.61
1:A:465:LEU:HB2	1:A:467[B]:PHE:CE2	2.35	0.61
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.84	0.60
8:A:1644:GOL:H32	9:A:2980:HOH:O	2.01	0.60
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.09	0.60
1:A:108:ARG:HE	8:A:1647:GOL:H32	1.67	0.60
2:A:1602:EDO:H22	9:A:2879:HOH:O	2.02	0.59
1:A:499:PHE:CD2	1:A:515[B]:LEU:HD12	2.37	0.59
1:A:136[A]:MET:HE3	9:A:1800:HOH:O	2.01	0.59
1:A:120:THR:H	1:A:123:GLN:HE21	1.50	0.58
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.02	0.58
8:A:1647:GOL:C1	9:A:1745:HOH:O	2.50	0.58
1:A:412[A]:MET:SD	9:A:2537:HOH:O	2.57	0.57
1:A:782:LYS:CE	1:A:793:GLU:CD	2.78	0.57
1:A:284[B]:GLN:HG2	9:A:1709:HOH:O	2.03	0.57
2:A:1602:EDO:H21	9:A:2879:HOH:O	2.02	0.57
1:A:465:LEU:HB2	1:A:467[B]:PHE:CZ	2.40	0.56
1:A:1206:ASP:HB3	9:A:2825:HOH:O	2.05	0.56
1:A:1076:LEU:HD21	9:A:1765:HOH:O	2.03	0.56
1:A:680:CYS:SG	1:A:726[A]:THR:HG21	2.46	0.56
1:A:499:PHE:HA	9:A:2187:HOH:O	2.06	0.56
1:A:2[B]:MET:HE1	1:A:146:ALA:HB3	1.88	0.54
1:A:657[A]:ASP:OD2	1:A:660:VAL:HG12	2.07	0.54
8:A:1653:GOL:H11	9:A:2927:HOH:O	2.07	0.54
1:A:298:HIS:HE1	1:A:469:SER:OG	1.90	0.54
5:A:1618:GLN:NE2	9:A:1717:HOH:O	2.39	0.54
1:A:-7:GLY:O	1:A:3:GLU:HA	2.08	0.54
1:A:787:GLU:HG2	1:A:792[B]:ARG:HD2	1.90	0.54
1:A:877[B]:ARG:NH1	9:A:1713:HOH:O	2.35	0.53
1:A:251:TYR:H	8:A:1653:GOL:C3	2.21	0.53
1:A:298:HIS:CD2	9:A:2732:HOH:O	2.61	0.53
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.91	0.53
1:A:39:HIS:HD2	9:A:2101:HOH:O	1.91	0.53
1:A:447:GLY:HA2	1:A:468:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767[B]:GLN:NE2	9:A:1724:HOH:O	2.42	0.53
1:A:219:HIS:N	9:A:1721:HOH:O	2.43	0.52
1:A:329[B]:LYS:O	1:A:383:PRO:HD2	2.10	0.52
1:A:864[A]:LYS:HD3	9:A:2263:HOH:O	2.10	0.51
1:A:219:HIS:N	9:A:1723:HOH:O	2.43	0.50
1:A:108:ARG:NE	8:A:1647:GOL:H31	2.23	0.50
1:A:907[B]:VAL:HG11	1:A:966[B]:ILE:CD1	2.41	0.50
1:A:2[B]:MET:HE3	1:A:40:PHE:CD1	2.47	0.49
1:A:251:TYR:H	8:A:1653:GOL:H32	1.77	0.49
1:A:545:ASN:ND2	1:A:547:SER:H	2.06	0.49
1:A:767[B]:GLN:CD	9:A:1724:HOH:O	2.55	0.49
1:A:1045[A]:LEU:HD11	1:A:1072[A]:MET:SD	2.52	0.49
1:A:296[A]:HIS:HD2	1:A:307:GLY:O	1.95	0.49
1:A:873:LEU:CD2	1:A:942[B]:LEU:HD23	2.43	0.49
1:A:335:PHE:CE1	1:A:412[B]:MET:SD	3.06	0.49
1:A:354:GLY:O	1:A:408:HIS:HE1	1.95	0.49
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.48	0.49
1:A:877[B]:ARG:HH11	1:A:877[B]:ARG:HG3	1.78	0.48
1:A:175:ASN:ND2	1:A:180:LEU:HB2	2.27	0.48
1:A:216:HIS:C	9:A:1721:HOH:O	2.56	0.48
1:A:1072[B]:MET:CE	9:A:2829:HOH:O	2.58	0.48
1:A:108:ARG:HB3	8:A:1647:GOL:H32	1.96	0.47
1:A:329[B]:LYS:NZ	1:A:419:ASN:HD21	2.12	0.47
1:A:782:LYS:CE	1:A:793:GLU:CG	2.92	0.47
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.12	0.47
1:A:1006:HIS:HE1	9:A:1965:HOH:O	1.97	0.47
1:A:1266[A]:ARG:CZ	9:A:1706:HOH:O	2.62	0.47
8:A:1654:GOL:H32	9:A:1741:HOH:O	2.14	0.47
1:A:216:HIS:HE1	7:A:1633[B]:SO4:O2	1.97	0.47
1:A:1006:HIS:HD2	9:A:2304:HOH:O	1.98	0.47
1:A:1266[A]:ARG:NH2	9:A:1706:HOH:O	2.47	0.47
1:A:298:HIS:CE1	1:A:469:SER:OG	2.67	0.46
1:A:782:LYS:HE3	1:A:793:GLU:HG2	1.98	0.46
1:A:338:SER:OG	1:A:408:HIS:HD2	1.98	0.45
1:A:1104[B]:GLU:OE2	1:A:1143[B]:ASN:OD1	2.33	0.45
1:A:585:HIS:CE1	1:A:599:ASP:OD1	2.65	0.45
1:A:1018:ASN:CB	8:A:1655:GOL:H2	2.45	0.45
1:A:96:HIS:CE1	1:A:103:VAL:O	2.64	0.44
1:A:279:ARG:CZ	9:A:2491:HOH:O	2.65	0.44
1:A:873:LEU:HD21	1:A:942[B]:LEU:HD23	2.00	0.44
1:A:219:HIS:HD2	1:A:777:ASP:OD1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:GLN:HG2	4:A:1617:ADP:H1'	2.01	0.43
1:A:1018:ASN:HB3	8:A:1655:GOL:H2	2.01	0.43
1:A:767[B]:GLN:CG	9:A:1724:HOH:O	2.66	0.43
1:A:1000[B]:GLN:OE1	9:A:1702:HOH:O	2.21	0.43
1:A:283:HIS:CE1	9:A:2398:HOH:O	2.71	0.43
1:A:402:GLU:HG3	9:A:2567:HOH:O	2.18	0.43
1:A:860:VAL:CB	8:A:1642:GOL:H12	2.48	0.43
1:A:623:GLY:HA3	1:A:852[A]:ASP:HA	2.01	0.43
1:A:368:GLU:HG3	2:A:1610:EDO:C2	2.43	0.42
1:A:1019[A]:VAL:HG12	1:A:1021:LEU:HG	2.01	0.42
1:A:782:LYS:NZ	1:A:793:GLU:CD	2.78	0.42
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.38	0.42
1:A:218:ARG:HD2	9:A:2934:HOH:O	2.19	0.42
1:A:1221:ARG:HH21	8:A:1651:GOL:H12	1.83	0.41
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.20	0.41
1:A:96:HIS:HD2	9:A:1728:HOH:O	2.04	0.41
1:A:936:ARG:HH22	2:A:1602:EDO:C1	2.33	0.41
2:A:1601:EDO:H21	9:A:2242:HOH:O	2.19	0.41
8:A:1647:GOL:H12	9:A:1745:HOH:O	2.16	0.41
1:A:339:ASN:HB3	1:A:350:GLU:OE2	2.21	0.41
1:A:499:PHE:HD2	1:A:515[B]:LEU:HD12	1.85	0.41
1:A:619[B]:LEU:HD13	8:A:1644:GOL:O3	2.21	0.41
1:A:782:LYS:HE2	1:A:793:GLU:CG	2.50	0.41
1:A:787:GLU:HB3	1:A:792[B]:ARG:HG3	2.02	0.41
1:A:34:TYR:HE2	9:A:2778:HOH:O	2.03	0.41
1:A:444:MET:HE1	1:A:472:ARG:CZ	2.51	0.41
1:A:891:LEU:C	1:A:891:LEU:HD13	2.46	0.41
1:A:275:HIS:HE1	9:A:2964:HOH:O	2.04	0.40
1:A:596:GLN:HG2	1:A:599:ASP:HB2	2.03	0.40
8:A:1650:GOL:H32	9:A:1871:HOH:O	2.20	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	1364/1305 (104%)	1324 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1103/1041 (106%)	1083 (98%)	20 (2%)	51	36

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	104	ASP
1	A	119	LEU
1	A	296[A]	HIS
1	A	296[B]	HIS
1	A	471	GLN
1	A	596	GLN
1	A	726[A]	THR
1	A	726[B]	THR
1	A	782	LYS
1	A	1136	ASN
1	A	1144[A]	LEU
1	A	1144[B]	LEU
1	A	1190[A]	MET
1	A	1190[B]	MET
1	A	1194	VAL
1	A	1195[A]	SER
1	A	1195[B]	SER
1	A	1251	ASN
1	A	1276	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	39	HIS
1	A	96	HIS
1	A	101	GLN
1	A	123	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	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	585	HIS
1	A	739	ASN
1	A	746	HIS
1	A	824	ASN
1	A	883	HIS
1	A	906	GLN
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS
1	A	1293	GLN

5.3.3 RNA ⓘ

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 59 ligands modelled in this entry, 4 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	$\# Z > 2$
2	EDO	A	1614	-	3,3,3	0.74	0	2,2,2	0.58	0
7	SO4	A	1637	-	4,4,4	0.67	0	6,6,6	0.75	0
2	EDO	A	1604	-	3,3,3	0.57	0	2,2,2	0.61	0
2	EDO	A	1613	-	3,3,3	0.56	0	2,2,2	0.15	0
8	GOL	A	1646	-	5,5,5	1.03	0	5,5,5	0.56	0
8	GOL	A	1655	-	5,5,5	0.70	0	5,5,5	1.01	0
2	EDO	A	1602	-	3,3,3	0.43	0	2,2,2	1.27	0
2	EDO	A	1603	-	3,3,3	0.30	0	2,2,2	0.71	0
7	SO4	A	1634	-	4,4,4	0.84	0	6,6,6	0.67	0
7	SO4	A	1623	-	4,4,4	0.20	0	6,6,6	0.86	0
7	SO4	A	1626	-	4,4,4	0.31	0	6,6,6	1.17	0
8	GOL	A	1641[B]	-	5,5,5	0.54	0	5,5,5	0.79	0
7	SO4	A	1633[B]	-	4,4,4	0.33	0	6,6,6	1.14	1 (16%)
7	SO4	A	1638	-	4,4,4	0.60	0	6,6,6	0.40	0
7	SO4	A	1629	-	4,4,4	0.55	0	6,6,6	0.98	0
7	SO4	A	1628	-	4,4,4	0.67	0	6,6,6	0.22	0
8	GOL	A	1656	-	5,5,5	0.53	0	5,5,5	1.33	1 (20%)
2	EDO	A	1616	-	3,3,3	0.64	0	2,2,2	0.18	0
2	EDO	A	1612	-	3,3,3	0.36	0	2,2,2	1.51	0
2	EDO	A	1610	-	3,3,3	0.46	0	2,2,2	0.99	0
2	EDO	A	1601	-	3,3,3	0.55	0	2,2,2	0.93	0
7	SO4	A	1627	-	4,4,4	0.45	0	6,6,6	1.23	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	1647	-	5,5,5	2.71	2 (40%)	5,5,5	3.32	2 (40%)
7	SO4	A	1625	-	4,4,4	0.29	0	6,6,6	0.91	0
8	GOL	A	1649[B]	-	5,5,5	0.53	0	5,5,5	0.50	0
7	SO4	A	1630	-	4,4,4	0.59	0	6,6,6	0.74	0
8	GOL	A	1648	-	5,5,5	1.28	1 (20%)	5,5,5	1.58	1 (20%)
8	GOL	A	1645	-	5,5,5	1.14	0	5,5,5	1.27	1 (20%)
7	SO4	A	1636	-	4,4,4	0.51	0	6,6,6	0.58	0
8	GOL	A	1641[A]	-	5,5,5	1.08	0	5,5,5	0.66	0
7	SO4	A	1633[A]	-	4,4,4	0.36	0	6,6,6	0.34	0
8	GOL	A	1640	-	5,5,5	0.98	0	5,5,5	1.29	1 (20%)
7	SO4	A	1639	-	4,4,4	0.58	0	6,6,6	0.33	0
2	EDO	A	1607	-	3,3,3	0.92	0	2,2,2	0.39	0
7	SO4	A	1632	-	4,4,4	1.08	0	6,6,6	0.84	0
8	GOL	A	1643	-	5,5,5	0.75	0	5,5,5	1.07	0
8	GOL	A	1653	-	5,5,5	0.71	0	5,5,5	1.51	0
7	SO4	A	1635	-	4,4,4	0.77	0	6,6,6	0.45	0
8	GOL	A	1644	-	5,5,5	0.38	0	5,5,5	0.64	0
4	ADP	A	1617	6	28,29,29	1.23	3 (10%)	43,45,45	1.13	3 (6%)
8	GOL	A	1649[A]	-	5,5,5	0.63	0	5,5,5	2.05	3 (60%)
5	GLN	A	1618	-	8,9,9	0.65	0	8,11,11	1.02	1 (12%)
7	SO4	A	1631	-	4,4,4	0.63	0	6,6,6	0.64	0
3	IMD	A	1611	-	5,5,5	0.44	0	5,5,5	0.62	0
2	EDO	A	1605	-	3,3,3	0.74	0	2,2,2	0.47	0
8	GOL	A	1651	-	5,5,5	2.61	3 (60%)	5,5,5	5.32	4 (80%)
8	GOL	A	1652	-	5,5,5	0.64	0	5,5,5	0.94	0
8	GOL	A	1642	-	5,5,5	1.60	1 (20%)	5,5,5	1.70	1 (20%)
8	GOL	A	1654	-	5,5,5	0.22	0	5,5,5	0.29	0
8	GOL	A	1650	-	5,5,5	0.37	0	5,5,5	0.74	0
2	EDO	A	1615	-	3,3,3	0.59	0	2,2,2	0.24	0
2	EDO	A	1609	-	3,3,3	0.43	0	2,2,2	0.50	0
2	EDO	A	1606	-	3,3,3	0.29	0	2,2,2	0.45	0
7	SO4	A	1624	-	4,4,4	0.71	0	6,6,6	0.49	0
2	EDO	A	1608	-	3,3,3	0.57	0	2,2,2	0.31	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
2	EDO	A	1614	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1604	-	-	1/1/1/1	-
2	EDO	A	1613	-	-	1/1/1/1	-
8	GOL	A	1646	-	-	0/4/4/4	-
8	GOL	A	1655	-	-	3/4/4/4	-
2	EDO	A	1602	-	-	1/1/1/1	-
2	EDO	A	1603	-	-	0/1/1/1	-
8	GOL	A	1641[B]	-	-	0/4/4/4	-
8	GOL	A	1656	-	-	2/4/4/4	-
2	EDO	A	1616	-	-	1/1/1/1	-
2	EDO	A	1612	-	-	0/1/1/1	-
2	EDO	A	1610	-	-	1/1/1/1	-
2	EDO	A	1601	-	-	1/1/1/1	-
8	GOL	A	1647	-	-	1/4/4/4	-
8	GOL	A	1649[B]	-	-	2/4/4/4	-
8	GOL	A	1648	-	-	2/4/4/4	-
8	GOL	A	1645	-	-	0/4/4/4	-
8	GOL	A	1641[A]	-	-	0/4/4/4	-
8	GOL	A	1640	-	-	0/4/4/4	-
2	EDO	A	1607	-	-	1/1/1/1	-
8	GOL	A	1653	-	-	2/4/4/4	-
8	GOL	A	1643	-	-	0/4/4/4	-
8	GOL	A	1644	-	-	2/4/4/4	-
4	ADP	A	1617	6	-	1/16/32/32	0/3/3/3
8	GOL	A	1649[A]	-	-	0/4/4/4	-
5	GLN	A	1618	-	-	1/9/9/9	-
8	GOL	A	1651	-	-	2/4/4/4	-
2	EDO	A	1605	-	-	1/1/1/1	-
8	GOL	A	1652	-	-	0/4/4/4	-
3	IMD	A	1611	-	-	-	0/1/1/1
8	GOL	A	1642	-	-	0/4/4/4	-
8	GOL	A	1654	-	-	3/4/4/4	-
8	GOL	A	1650	-	-	2/4/4/4	-
2	EDO	A	1615	-	-	0/1/1/1	-
2	EDO	A	1609	-	-	0/1/1/1	-
2	EDO	A	1606	-	-	1/1/1/1	-
2	EDO	A	1608	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1647	GOL	O2-C2	5.23	1.58	1.43
8	A	1651	GOL	O2-C2	4.14	1.55	1.43
8	A	1642	GOL	O1-C1	-3.16	1.29	1.42
8	A	1651	GOL	C3-C2	2.96	1.63	1.51
4	A	1617	ADP	C4-N9	-2.93	1.31	1.37
4	A	1617	ADP	C5-C4	2.92	1.44	1.39
8	A	1651	GOL	O3-C3	2.62	1.53	1.42
8	A	1648	GOL	C1-C2	2.50	1.61	1.51
8	A	1647	GOL	O3-C3	2.29	1.52	1.42
4	A	1617	ADP	C2-N3	2.04	1.37	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1651	GOL	O2-C2-C1	-6.54	82.09	109.18
8	A	1651	GOL	O2-C2-C3	6.50	136.08	109.18
8	A	1647	GOL	O3-C3-C2	6.36	139.00	110.38
8	A	1651	GOL	O3-C3-C2	5.88	136.83	110.38
8	A	1651	GOL	O1-C1-C2	4.48	130.53	110.38
8	A	1647	GOL	O2-C2-C1	2.81	120.83	109.18
8	A	1649[A]	GOL	O3-C3-C2	-2.79	97.82	110.38
4	A	1617	ADP	O2A-PA-O1A	2.76	125.27	112.44
8	A	1642	GOL	O2-C2-C3	2.57	119.84	109.18
4	A	1617	ADP	C4-C5-N7	-2.54	107.68	110.58
8	A	1656	GOL	O1-C1-C2	2.41	121.25	110.38
8	A	1649[A]	GOL	O2-C2-C3	-2.40	99.26	109.18
7	A	1627	SO4	O3-S-O1	2.37	121.96	109.56
7	A	1633[B]	SO4	O3-S-O2	-2.32	97.44	109.56
4	A	1617	ADP	C4-N9-C8	2.15	108.00	105.74
8	A	1640	GOL	C3-C2-C1	2.14	119.65	111.80
5	A	1618	GLN	OXT-C-O	-2.11	119.30	124.08
8	A	1648	GOL	O2-C2-C1	2.10	117.88	109.18
8	A	1645	GOL	O3-C3-C2	-2.09	100.96	110.38
8	A	1649[A]	GOL	O2-C2-C1	2.04	117.64	109.18

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1644	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	1644	GOL	O1-C1-C2-C3
8	A	1648	GOL	O1-C1-C2-C3
8	A	1649[B]	GOL	C1-C2-C3-O3
8	A	1651	GOL	C1-C2-C3-O3
8	A	1654	GOL	O1-C1-C2-C3
8	A	1655	GOL	O1-C1-C2-O2
8	A	1655	GOL	O1-C1-C2-C3
8	A	1656	GOL	C1-C2-C3-O3
8	A	1650	GOL	O1-C1-C2-C3
8	A	1651	GOL	O1-C1-C2-C3
8	A	1653	GOL	C1-C2-C3-O3
2	A	1601	EDO	O1-C1-C2-O2
2	A	1602	EDO	O1-C1-C2-O2
2	A	1605	EDO	O1-C1-C2-O2
2	A	1608	EDO	O1-C1-C2-O2
8	A	1648	GOL	O1-C1-C2-O2
8	A	1654	GOL	O1-C1-C2-O2
2	A	1607	EDO	O1-C1-C2-O2
2	A	1613	EDO	O1-C1-C2-O2
2	A	1616	EDO	O1-C1-C2-O2
8	A	1649[B]	GOL	O2-C2-C3-O3
8	A	1656	GOL	O2-C2-C3-O3
8	A	1653	GOL	O2-C2-C3-O3
8	A	1654	GOL	O2-C2-C3-O3
8	A	1655	GOL	O2-C2-C3-O3
5	A	1618	GLN	CA-CB-CG-CD
8	A	1650	GOL	O1-C1-C2-O2
4	A	1617	ADP	PA-O3A-PB-O1B
2	A	1610	EDO	O1-C1-C2-O2
2	A	1604	EDO	O1-C1-C2-O2
8	A	1647	GOL	O1-C1-C2-O2
2	A	1606	EDO	O1-C1-C2-O2
2	A	1614	EDO	O1-C1-C2-O2

There are no ring outliers.

16 monomers are involved in 34 short contacts:

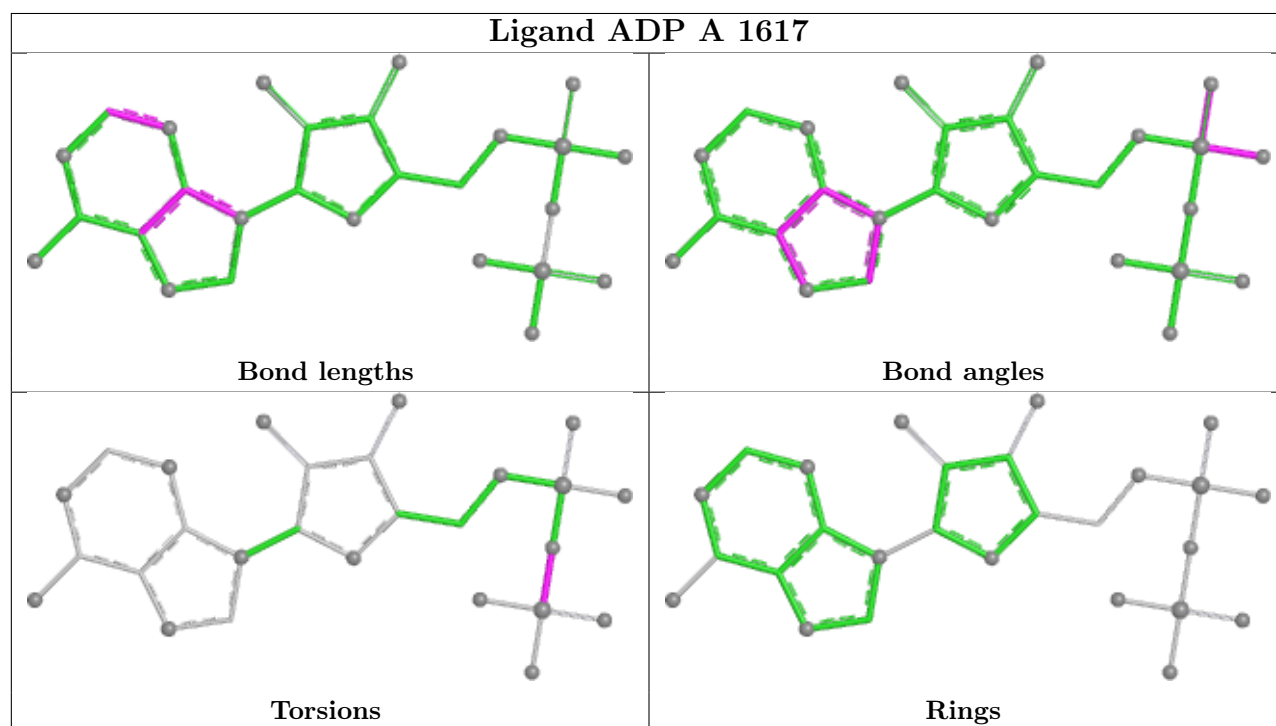
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1655	GOL	2	0
2	A	1602	EDO	4	0
7	A	1633[B]	SO4	1	0
8	A	1656	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1610	EDO	2	0
2	A	1601	EDO	1	0
8	A	1647	GOL	7	0
8	A	1653	GOL	3	0
8	A	1644	GOL	3	0
4	A	1617	ADP	1	0
5	A	1618	GLN	2	0
8	A	1651	GOL	2	0
8	A	1642	GOL	2	0
8	A	1654	GOL	1	0
8	A	1650	GOL	1	0
2	A	1608	EDO	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	1293/1305 (99%)	-0.26	25 (1%) 66 71	7, 17, 37, 68	75 (5%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-9	ALA	6.5
1	A	-7	GLY	6.3
1	A	-5	VAL	5.0
1	A	451	GLY	4.3
1	A	-8	SER	4.1
1	A	450	GLY	4.1
1	A	-6	LEU	4.0
1	A	789	ASN	4.0
1	A	-4	PRO	3.9
1	A	465	LEU	3.4
1	A	464	ASP	3.3
1	A	-1	SER	2.8
1	A	259	ASN	2.6
1	A	-3	ARG	2.6
1	A	788	GLY	2.5
1	A	67	SER	2.5
1	A	449	GLY	2.5
1	A	-2	GLY	2.3
1	A	448	LEU	2.3
1	A	118	THR	2.3
1	A	22	ARG	2.2
1	A	152	HIS	2.1
1	A	428	GLY	2.1
1	A	6	ARG	2.1
1	A	623	GLY	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	SO4	A	1639	5/5	0.67	0.20	88,99,114,128	0
2	EDO	A	1613	4/4	0.70	0.31	56,59,70,72	0
2	EDO	A	1614	4/4	0.71	0.22	58,60,60,72	0
2	EDO	A	1615	4/4	0.72	0.30	67,69,78,83	0
2	EDO	A	1601	4/4	0.77	0.21	52,55,55,56	0
7	SO4	A	1637	5/5	0.78	0.13	55,65,80,86	0
8	GOL	A	1646	6/6	0.79	0.17	33,37,41,42	0
8	GOL	A	1650	6/6	0.79	0.15	44,45,51,51	0
8	GOL	A	1656	6/6	0.79	0.18	44,51,55,64	0
2	EDO	A	1616	4/4	0.80	0.16	46,46,51,56	0
8	GOL	A	1655	6/6	0.80	0.20	49,53,57,65	0
2	EDO	A	1607	4/4	0.80	0.17	42,43,50,51	0
2	EDO	A	1606	4/4	0.81	0.20	46,48,52,58	0
2	EDO	A	1610	4/4	0.81	0.17	40,48,49,49	0
8	GOL	A	1644	6/6	0.82	0.16	24,37,42,47	1
2	EDO	A	1609	4/4	0.83	0.20	47,63,64,64	0
3	IMD	A	1611	5/5	0.84	0.17	46,55,58,65	0
2	EDO	A	1608	4/4	0.84	0.17	32,39,41,48	0
7	SO4	A	1638	5/5	0.84	0.11	57,67,79,80	0
8	GOL	A	1653	6/6	0.85	0.15	37,43,49,50	0
8	GOL	A	1654	6/6	0.85	0.16	46,59,60,81	0
8	GOL	A	1647	6/6	0.85	0.15	28,34,43,46	0
8	GOL	A	1652	6/6	0.85	0.18	30,51,55,62	0
2	EDO	A	1602	4/4	0.86	0.15	33,37,42,43	0
7	SO4	A	1636	5/5	0.86	0.11	70,71,85,85	0
8	GOL	A	1649[A]	6/6	0.86	0.15	21,30,33,35	6
8	GOL	A	1649[B]	6/6	0.86	0.15	30,35,37,39	6

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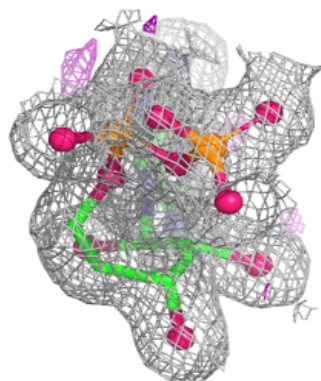
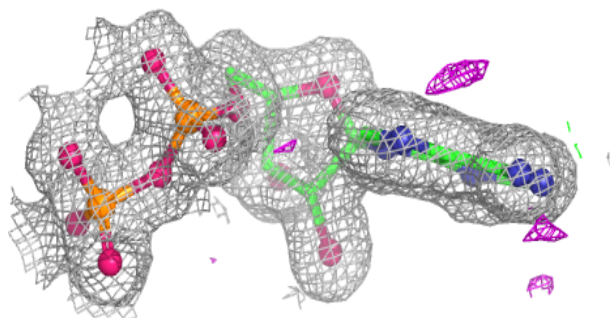
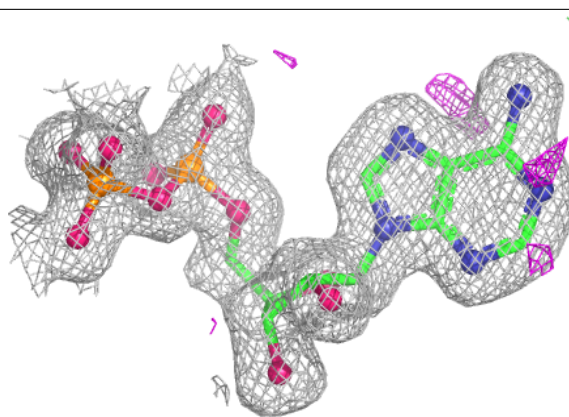
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	1612	4/4	0.86	0.15	34,44,51,54	0
7	SO4	A	1635	5/5	0.89	0.11	45,47,50,55	1
2	EDO	A	1605	4/4	0.89	0.15	37,42,45,52	0
7	SO4	A	1633[B]	5/5	0.90	0.14	27,28,31,33	5
8	GOL	A	1645	6/6	0.90	0.11	31,35,40,40	0
7	SO4	A	1633[A]	5/5	0.90	0.14	35,37,42,44	5
7	SO4	A	1634	5/5	0.92	0.09	34,39,43,45	1
8	GOL	A	1651	6/6	0.92	0.11	27,32,36,36	0
2	EDO	A	1604	4/4	0.92	0.13	33,38,40,43	0
8	GOL	A	1641[A]	6/6	0.92	0.12	20,25,26,27	6
8	GOL	A	1641[B]	6/6	0.92	0.12	21,29,32,33	6
8	GOL	A	1642	6/6	0.92	0.11	24,33,43,43	0
8	GOL	A	1643	6/6	0.92	0.12	21,25,27,30	1
2	EDO	A	1603	4/4	0.94	0.14	24,37,47,50	0
7	SO4	A	1625	5/5	0.94	0.10	28,32,40,45	1
8	GOL	A	1648	6/6	0.94	0.11	18,22,29,37	0
7	SO4	A	1626	5/5	0.95	0.12	26,26,37,42	1
7	SO4	A	1630	5/5	0.96	0.06	33,35,44,44	0
8	GOL	A	1640	6/6	0.96	0.08	19,22,29,31	0
7	SO4	A	1632	5/5	0.96	0.09	21,27,30,39	1
7	SO4	A	1629	5/5	0.96	0.08	25,28,35,37	1
7	SO4	A	1627	5/5	0.97	0.07	24,24,29,32	1
5	GLN	A	1618	10/10	0.97	0.06	12,13,16,16	2
6	MG	A	1622	1/1	0.97	0.06	31,31,31,31	0
7	SO4	A	1631	5/5	0.97	0.06	36,36,47,48	0
7	SO4	A	1628	5/5	0.98	0.06	29,34,40,41	0
7	SO4	A	1623	5/5	0.98	0.05	16,19,21,24	1
7	SO4	A	1624	5/5	0.99	0.04	22,24,25,29	0
6	MG	A	1621	1/1	0.99	0.01	12,12,12,12	0
4	ADP	A	1617	27/27	0.99	0.03	11,12,14,14	0
6	MG	A	1619	1/1	0.99	0.02	13,13,13,13	0
6	MG	A	1620	1/1	1.00	0.01	13,13,13,13	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 1617:

$2mF_o-DF_c$ (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.