WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 06:52 PM JST

PDB ID	:	6JTA
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)

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

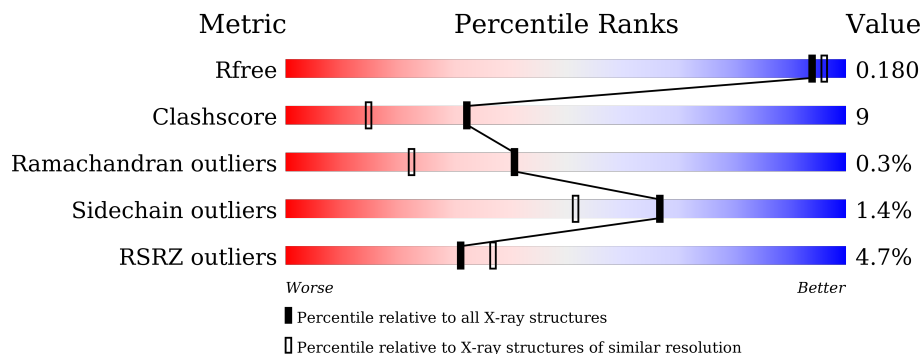|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.180
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		1.4%
RSRZ outliers		4.7%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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	5% ■ / 89% / 9% •

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	-
5	EDO	A	1319	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 Phosphoribosylformylglycinamidine 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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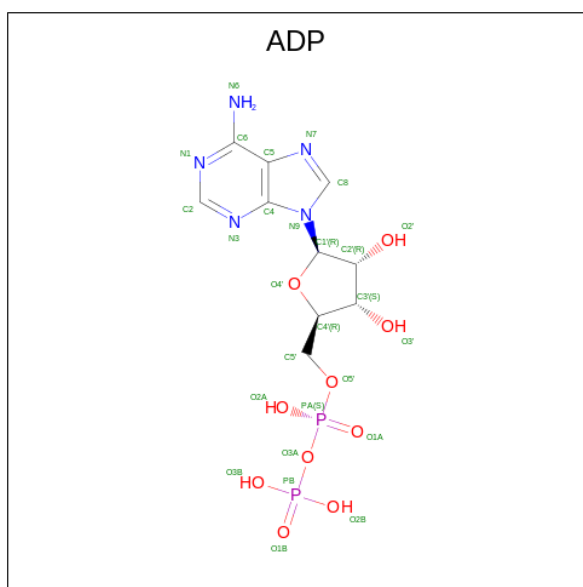
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).

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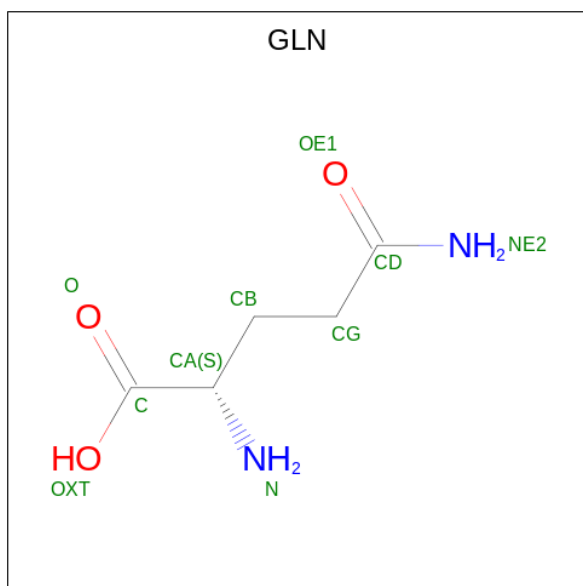
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	5	2	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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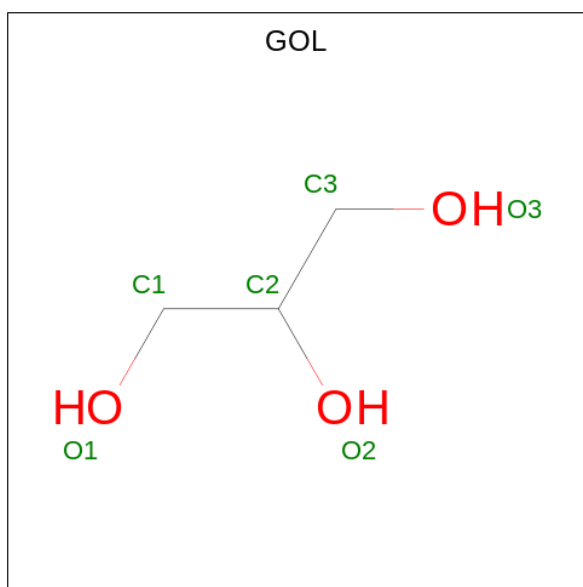
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1

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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- 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: Phosphoribosylformylglycinamidine synthase
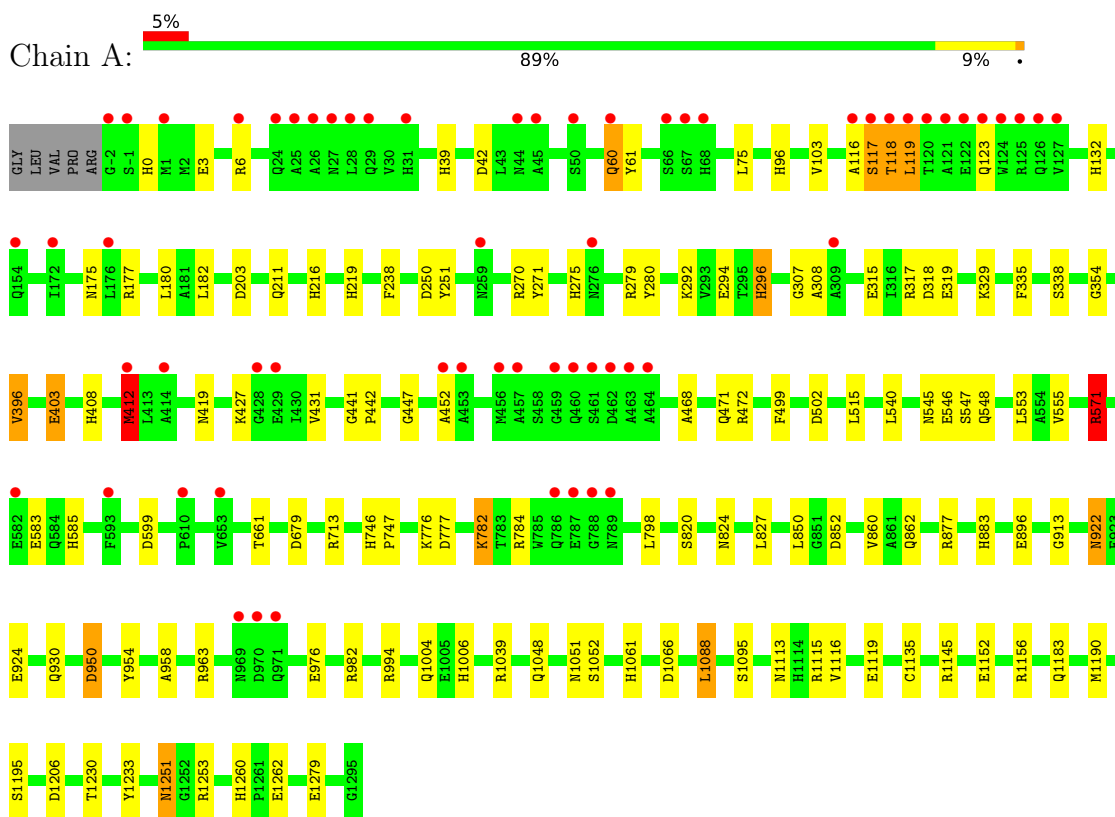
4 Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [1]	3.25 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.151 , 0.181 0.155 , 0.180	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)	0.35 , 40.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, MG, SO4, GOL, EDO

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	1.17	6/10438 (0.1%)	1.08	8/14168 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1119	GLU	CD-OE2	-6.45	1.18	1.25
1	A	403	GLU	CD-OE2	-5.81	1.19	1.25
1	A	571[A]	ARG	CA-C	5.36	1.66	1.52
1	A	571[B]	ARG	CA-C	5.36	1.66	1.52
1	A	412[A]	MET	CA-C	5.21	1.66	1.52
1	A	412[B]	MET	CA-C	5.21	1.66	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1156	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	1088	LEU	CA-CB-CG	7.57	132.71	115.30
1	A	412[A]	MET	CG-SD-CE	6.70	110.93	100.20
1	A	412[B]	MET	CG-SD-CE	6.70	110.93	100.20
1	A	994	ARG	CG-CD-NE	-5.71	99.81	111.80
1	A	203	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	950	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	1156	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	157	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	56	0
6	A	3	0	0	0	0
7	A	90	0	0	0	0
8	A	1204	0	0	57	0
All	All	11632	0	10212	182	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 (182) 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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1135:CYS:SG	3:A:1302:GLN:CD	2.69	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
1:A:412[A]:MET:HE1	8:A:2219:HOH:O	1.95	0.67
5:A:1323:EDO:H21	8:A:1652:HOH:O	1.94	0.66
1:A:412[A]:MET:CE	8:A:2219:HOH:O	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:308:ALA:O	1:A:412[A]:MET:HE3	2.07	0.54
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:335:PHE:CE1	1:A:412[B]:MET:CE	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:540:LEU:C	1:A:540:LEU:HD23	2.32	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:784[A]:ARG:NH2	5:A:1330:EDO:O1	2.38	0.47
1:A:412[A]:MET:HE2	8:A:2219:HOH:O	2.11	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
1:A:747:PRO:HA	4:A:1305:GOL:H12	1.96	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:308:ALA:HA	1:A:412[A]:MET:HE3	1.98	0.45
1:A:96:HIS:CE1	1:A:103:VAL:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:396[A]:VAL:CG1	1:A:850:LEU:HD22	2.46	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
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.23	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:827:LEU:HD23	1:A:954:TYR:HA	2.02	0.41
1:A:1135:CYS:SG	3:A:1302:GLN:OE1	2.77	0.41
1:A:1113:ASN:HD21	1:A:1115:ARG:HB3	1.85	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
1:A:318:ASP:OD2	1:A:502[B]:ASP:CG	2.59	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1330/1303 (102%)	1293 (97%)	33 (2%)	4 (0%)	41	22

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 ⓘ

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%)	1043 (98%)	17 (2%)	62	45

All (17) 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	412[A]	MET
1	A	412[B]	MET

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Mol	Chain	Res	Type
1	A	571[A]	ARG
1	A	571[B]	ARG
1	A	782	LYS
1	A	922	ASN
1	A	982	ARG
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 (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	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	233	GLN
1	A	243	ASN
1	A	275	HIS
1	A	296	HIS
1	A	298	HIS
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	674	GLN
1	A	739	ASN
1	A	746	HIS
1	A	818	GLN
1	A	824	ASN
1	A	862	GLN
1	A	883	HIS

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Mol	Chain	Res	Type
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	1026	ASN
1	A	1061	HIS
1	A	1113	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
7	SO4	A	1351	-	4,4,4	0.79	0	6,6,6	1.26	1 (16%)
3	GLN	A	1302	-	8,9,9	1.35	1 (12%)	10,11,11	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	GOL	A	1311	-	5,5,5	0.81	0	5,5,5	1.23	0
5	EDO	A	1316	-	3,3,3	0.63	0	2,2,2	0.26	0
4	GOL	A	1304	-	5,5,5	1.13	0	5,5,5	0.96	0
5	EDO	A	1317	-	3,3,3	0.61	0	2,2,2	0.17	0
7	SO4	A	1346	-	4,4,4	0.67	0	6,6,6	1.35	1 (16%)
7	SO4	A	1341	-	4,4,4	0.89	0	6,6,6	0.83	0
4	GOL	A	1314	-	5,5,5	0.48	0	5,5,5	0.75	0
7	SO4	A	1347	-	4,4,4	0.43	0	6,6,6	1.04	0
5	EDO	A	1315	-	3,3,3	0.86	0	2,2,2	0.25	0
5	EDO	A	1319	-	3,3,3	0.76	0	2,2,2	1.91	1 (50%)
7	SO4	A	1344	-	4,4,4	0.38	0	6,6,6	1.10	1 (16%)
5	EDO	A	1333	-	3,3,3	0.35	0	2,2,2	0.37	0
5	EDO	A	1334	-	3,3,3	0.33	0	2,2,2	0.10	0
7	SO4	A	1353	-	4,4,4	0.27	0	6,6,6	0.64	0
5	EDO	A	1328	-	3,3,3	0.39	0	2,2,2	0.49	0
4	GOL	A	1308	-	5,5,5	0.55	0	5,5,5	1.10	0
5	EDO	A	1332	-	3,3,3	0.28	0	2,2,2	0.93	0
7	SO4	A	1342	-	4,4,4	0.45	0	6,6,6	0.56	0
5	EDO	A	1324	-	3,3,3	0.74	0	2,2,2	0.69	0
5	EDO	A	1329	-	3,3,3	0.22	0	2,2,2	0.68	0
7	SO4	A	1352	-	4,4,4	0.87	0	6,6,6	0.60	0
4	GOL	A	1331	-	5,5,5	1.15	1 (20%)	5,5,5	0.94	0
7	SO4	A	1350	-	4,4,4	1.09	1 (25%)	6,6,6	1.51	1 (16%)
4	GOL	A	1306	-	5,5,5	0.83	0	5,5,5	2.84	3 (60%)
5	EDO	A	1323	-	3,3,3	0.25	0	2,2,2	0.18	0
7	SO4	A	1354	-	4,4,4	0.51	0	6,6,6	0.64	0
7	SO4	A	1356	-	4,4,4	0.39	0	6,6,6	0.40	0
5	EDO	A	1330	-	3,3,3	0.27	0	2,2,2	0.28	0
7	SO4	A	1348	-	4,4,4	0.96	0	6,6,6	1.02	0
7	SO4	A	1355	-	4,4,4	0.41	0	6,6,6	0.60	0
7	SO4	A	1349	-	4,4,4	0.54	0	6,6,6	0.64	0
7	SO4	A	1343	-	4,4,4	0.73	0	6,6,6	1.44	1 (16%)
5	EDO	A	1313	-	3,3,3	0.42	0	2,2,2	0.39	0
4	GOL	A	1303	-	5,5,5	0.61	0	5,5,5	1.11	0
4	GOL	A	1307	-	5,5,5	0.46	0	5,5,5	1.25	0
5	EDO	A	1336	-	3,3,3	0.37	0	2,2,2	0.44	0
5	EDO	A	1322	-	3,3,3	0.30	0	2,2,2	1.10	0
5	EDO	A	1321	-	3,3,3	0.45	0	2,2,2	1.04	0
7	SO4	A	1358	-	4,4,4	0.39	0	6,6,6	0.64	0
4	GOL	A	1335	-	5,5,5	0.59	0	5,5,5	1.19	1 (20%)
5	EDO	A	1327	-	3,3,3	0.30	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	EDO	A	1326	-	3,3,3	0.62	0	2,2,2	0.16	0
5	EDO	A	1318	-	3,3,3	0.70	0	2,2,2	1.15	0
5	EDO	A	1312	-	3,3,3	0.28	0	2,2,2	0.20	0
7	SO4	A	1345	-	4,4,4	0.34	0	6,6,6	0.80	0
2	ADP	A	1301	6	24,29,29	1.36	5 (20%)	29,45,45	1.17	2 (6%)
5	EDO	A	1337	-	3,3,3	0.22	0	2,2,2	0.27	0
4	GOL	A	1309	-	5,5,5	0.53	0	5,5,5	0.62	0
4	GOL	A	1310	-	5,5,5	0.44	0	5,5,5	0.82	0
4	GOL	A	1305	-	5,5,5	1.24	1 (20%)	5,5,5	1.48	1 (20%)
5	EDO	A	1325	-	3,3,3	0.41	0	2,2,2	0.36	0
7	SO4	A	1357	-	4,4,4	0.69	0	6,6,6	0.38	0
5	EDO	A	1320	-	3,3,3	0.64	0	2,2,2	0.23	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	GLN	A	1302	-	-	1/9/9/9	-
4	GOL	A	1311	-	-	4/4/4/4	-
5	EDO	A	1316	-	-	1/1/1/1	-
4	GOL	A	1304	-	-	2/4/4/4	-
5	EDO	A	1317	-	-	1/1/1/1	-
4	GOL	A	1314	-	-	2/4/4/4	-
5	EDO	A	1315	-	-	1/1/1/1	-
5	EDO	A	1319	-	-	0/1/1/1	-
5	EDO	A	1333	-	-	0/1/1/1	-
5	EDO	A	1334	-	-	1/1/1/1	-
5	EDO	A	1328	-	-	0/1/1/1	-
4	GOL	A	1308	-	-	0/4/4/4	-
5	EDO	A	1332	-	-	1/1/1/1	-
5	EDO	A	1324	-	-	1/1/1/1	-
5	EDO	A	1329	-	-	0/1/1/1	-
4	GOL	A	1331	-	-	2/4/4/4	-
4	GOL	A	1306	-	-	0/4/4/4	-
5	EDO	A	1323	-	-	0/1/1/1	-
5	EDO	A	1330	-	-	1/1/1/1	-
5	EDO	A	1313	-	-	1/1/1/1	-
4	GOL	A	1303	-	-	1/4/4/4	-
4	GOL	A	1307	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1336	-	-	1/1/1/1	-
5	EDO	A	1322	-	-	1/1/1/1	-
5	EDO	A	1321	-	-	1/1/1/1	-
4	GOL	A	1335	-	-	2/4/4/4	-
5	EDO	A	1327	-	-	0/1/1/1	-
5	EDO	A	1326	-	-	1/1/1/1	-
5	EDO	A	1318	-	-	0/1/1/1	-
5	EDO	A	1312	-	-	1/1/1/1	-
2	ADP	A	1301	6	-	2/12/32/32	0/3/3/3
5	EDO	A	1337	-	-	1/1/1/1	-
4	GOL	A	1309	-	-	3/4/4/4	-
4	GOL	A	1310	-	-	2/4/4/4	-
4	GOL	A	1305	-	-	2/4/4/4	-
5	EDO	A	1325	-	-	1/1/1/1	-
5	EDO	A	1320	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1302	GLN	OXT-C	-3.24	1.19	1.30
2	A	1301	ADP	C2-N3	2.89	1.36	1.32
4	A	1305	GOL	O2-C2	-2.51	1.35	1.43
2	A	1301	ADP	C2'-C1'	2.49	1.57	1.53
2	A	1301	ADP	C8-N7	-2.47	1.30	1.34
2	A	1301	ADP	PA-O1A	-2.20	1.43	1.50
4	A	1331	GOL	O2-C2	-2.11	1.37	1.43
2	A	1301	ADP	O4'-C1'	2.08	1.44	1.41
7	A	1350	SO4	O2-S	2.04	1.57	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1306	GOL	O2-C2-C3	-4.88	87.65	109.12
2	A	1301	ADP	O4'-C1'-C2'	-3.28	102.13	106.93
4	A	1306	GOL	O3-C3-C2	-3.26	94.58	110.20
5	A	1319	EDO	O1-C1-C2	2.61	130.70	111.91
7	A	1343	SO4	O3-S-O1	2.57	122.71	109.31
7	A	1350	SO4	O4-S-O1	2.36	121.63	109.31
2	A	1301	ADP	O3B-PB-O2B	2.34	116.60	107.64
7	A	1346	SO4	O4-S-O3	-2.31	99.20	109.06
7	A	1351	SO4	O4-S-O2	2.31	121.35	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1335	GOL	O1-C1-C2	2.28	121.13	110.20
4	A	1305	GOL	C3-C2-C1	2.22	120.33	111.70
7	A	1344	SO4	O4-S-O2	2.16	120.60	109.31
4	A	1306	GOL	C3-C2-C1	2.14	120.02	111.70

There are no chirality outliers.

All (40) 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	1312	EDO	O1-C1-C2-O2
5	A	1313	EDO	O1-C1-C2-O2
5	A	1315	EDO	O1-C1-C2-O2
5	A	1322	EDO	O1-C1-C2-O2
5	A	1325	EDO	O1-C1-C2-O2
5	A	1337	EDO	O1-C1-C2-O2
5	A	1316	EDO	O1-C1-C2-O2
5	A	1321	EDO	O1-C1-C2-O2
4	A	1309	GOL	O2-C2-C3-O3
5	A	1317	EDO	O1-C1-C2-O2
5	A	1320	EDO	O1-C1-C2-O2
3	A	1302	GLN	CA-CB-CG-CD
4	A	1314	GOL	O2-C2-C3-O3
4	A	1314	GOL	O1-C1-C2-C3
5	A	1324	EDO	O1-C1-C2-O2
5	A	1330	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1334	EDO	O1-C1-C2-O2
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
4	A	1303	GOL	O1-C1-C2-C3

There are no ring outliers.

25 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1302	GLN	4	0
5	A	1316	EDO	2	0
4	A	1304	GOL	2	0
5	A	1317	EDO	1	0
4	A	1314	GOL	1	0
5	A	1315	EDO	1	0
5	A	1319	EDO	6	0
5	A	1333	EDO	2	0
5	A	1328	EDO	7	0
4	A	1308	GOL	3	0
5	A	1332	EDO	3	0
5	A	1324	EDO	2	0
4	A	1331	GOL	2	0
4	A	1306	GOL	2	0
5	A	1323	EDO	13	0
5	A	1330	EDO	1	0
4	A	1307	GOL	1	0
5	A	1336	EDO	2	0
4	A	1335	GOL	3	0
5	A	1312	EDO	7	0
5	A	1337	EDO	3	0
4	A	1309	GOL	2	0
4	A	1310	GOL	3	0
4	A	1305	GOL	2	0
5	A	1325	EDO	9	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 then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1301

Bond lengths

Bond angles

Torsions

Rings
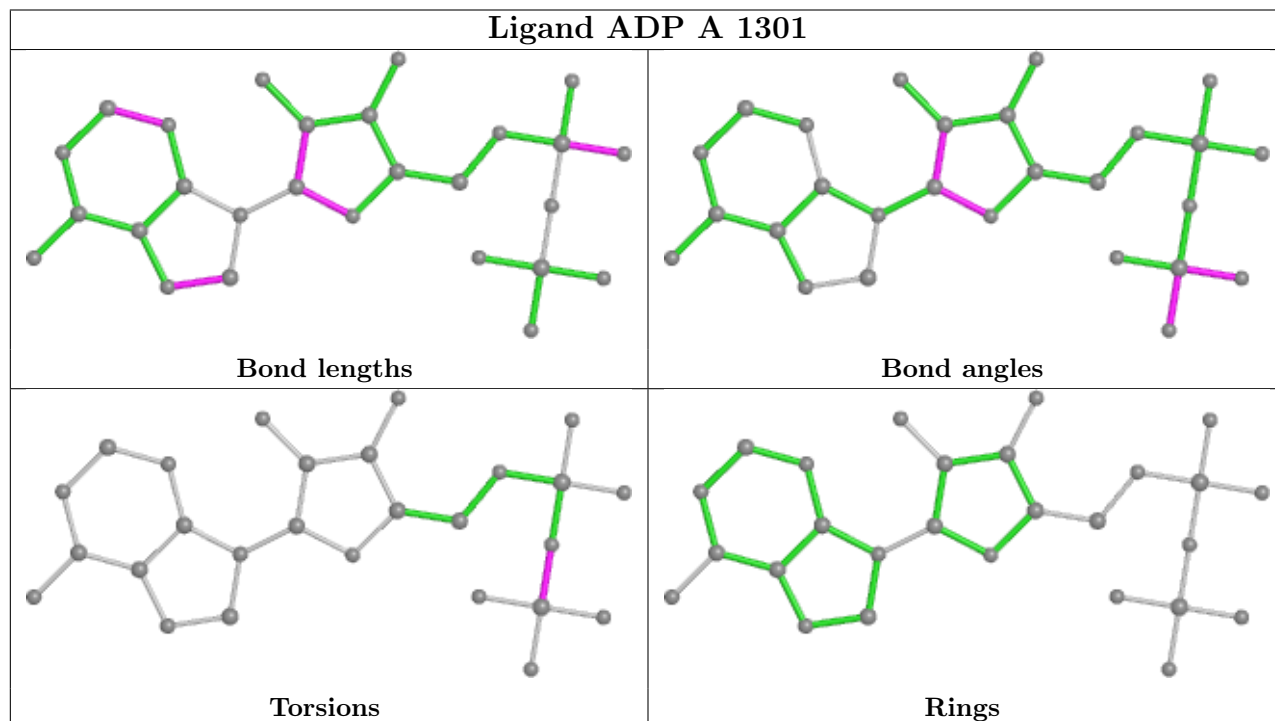
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	1298/1303 (99%)	0.26	61 (4%)	31	37	13, 20, 42, 72	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	7.0
1	A	117	SER	5.6
1	A	119	LEU	5.3
1	A	463	ALA	5.1
1	A	-1	SER	4.9
1	A	120	THR	4.9
1	A	461	SER	4.7
1	A	460	GLN	4.6
1	A	121	ALA	4.6
1	A	789	ASN	4.6
1	A	-2	GLY	4.4
1	A	25	ALA	4.3
1	A	176	LEU	4.2
1	A	122	GLU	4.1
1	A	66	SER	4.0
1	A	27	ASN	3.9
1	A	788	GLY	3.9
1	A	116	ALA	3.6
1	A	1	MET	3.6
1	A	462	ASP	3.6
1	A	28	LEU	3.4
1	A	459	GLY	3.4
1	A	154	GLN	3.4
1	A	123	GLN	3.3
1	A	464	ALA	3.3
1	A	31	HIS	3.0
1	A	969	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	29	GLN	2.9
1	A	309	ALA	2.8
1	A	24	GLN	2.8
1	A	429	GLU	2.7
1	A	787	GLU	2.6
1	A	276	ASN	2.6
1	A	68	HIS	2.6
1	A	124	TRP	2.6
1	A	259	ASN	2.6
1	A	60	GLN	2.6
1	A	125	ARG	2.5
1	A	970	ASP	2.5
1	A	786	GLN	2.4
1	A	428	GLY	2.4
1	A	457	ALA	2.4
1	A	593	PHE	2.4
1	A	50	SER	2.4
1	A	610	PRO	2.3
1	A	126	GLN	2.3
1	A	653	VAL	2.3
1	A	412[A]	MET	2.3
1	A	45	ALA	2.3
1	A	414	ALA	2.3
1	A	582	GLU	2.2
1	A	127	VAL	2.2
1	A	172	ILE	2.2
1	A	452	ALA	2.2
1	A	456	MET	2.1
1	A	67	SER	2.1
1	A	26	ALA	2.1
1	A	971	GLN	2.1
1	A	6	ARG	2.1
1	A	453	ALA	2.1
1	A	44	ASN	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 monosaccharides 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.
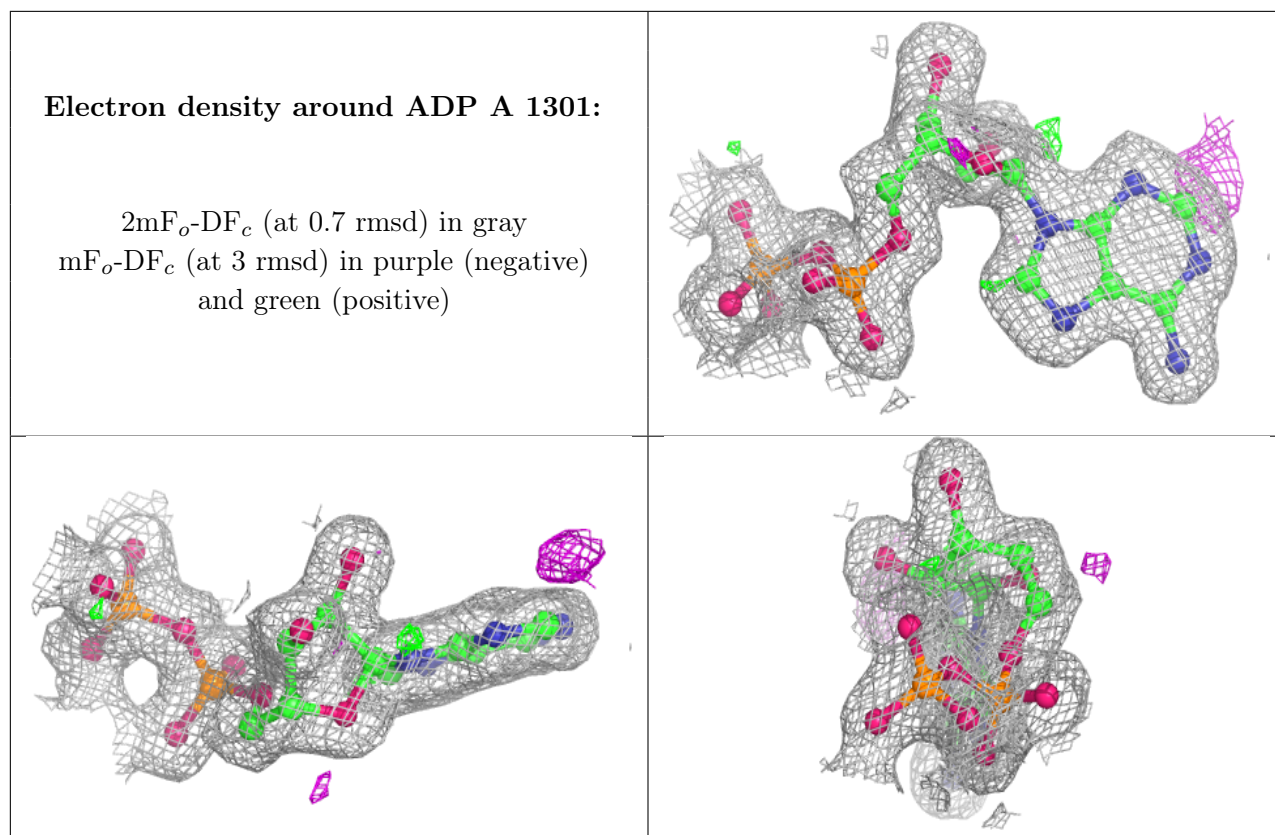
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	EDO	A	1336	4/4	0.64	0.31	51,62,62,66	0
5	EDO	A	1333	4/4	0.66	0.37	45,56,60,73	0
5	EDO	A	1320	4/4	0.70	0.21	57,58,61,62	0
5	EDO	A	1324	4/4	0.70	0.29	47,49,53,59	0
4	GOL	A	1307	6/6	0.73	0.19	34,47,57,61	0
5	EDO	A	1317	4/4	0.73	0.19	44,51,54,55	0
5	EDO	A	1337	4/4	0.73	0.34	60,67,68,73	0
4	GOL	A	1308	6/6	0.74	0.21	40,46,54,55	0
4	GOL	A	1335	6/6	0.74	0.16	33,48,52,53	0
4	GOL	A	1311	6/6	0.76	0.16	36,42,54,57	0
5	EDO	A	1327	4/4	0.76	0.32	56,68,71,76	0
5	EDO	A	1332	4/4	0.76	0.13	48,50,59,65	0
4	GOL	A	1309	6/6	0.78	0.24	40,65,69,75	0
5	EDO	A	1325	4/4	0.78	0.17	42,55,61,63	0
5	EDO	A	1326	4/4	0.78	0.39	47,58,58,66	0
5	EDO	A	1321	4/4	0.78	0.20	44,49,50,50	0
4	GOL	A	1314	6/6	0.80	0.17	25,36,39,42	0
5	EDO	A	1334	4/4	0.81	0.37	58,59,61,63	0
5	EDO	A	1323	4/4	0.82	0.21	44,52,53,71	0
4	GOL	A	1303	6/6	0.82	0.18	23,24,38,41	0
5	EDO	A	1329	4/4	0.82	0.17	61,62,64,67	0
5	EDO	A	1322	4/4	0.82	0.11	48,55,57,58	0
5	EDO	A	1330	4/4	0.83	0.10	60,61,64,65	0
4	GOL	A	1310	6/6	0.83	0.29	38,61,63,64	0
5	EDO	A	1315	4/4	0.83	0.19	35,36,37,52	0
5	EDO	A	1318	4/4	0.86	0.28	39,39,45,53	0
5	EDO	A	1328	4/4	0.87	0.19	38,52,54,56	0
5	EDO	A	1316	4/4	0.87	0.26	39,42,42,44	0
5	EDO	A	1313	4/4	0.88	0.18	37,47,47,60	0
4	GOL	A	1306	6/6	0.89	0.11	30,39,45,47	0
4	GOL	A	1304	6/6	0.90	0.23	27,45,54,65	0
7	SO4	A	1355	5/5	0.90	0.31	59,84,93,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	1319	4/4	0.91	0.17	36,38,41,42	0
3	GLN	A	1302	10/10	0.91	0.12	13,16,18,19	2
5	EDO	A	1312	4/4	0.92	0.20	42,44,45,65	0
7	SO4	A	1356	5/5	0.92	0.27	68,74,80,93	0
4	GOL	A	1305	6/6	0.93	0.20	29,37,44,53	0
7	SO4	A	1357	5/5	0.93	0.43	64,73,79,81	0
7	SO4	A	1358	5/5	0.93	0.34	66,79,86,95	0
7	SO4	A	1352	5/5	0.94	0.34	39,49,53,56	0
7	SO4	A	1354	5/5	0.94	0.28	68,68,73,76	0
4	GOL	A	1331	6/6	0.94	0.14	20,28,33,36	0
7	SO4	A	1348	5/5	0.95	0.19	25,32,38,39	0
7	SO4	A	1353	5/5	0.96	0.22	54,62,72,74	0
7	SO4	A	1350	5/5	0.96	0.10	35,35,45,47	0
7	SO4	A	1351	5/5	0.97	0.20	29,37,41,43	0
2	ADP	A	1301	27/27	0.97	0.09	12,14,15,16	0
7	SO4	A	1349	5/5	0.97	0.24	40,44,49,54	0
7	SO4	A	1346	5/5	0.97	0.08	33,34,46,58	0
7	SO4	A	1347	5/5	0.98	0.18	30,38,44,44	0
7	SO4	A	1342	5/5	0.98	0.10	21,26,27,31	0
7	SO4	A	1343	5/5	0.98	0.12	32,36,38,44	0
7	SO4	A	1344	5/5	0.98	0.08	27,36,40,47	0
7	SO4	A	1345	5/5	0.98	0.24	38,39,47,52	0
6	MG	A	1340	1/1	0.98	0.07	15,15,15,15	0
7	SO4	A	1341	5/5	0.99	0.05	21,21,24,25	0
6	MG	A	1339	1/1	0.99	0.08	15,15,15,15	0
6	MG	A	1338	1/1	0.99	0.05	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:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.