Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 06:44 PM JST

PDB ID	:	6JT9
Title	:	Crystal Structure of D464A mutant of FGAM Synthetase
Authors	:	Sharma, N.; Ahalawat, N.; Sandhu, P.; Mondal, J.; Anand, R.
Deposited on	:	2019-04-10
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

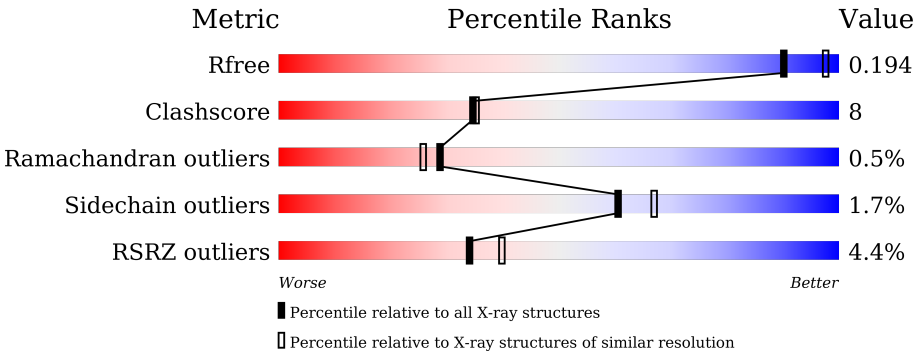
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	1305	4% 87% 11% ••

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
3	SO4	A	1314	-	X	-	-
5	GOL	A	1320	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1321	-	X	-	-
5	GOL	A	1322	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11047 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	1286	Total	C	N	O	S	0	26	0
			10051	6316	1785	1899	51			

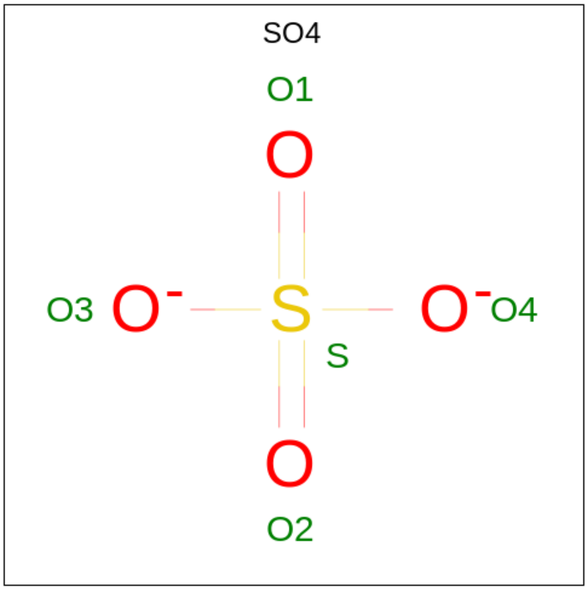
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-8	SER	-	expression tag	UNP A0A0D6F9Y3
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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

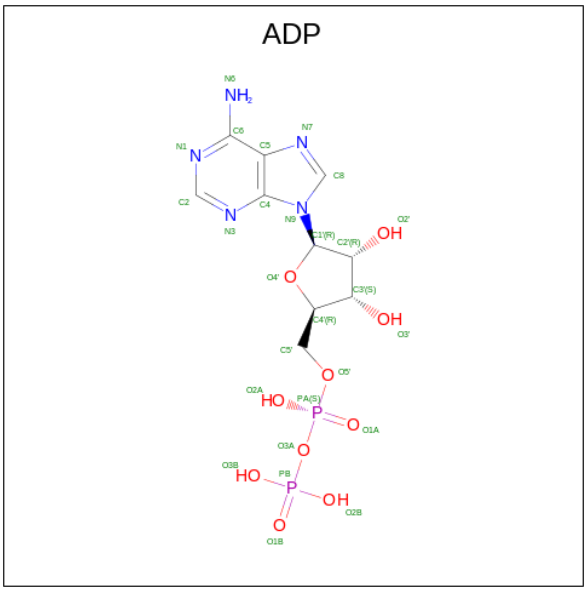
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



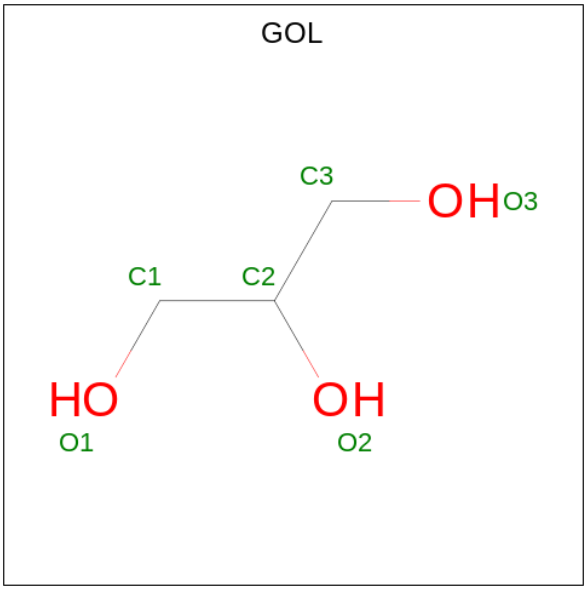
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

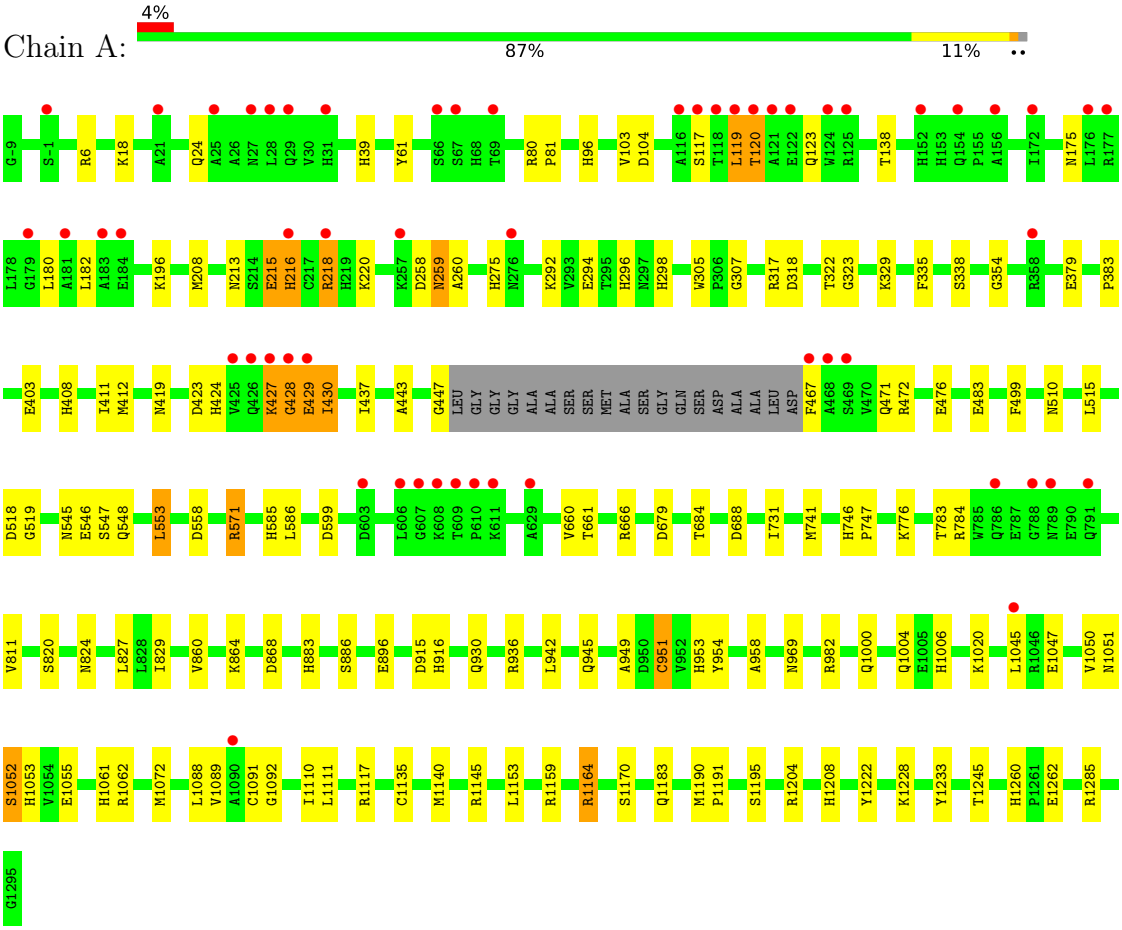
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	855	Total O 855 855	0	0

3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	146.46Å 146.46Å 141.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.52 – 2.10 32.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.52-2.10) 100.0 (32.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.145 , 0.189 0.158 , 0.194	Depositor DCC
R_{free} test set	5004 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11047	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, SO4, GOL, MG, CL, CYG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.94	2/10300 (0.0%)	0.92	10/13978 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	951	CYS	CB-SG	-5.32	1.73	1.81
1	A	1091	CYS	CB-SG	-5.14	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	688	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	216	HIS	N-CA-C	-6.31	93.96	111.00
1	A	666	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	868	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	215	GLU	N-CA-C	-5.46	96.27	111.00
1	A	119	LEU	N-CA-C	5.37	125.50	111.00
1	A	558	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	660	VAL	C-N-CA	5.24	134.81	121.70
1	A	18	LYS	CD-CE-NZ	5.18	123.61	111.70
1	A	1164	ARG	NE-CZ-NH1	5.11	122.86	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	10051	0	9843	163	0
2	A	3	0	0	0	0
3	A	60	0	0	1	0
4	A	27	0	12	0	0
5	A	48	0	64	19	0
6	A	3	0	0	0	0
7	A	855	0	0	47	0
All	All	11047	0	9919	166	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 8.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:HIS:HB3	7:A:1414:HOH:O	1.32	1.23
5:A:1322:GOL:H31	7:A:1973:HOH:O	1.48	1.13
1:A:1045[B]:LEU:HD11	1:A:1072[B]:MET:CE	1.79	1.12
1:A:1159:ARG:HH22	5:A:1320:GOL:H2	1.16	1.07
1:A:1045[A]:LEU:HD12	1:A:1088[A]:LEU:HD21	1.33	1.05
1:A:1045[A]:LEU:CD1	1:A:1088[A]:LEU:HD21	1.92	0.98
1:A:215:GLU:HB2	1:A:220:LYS:HE3	1.46	0.97
1:A:1204[B]:ARG:H	1:A:1208[B]:HIS:HD2	1.03	0.97
1:A:120:THR:HG22	1:A:123:GLN:HE21	1.29	0.95
1:A:1204[B]:ARG:H	1:A:1208[B]:HIS:CD2	1.85	0.95
1:A:747:PRO:HD3	5:A:1324:GOL:H2	1.52	0.92
1:A:1052:SER:HB3	7:A:1412:HOH:O	1.67	0.91
1:A:1062:ARG:HA	5:A:1322:GOL:H32	1.54	0.89
1:A:942:LEU:HG	7:A:2015:HOH:O	1.74	0.86
1:A:1045[B]:LEU:HD11	1:A:1072[B]:MET:HE1	1.59	0.85
1:A:824:ASN:HD21	1:A:958:ALA:H	1.24	0.84
1:A:820:SER:H	1:A:930:GLN:HE22	1.27	0.83
1:A:1045[B]:LEU:HD11	1:A:1072[B]:MET:HE2	1.63	0.81
1:A:120:THR:HG23	1:A:123:GLN:H	1.47	0.80
1:A:81:PRO:HD3	1:A:138[A]:THR:HG21	1.63	0.79
1:A:1045[B]:LEU:HD21	7:A:1427:HOH:O	1.83	0.77
1:A:437:ILE:HB	1:A:553:LEU:HD12	1.66	0.77
1:A:305:TRP:CD1	7:A:1401:HOH:O	2.39	0.75
1:A:215:GLU:HG2	1:A:220:LYS:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412[B]:MET:SD	7:A:2064:HOH:O	2.47	0.73
1:A:215:GLU:HB2	1:A:220:LYS:CE	2.18	0.73
1:A:96:HIS:HE1	1:A:103:VAL:O	1.71	0.72
1:A:1055:GLU:HB2	7:A:1571:HOH:O	1.89	0.72
1:A:437:ILE:HB	1:A:553:LEU:CD1	2.20	0.71
1:A:80:ARG:HA	1:A:138[B]:THR:HG23	1.73	0.70
1:A:259:ASN:ND2	1:A:259:ASN:H	1.90	0.70
1:A:218:ARG:HG2	1:A:220:LYS:HG3	1.74	0.69
1:A:1045[A]:LEU:HD12	1:A:1088[A]:LEU:CD2	2.18	0.69
1:A:784:ARG:NH2	5:A:1324:GOL:H31	2.09	0.68
1:A:499[B]:PHE:CD2	1:A:515:LEU:HD12	2.29	0.68
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.75	0.67
1:A:1045[A]:LEU:CD1	1:A:1088[A]:LEU:CD2	2.70	0.67
1:A:829:ILE:HG23	7:A:2115:HOH:O	1.95	0.67
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.78	0.66
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:CG	2.26	0.65
1:A:1204[B]:ARG:N	1:A:1208[B]:HIS:HD2	1.86	0.65
1:A:335:PHE:CE1	1:A:412[A]:MET:SD	2.90	0.64
1:A:954:TYR:CD2	5:A:1323:GOL:H2	2.32	0.64
1:A:429:GLU:N	1:A:499[A]:PHE:HE1	1.95	0.64
1:A:429:GLU:OE2	1:A:429:GLU:HA	1.96	0.64
1:A:467:PHE:N	7:A:1404:HOH:O	2.31	0.64
1:A:545:ASN:HD22	1:A:547:SER:H	1.46	0.63
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.81	0.63
1:A:936:ARG:HH22	5:A:1323:GOL:H11	1.64	0.62
1:A:292:LYS:HE3	7:A:1799:HOH:O	2.00	0.62
1:A:215:GLU:CG	1:A:220:LYS:HB2	2.30	0.61
1:A:429:GLU:N	1:A:499[A]:PHE:CE1	2.68	0.61
1:A:1088[A]:LEU:HD23	1:A:1089:VAL:N	2.16	0.61
1:A:215:GLU:CB	1:A:220:LYS:HE3	2.26	0.61
1:A:305:TRP:HD1	7:A:1401:HOH:O	1.79	0.59
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:HD11	1.84	0.59
1:A:1159:ARG:NH2	5:A:1320:GOL:H2	2.02	0.58
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.68	0.58
1:A:275:HIS:HD2	7:A:2202:HOH:O	1.86	0.58
1:A:259:ASN:HD22	1:A:260:ALA:H	1.50	0.58
1:A:218:ARG:CG	1:A:220:LYS:HG3	2.34	0.58
1:A:258:ASP:OD2	1:A:259:ASN:ND2	2.37	0.58
1:A:1183:GLN:HE22	1:A:1285:ARG:HH21	1.51	0.57
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.87	0.57
1:A:1062:ARG:HB2	5:A:1322:GOL:H12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:ILE:HD11	7:A:1427:HOH:O	2.05	0.57
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:HD21	1.83	0.56
1:A:428:GLY:C	1:A:499[A]:PHE:CZ	2.80	0.55
1:A:1204[B]:ARG:N	1:A:1208[B]:HIS:CD2	2.66	0.55
1:A:81:PRO:CD	1:A:138[A]:THR:HG21	2.36	0.54
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.91	0.53
1:A:949:ALA:N	7:A:1416:HOH:O	2.42	0.53
1:A:969:ASN:HA	7:A:1418:HOH:O	2.07	0.53
1:A:1051:ASN:HB3	7:A:1408:HOH:O	2.09	0.53
1:A:1061:HIS:ND1	5:A:1322:GOL:H11	2.24	0.52
1:A:427:LYS:HB2	1:A:499[A]:PHE:CE2	2.45	0.52
1:A:510:ASN:HB2	7:A:2080:HOH:O	2.09	0.52
1:A:39:HIS:CE1	1:A:61:TYR:OH	2.61	0.52
1:A:81:PRO:HD3	1:A:138[A]:THR:CG2	2.38	0.52
1:A:471:GLN:HE21	1:A:472:ARG:H	1.58	0.51
1:A:1164:ARG:HD3	5:A:1320:GOL:O3	2.09	0.51
1:A:215:GLU:HG2	1:A:220:LYS:H	1.75	0.51
1:A:951:CYS:HB2	7:A:2115:HOH:O	2.11	0.51
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:CD1	2.40	0.51
1:A:1051:ASN:ND2	7:A:1408:HOH:O	2.43	0.51
1:A:96:HIS:CE1	1:A:103:VAL:O	2.58	0.50
1:A:954:TYR:HD2	5:A:1323:GOL:H2	1.73	0.50
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.93	0.50
1:A:969:ASN:ND2	7:A:1418:HOH:O	2.43	0.50
1:A:354:GLY:O	1:A:408:HIS:HE1	1.94	0.50
1:A:499[B]:PHE:HD2	1:A:515:LEU:HD12	1.75	0.50
1:A:1228:LYS:HB3	7:A:2136:HOH:O	2.12	0.50
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.95	0.49
1:A:1020:LYS:HE2	7:A:2191:HOH:O	2.12	0.49
1:A:39:HIS:HD2	7:A:1524:HOH:O	1.95	0.49
1:A:294:GLU:OE2	1:A:318:ASP:OD1	2.31	0.49
1:A:969:ASN:CA	7:A:1418:HOH:O	2.61	0.49
1:A:80:ARG:HA	1:A:138[A]:THR:HG22	1.95	0.49
1:A:296:HIS:HD2	1:A:307:GLY:O	1.95	0.49
1:A:175:ASN:HD21	1:A:182:LEU:H	1.60	0.48
1:A:731:ILE:HG21	1:A:864[B]:LYS:HE2	1.94	0.48
1:A:259:ASN:HD21	1:A:322:THR:HA	1.77	0.48
1:A:1153:LEU:O	1:A:1208[B]:HIS:HE1	1.97	0.48
1:A:218:ARG:HG2	1:A:220:LYS:CG	2.42	0.48
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:CD2	2.40	0.48
1:A:1072[B]:MET:HE2	1:A:1072[B]:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HE3	1:A:419:ASN:ND2	2.28	0.48
1:A:208[B]:MET:HE2	1:A:586:LEU:CD2	2.44	0.47
1:A:1006:HIS:HE1	7:A:1456:HOH:O	1.98	0.47
1:A:429:GLU:C	7:A:1469:HOH:O	2.53	0.47
1:A:953:HIS:ND1	3:A:1311:SO4:O4	2.33	0.47
1:A:120:THR:HG22	1:A:123:GLN:NE2	2.13	0.47
1:A:1050:VAL:HG13	1:A:1092:GLY:O	2.14	0.47
1:A:1062:ARG:CA	5:A:1322:GOL:H12	2.45	0.46
1:A:215:GLU:HG2	1:A:220:LYS:CB	2.43	0.46
1:A:1000:GLN:NE2	7:A:1428:HOH:O	2.47	0.46
1:A:379:GLU:HG3	7:A:1725:HOH:O	2.14	0.46
1:A:428:GLY:C	1:A:499[A]:PHE:CE1	2.90	0.45
1:A:447:GLY:HA2	1:A:546:GLU:HB2	1.97	0.45
1:A:427:LYS:HG3	1:A:499[B]:PHE:CE1	2.52	0.45
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.15	0.45
1:A:80:ARG:HA	1:A:138[B]:THR:CG2	2.44	0.45
1:A:1006:HIS:HD2	7:A:1771:HOH:O	1.99	0.45
1:A:323:GLY:HA3	1:A:424:HIS:O	2.17	0.45
1:A:1020:LYS:CE	7:A:2191:HOH:O	2.64	0.45
1:A:1045[A]:LEU:HD11	1:A:1088[A]:LEU:HG	1.97	0.45
1:A:298:HIS:HD2	7:A:2192:HOH:O	1.98	0.44
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	1.99	0.44
1:A:1159:ARG:HH22	5:A:1320:GOL:C2	2.07	0.44
1:A:329:LYS:O	1:A:383:PRO:HD2	2.17	0.44
1:A:915:ASP:HB3	5:A:1317:GOL:H31	1.99	0.44
1:A:6:ARG:CB	7:A:2082:HOH:O	2.64	0.44
1:A:942:LEU:CG	7:A:2015:HOH:O	2.46	0.44
1:A:430:ILE:HG12	1:A:499[A]:PHE:CD1	2.53	0.44
1:A:860:VAL:HB	5:A:1319:GOL:H2	2.00	0.43
1:A:684:THR:HG22	1:A:811:VAL:HG21	2.00	0.43
1:A:338:SER:OG	1:A:408:HIS:HD2	2.01	0.43
1:A:571[A]:ARG:NH1	1:A:1047:GLU:OE2	2.49	0.43
1:A:427:LYS:CE	7:A:1840:HOH:O	2.66	0.43
1:A:483:GLU:OE2	1:A:1053:HIS:HE1	2.01	0.43
1:A:427:LYS:HB3	7:A:1840:HOH:O	2.18	0.42
1:A:218:ARG:CG	1:A:220:LYS:CG	2.97	0.42
1:A:427:LYS:HE3	7:A:1840:HOH:O	2.20	0.42
1:A:864[A]:LYS:HD3	7:A:1421:HOH:O	2.18	0.42
1:A:1062:ARG:N	5:A:1322:GOL:H12	2.34	0.42
1:A:1140:MET:HE2	7:A:1427:HOH:O	2.19	0.42
5:A:1319:GOL:C3	7:A:1518:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499[B]:PHE:CE1	1:A:518:ASP:HB3	2.55	0.41
1:A:916:HIS:HD2	7:A:1494:HOH:O	2.03	0.41
1:A:1222:TYR:CE2	1:A:1245:THR:HB	2.55	0.41
1:A:80:ARG:HG2	1:A:138[B]:THR:CG2	2.50	0.41
1:A:945[B]:GLN:NE2	7:A:1423:HOH:O	2.54	0.41
1:A:430:ILE:HG13	1:A:519:GLY:HA3	2.03	0.41
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.69	0.41
1:A:275:HIS:CD2	7:A:2202:HOH:O	2.68	0.41
1:A:443:ALA:HB3	7:A:1829:HOH:O	2.20	0.41
1:A:1145:ARG:HH11	1:A:1145:ARG:HD2	1.72	0.41
1:A:411:ILE:HG12	1:A:741:MET:HG2	2.01	0.41
1:A:864[A]:LYS:CD	7:A:1421:HOH:O	2.68	0.41
1:A:1260:HIS:CD2	1:A:1262:GLU:OE2	2.68	0.41
1:A:259:ASN:ND2	1:A:259:ASN:N	2.59	0.40
1:A:476:GLU:HB2	7:A:1725:HOH:O	2.22	0.40
1:A:1170:SER:O	1:A:1191:PRO:HA	2.21	0.40
1:A:408:HIS:CB	1:A:783[B]:THR:HG21	2.52	0.40
5:A:1319:GOL:H31	7:A:1518: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	1307/1305 (100%)	1260 (96%)	40 (3%)	7 (0%)	29 26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	SER
1	A	119	LEU
1	A	216	HIS

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Mol	Chain	Res	Type
1	A	661	THR
1	A	886	SER
1	A	428	GLY
1	A	430	ILE

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	1047/1040 (101%)	1029 (98%)	18 (2%)	60 67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	104	ASP
1	A	120	THR
1	A	196	LYS
1	A	213	ASN
1	A	218	ARG
1	A	259	ASN
1	A	423	ASP
1	A	427	LYS
1	A	429	GLU
1	A	553	LEU
1	A	571[A]	ARG
1	A	571[B]	ARG
1	A	776	LYS
1	A	982	ARG
1	A	1052	SER
1	A	1190	MET
1	A	1195	SER

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

Mol	Chain	Res	Type
1	A	39	HIS
1	A	96	HIS
1	A	123	GLN
1	A	175	ASN
1	A	191	GLN
1	A	211	GLN
1	A	233	GLN
1	A	259	ASN
1	A	275	HIS
1	A	276	ASN
1	A	296	HIS
1	A	298	HIS
1	A	408	HIS
1	A	419	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	883	HIS
1	A	916	HIS
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	1053	HIS
1	A	1183	GLN
1	A	1260	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CYG	A	1135	1	12,14,15	2.90	5 (41%)	11,17,19	2.64	4 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CYG	A	1135	1	-	4/14/16/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CD1-SG	-8.28	1.55	1.76
1	A	1135	CYG	O2-C1	-3.28	1.19	1.30
1	A	1135	CYG	CG1-CD1	2.79	1.53	1.50
1	A	1135	CYG	OE2-CD1	-2.50	1.17	1.21
1	A	1135	CYG	CB-SG	-2.39	1.75	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	CYG	CG1-CD1-SG	6.27	120.76	113.46
1	A	1135	CYG	OE2-CD1-SG	-4.32	117.00	122.61
1	A	1135	CYG	CB-SG-CD1	2.20	103.91	100.84
1	A	1135	CYG	CB1-CG1-CD1	-2.18	107.49	112.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	SG-CD1-CG1-CB1
1	A	1135	CYG	OE2-CD1-CG1-CB1

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Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	OE2-CD1-SG-CB
1	A	1135	CYG	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
3	SO4	A	1310	-	4,4,4	0.63	0	6,6,6	0.75	0
3	SO4	A	1314	-	4,4,4	1.62	1 (25%)	6,6,6	2.69	3 (50%)
3	SO4	A	1305	-	4,4,4	0.55	0	6,6,6	0.73	0
5	GOL	A	1322	-	5,5,5	0.53	0	5,5,5	1.03	0
5	GOL	A	1321	-	5,5,5	1.38	1 (20%)	5,5,5	1.71	2 (40%)
3	SO4	A	1313	-	4,4,4	0.56	0	6,6,6	0.95	0
3	SO4	A	1306	-	4,4,4	0.28	0	6,6,6	0.81	0
5	GOL	A	1318	-	5,5,5	1.13	0	5,5,5	0.91	0
5	GOL	A	1319	-	5,5,5	1.32	0	5,5,5	2.21	2 (40%)
3	SO4	A	1307	-	4,4,4	0.57	0	6,6,6	0.67	0
4	ADP	A	1316	2	24,29,29	0.82	0	29,45,45	1.18	3 (10%)
3	SO4	A	1309	-	4,4,4	0.60	0	6,6,6	0.64	0
5	GOL	A	1317	-	5,5,5	1.10	0	5,5,5	2.61	2 (40%)
3	SO4	A	1308	-	4,4,4	0.61	0	6,6,6	0.90	0
3	SO4	A	1312	-	4,4,4	1.08	0	6,6,6	0.61	0
5	GOL	A	1320	-	5,5,5	0.73	0	5,5,5	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	A	1324	-	5,5,5	0.31	0	5,5,5	1.05	0
3	SO4	A	1311	-	4,4,4	1.05	0	6,6,6	1.76	2 (33%)
3	SO4	A	1304	-	4,4,4	0.19	0	6,6,6	0.50	0
3	SO4	A	1315	-	4,4,4	0.31	0	6,6,6	0.43	0
5	GOL	A	1323	-	5,5,5	0.28	0	5,5,5	1.18	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
5	GOL	A	1318	-	-	4/4/4/4	-
5	GOL	A	1322	-	-	4/4/4/4	-
5	GOL	A	1319	-	-	2/4/4/4	-
4	ADP	A	1316	2	-	2/12/32/32	0/3/3/3
5	GOL	A	1323	-	-	1/4/4/4	-
5	GOL	A	1320	-	-	0/4/4/4	-
5	GOL	A	1317	-	-	2/4/4/4	-
5	GOL	A	1324	-	-	0/4/4/4	-
5	GOL	A	1321	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1314	SO4	O2-S	3.12	1.62	1.46
5	A	1321	GOL	O3-C3	2.27	1.52	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1314	SO4	O3-S-O1	-5.46	80.80	109.31
5	A	1317	GOL	O3-C3-C2	4.53	131.94	110.20
5	A	1319	GOL	O1-C1-C2	-3.92	91.43	110.20
3	A	1311	SO4	O3-S-O1	3.32	126.61	109.31
5	A	1317	GOL	O2-C2-C3	2.95	122.11	109.12
3	A	1314	SO4	O2-S-O1	2.83	130.36	109.43
4	A	1316	ADP	N3-C2-N1	-2.45	124.84	128.68
5	A	1319	GOL	O3-C3-C2	-2.41	98.62	110.20
5	A	1321	GOL	O3-C3-C2	2.40	121.69	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1316	ADP	O2A-PA-O1A	2.38	123.99	112.24
4	A	1316	ADP	PA-O3A-PB	-2.19	125.32	132.83
3	A	1311	SO4	O4-S-O1	-2.11	98.31	109.31
5	A	1321	GOL	C3-C2-C1	2.06	119.72	111.70
3	A	1314	SO4	O3-S-O2	2.02	119.87	109.31

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1317	GOL	O1-C1-C2-C3
5	A	1318	GOL	O1-C1-C2-C3
5	A	1319	GOL	O1-C1-C2-C3
5	A	1321	GOL	O1-C1-C2-O2
5	A	1321	GOL	O1-C1-C2-C3
5	A	1321	GOL	C1-C2-C3-O3
5	A	1322	GOL	O1-C1-C2-C3
5	A	1322	GOL	C1-C2-C3-O3
5	A	1318	GOL	O2-C2-C3-O3
5	A	1317	GOL	C1-C2-C3-O3
5	A	1318	GOL	C1-C2-C3-O3
5	A	1323	GOL	C1-C2-C3-O3
5	A	1318	GOL	O1-C1-C2-O2
5	A	1319	GOL	O1-C1-C2-O2
5	A	1321	GOL	O2-C2-C3-O3
5	A	1322	GOL	O2-C2-C3-O3
5	A	1322	GOL	O1-C1-C2-O2
4	A	1316	ADP	PA-O3A-PB-O3B
4	A	1316	ADP	C5'-O5'-PA-O3A

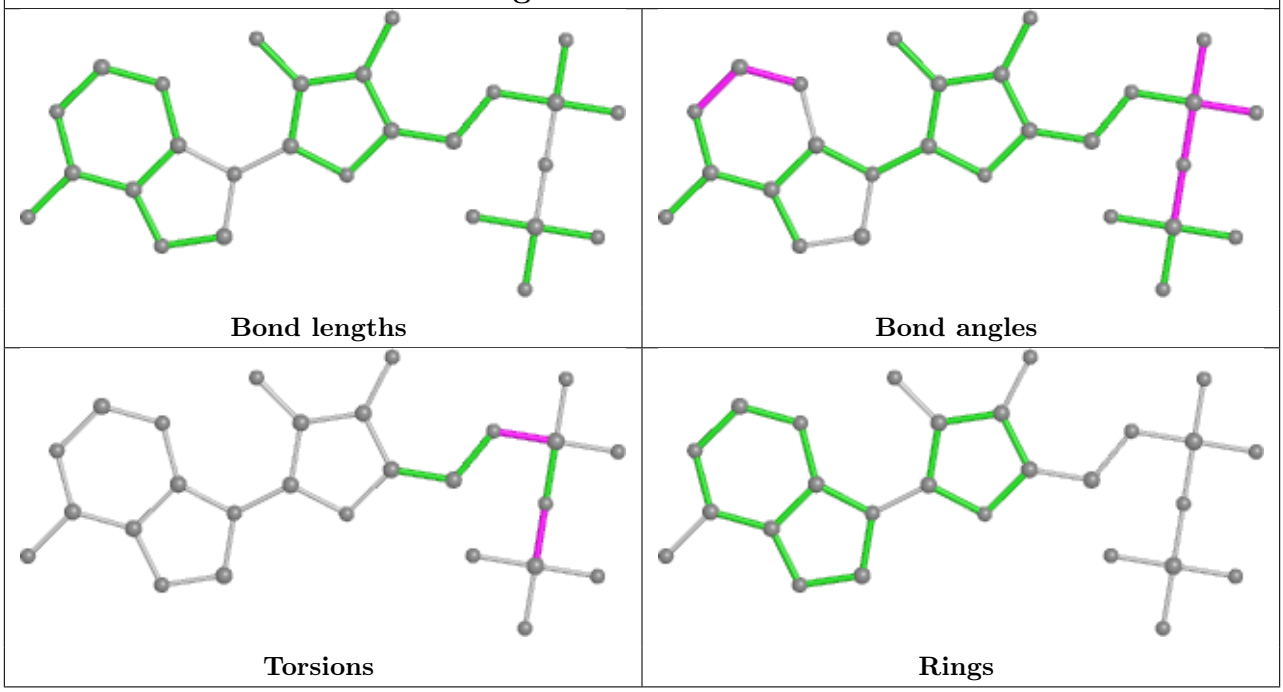
There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1322	GOL	6	0
5	A	1319	GOL	3	0
5	A	1317	GOL	1	0
5	A	1320	GOL	4	0
5	A	1324	GOL	2	0
3	A	1311	SO4	1	0
5	A	1323	GOL	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 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 1316



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, 95^{th} 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	1285/1305 (98%)	-0.29	56 (4%) 34 40	14, 23, 55, 93	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	LEU	5.9
1	A	117	SER	5.5
1	A	429	GLU	4.4
1	A	608	LYS	4.4
1	A	789	ASN	4.4
1	A	25	ALA	4.3
1	A	609	THR	4.2
1	A	607	GLY	3.7
1	A	610	PRO	3.6
1	A	181	ALA	3.6
1	A	469	SER	3.5
1	A	428	GLY	3.4
1	A	788	GLY	3.4
1	A	218	ARG	3.4
1	A	121	ALA	3.3
1	A	66	SER	3.2
1	A	786	GLN	2.9
1	A	120	THR	2.9
1	A	27	ASN	2.9
1	A	177	ARG	2.8
1	A	1045[A]	LEU	2.8
1	A	425	VAL	2.8
1	A	468	ALA	2.8
1	A	467	PHE	2.7
1	A	118	THR	2.7
1	A	122	GLU	2.7
1	A	125	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	791	GLN	2.6
1	A	179	GLY	2.6
1	A	154	GLN	2.6
1	A	31	HIS	2.5
1	A	216	HIS	2.5
1	A	611	LYS	2.5
1	A	172	ILE	2.5
1	A	124	TRP	2.4
1	A	426	GLN	2.4
1	A	69	THR	2.4
1	A	276	ASN	2.4
1	A	603	ASP	2.4
1	A	28	LEU	2.4
1	A	606	LEU	2.4
1	A	67	SER	2.4
1	A	427	LYS	2.4
1	A	183	ALA	2.3
1	A	-1	SER	2.3
1	A	152	HIS	2.3
1	A	156	ALA	2.3
1	A	184	GLU	2.2
1	A	119	LEU	2.2
1	A	257	LYS	2.1
1	A	21	ALA	2.1
1	A	629	ALA	2.1
1	A	1090	ALA	2.0
1	A	358	ARG	2.0
1	A	116	ALA	2.0
1	A	29	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CYG	A	1135	15/16	0.95	0.14	17,26,38,48	2

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

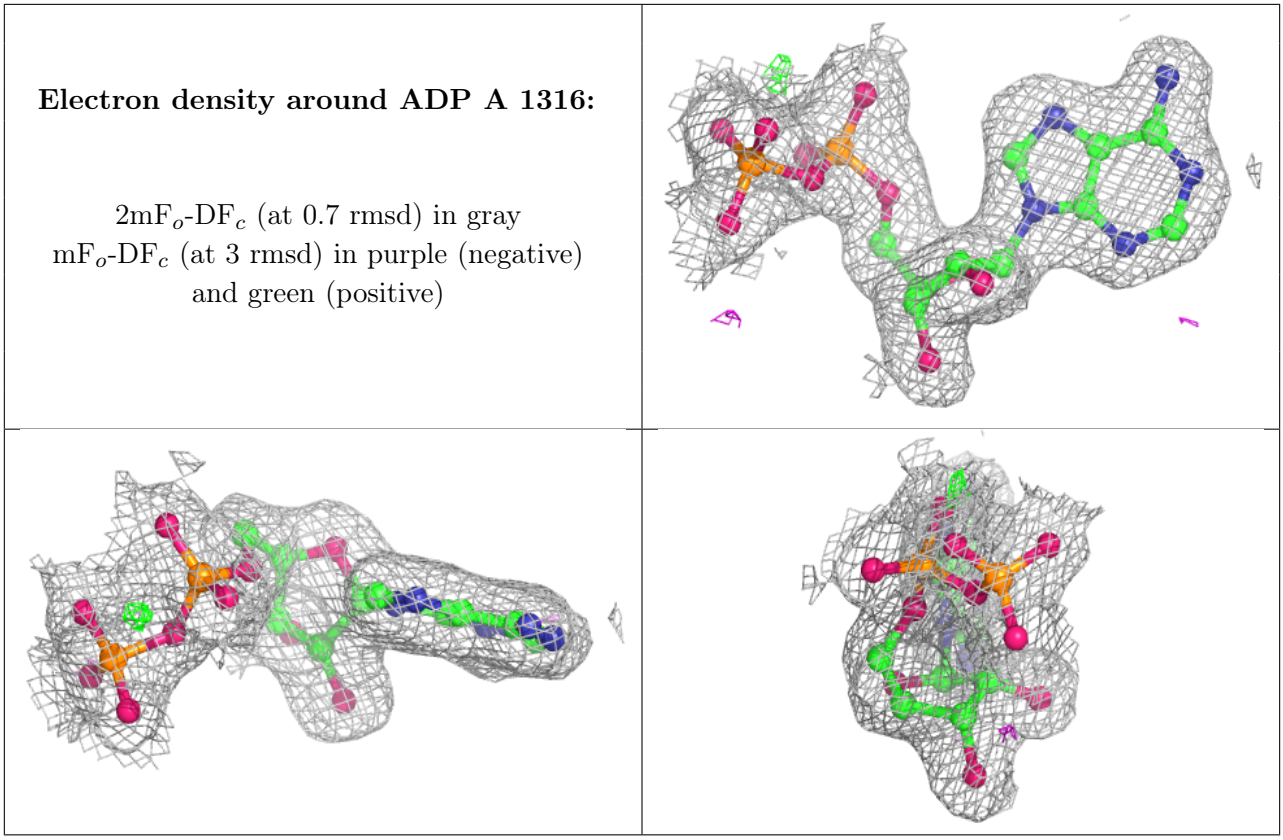
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	SO4	A	1311	5/5	0.64	0.24	49,52,57,73	0
5	GOL	A	1323	6/6	0.67	0.27	50,51,55,57	0
5	GOL	A	1324	6/6	0.70	0.32	22,45,48,55	0
6	CL	A	1326	1/1	0.75	0.07	66,66,66,66	0
5	GOL	A	1318	6/6	0.76	0.23	43,57,58,63	0
3	SO4	A	1314	5/5	0.79	0.20	38,47,64,73	0
3	SO4	A	1312	5/5	0.80	0.28	37,50,60,67	0
5	GOL	A	1321	6/6	0.81	0.19	29,40,46,51	0
5	GOL	A	1322	6/6	0.82	0.23	28,42,43,63	0
6	CL	A	1327	1/1	0.84	0.06	54,54,54,54	0
5	GOL	A	1317	6/6	0.85	0.19	27,41,43,55	0
5	GOL	A	1320	6/6	0.87	0.17	30,42,47,48	0
3	SO4	A	1310	5/5	0.90	0.28	55,58,63,81	0
3	SO4	A	1315	5/5	0.91	0.30	70,75,80,84	0
5	GOL	A	1319	6/6	0.94	0.19	26,33,40,49	0
3	SO4	A	1309	5/5	0.96	0.27	41,48,49,50	0
3	SO4	A	1313	5/5	0.96	0.20	41,42,54,60	0
3	SO4	A	1308	5/5	0.97	0.24	42,49,59,65	0
3	SO4	A	1306	5/5	0.98	0.14	32,34,45,51	0
3	SO4	A	1304	5/5	0.99	0.06	33,37,40,45	0
4	ADP	A	1316	27/27	0.99	0.08	13,16,19,20	0
3	SO4	A	1305	5/5	0.99	0.13	24,34,37,38	0
2	MG	A	1301	1/1	0.99	0.10	13,13,13,13	0
2	MG	A	1302	1/1	0.99	0.07	17,17,17,17	0
2	MG	A	1303	1/1	0.99	0.11	16,16,16,16	0
3	SO4	A	1307	5/5	1.00	0.06	24,28,29,30	0
6	CL	A	1325	1/1	1.00	0.07	27,27,27,27	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 1316:

$2mF_o$-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.