Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:43 PM JST

PDB ID	:	7DW7
Title	:	Crystal Structure of N1051A mutant of Formylglycinamidine Synthetase
Authors	:	Sharma, N.; Tanwar, A.S.; Anand, R.
Deposited on	:	2021-01-15
Resolution	:	1.80 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:

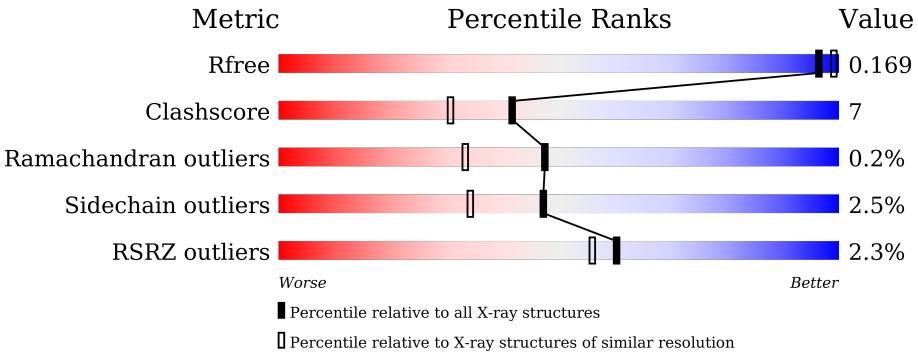
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	1304	2% 86% 12%

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	GOL	A	1302	-	X	-	-
3	GOL	A	1309	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1310	-	X	X	-
3	GOL	A	1319	-	-	X	-
3	GOL	A	1323	-	X	X	-
3	GOL	A	1330	-	-	X	-
3	GOL	A	1336	-	X	-	-
3	GOL	A	1339	-	-	X	-
4	SO4	A	1360	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11709 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.

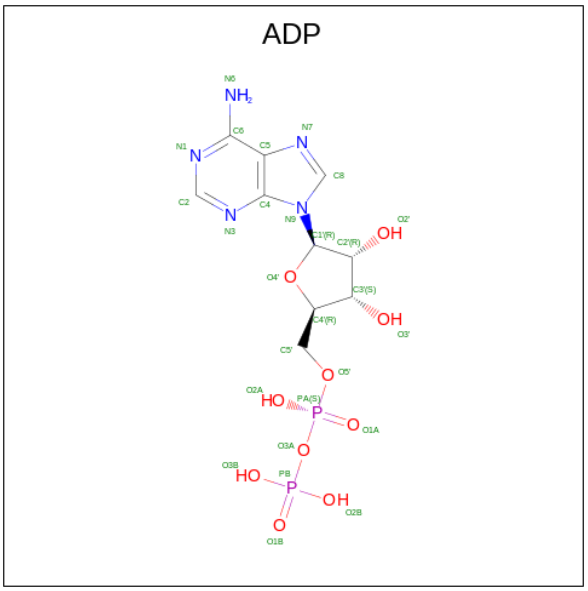
- Molecule 1 is a protein called Phosphoribosylformylglycinamidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1290	10135	6374	1806	1904	51	0	38	0

There are 10 discrepancies between the modelled and reference sequences:

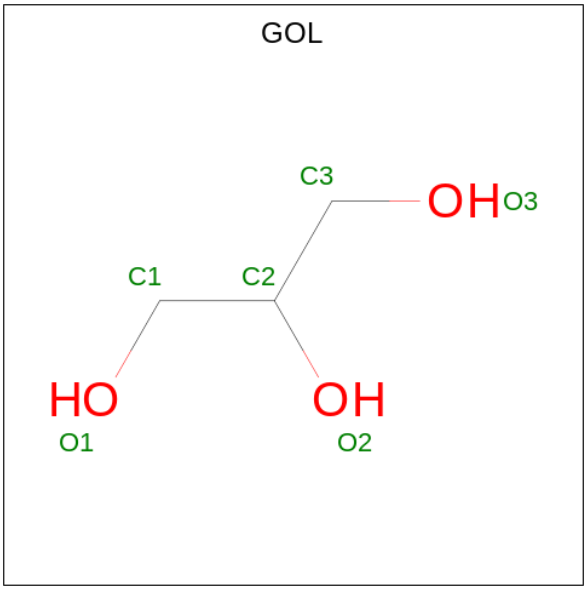
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	SER	-	expression tag	UNP A0A0D6F9Y3
A	-7	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-6	LEU	-	expression tag	UNP A0A0D6F9Y3
A	-5	VAL	-	expression tag	UNP A0A0D6F9Y3
A	-4	PRO	-	expression tag	UNP A0A0D6F9Y3
A	-3	ARG	-	expression tag	UNP A0A0D6F9Y3
A	-2	GLY	-	expression tag	UNP A0A0D6F9Y3
A	-1	SER	-	expression tag	UNP A0A0D6F9Y3
A	0	HIS	-	expression tag	UNP A0A0D6F9Y3
A	1051	ALA	ASN	engineered mutation	UNP A0A0D6F9Y3

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



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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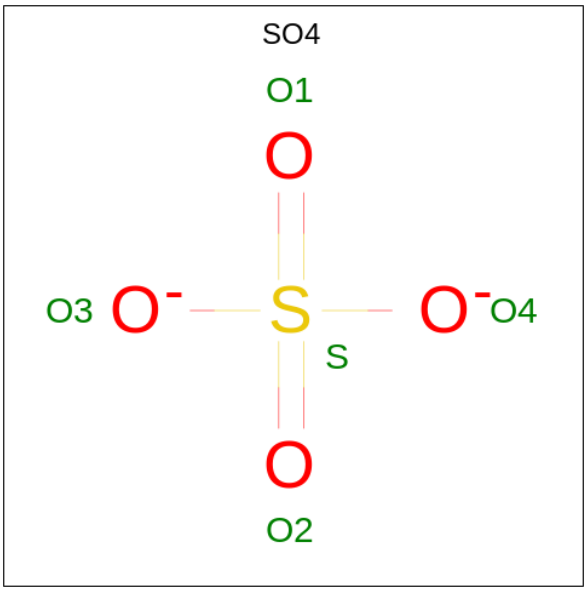
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

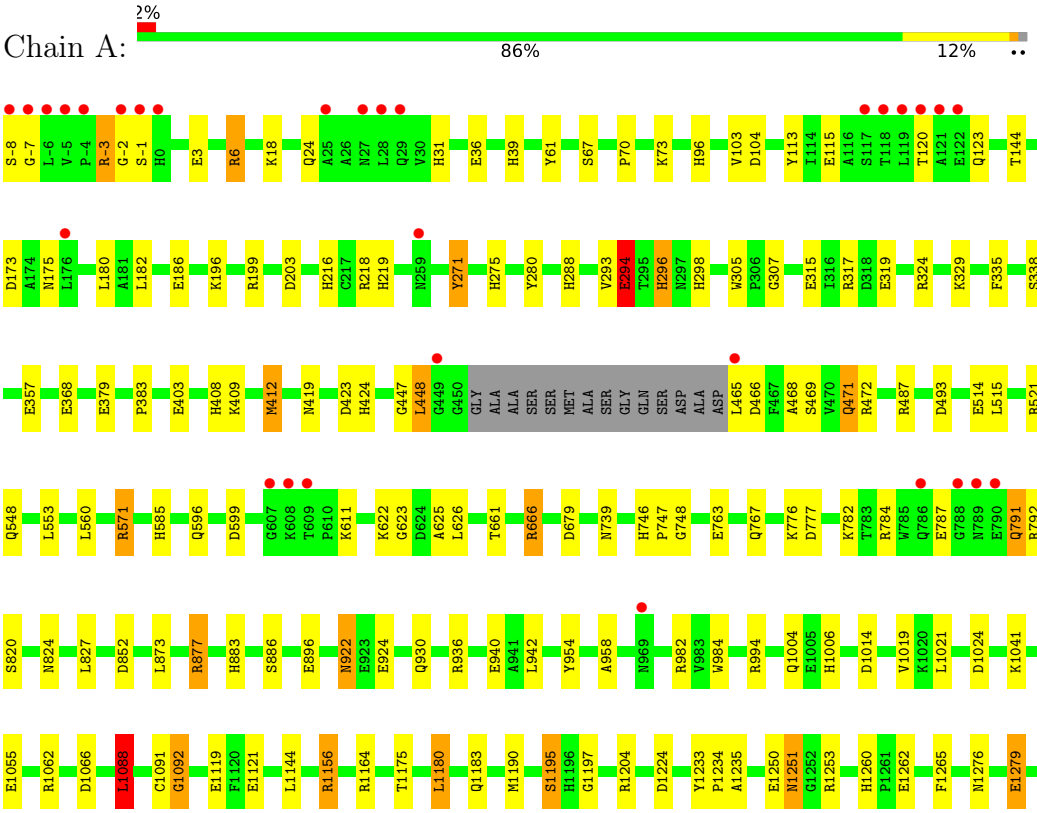
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1203	Total O 1203 1203	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	146.63Å 146.63Å 141.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.99 – 1.80 39.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.99-1.80) 99.8 (39.68-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.31 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.133 , 0.163 0.144 , 0.169	Depositor DCC
R_{free} test set	8052 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11709	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 2.43% 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

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	1.14	15/10447 (0.1%)	1.07	33/14171 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1119	GLU	CD-OE2	-7.37	1.17	1.25
1	A	294	GLU	CD-OE2	-6.78	1.18	1.25
1	A	1250	GLU	CD-OE1	-5.97	1.19	1.25
1	A	1121	GLU	CD-OE2	-5.90	1.19	1.25
1	A	1279	GLU	CD-OE2	5.85	1.32	1.25
1	A	115	GLU	CD-OE2	-5.79	1.19	1.25
1	A	796	SER	CB-OG	5.76	1.49	1.42
1	A	940	GLU	CD-OE2	-5.64	1.19	1.25
1	A	271	TYR	CE1-CZ	5.64	1.45	1.38
1	A	1195	SER	CB-OG	-5.56	1.35	1.42
1	A	186	GLU	CD-OE2	5.53	1.31	1.25
1	A	409	LYS	CD-CE	-5.26	1.38	1.51
1	A	412[A]	MET	CA-C	5.23	1.66	1.52
1	A	412[B]	MET	CA-C	5.23	1.66	1.52
1	A	-1	SER	N-CA	5.05	1.56	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1156[A]	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	1156[B]	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	A	1180	LEU	CB-CG-CD1	9.50	127.16	111.00
1	A	412[A]	MET	CG-SD-CE	8.31	113.50	100.20
1	A	412[B]	MET	CG-SD-CE	8.31	113.50	100.20
1	A	1156[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	1156[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	666	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	877[A]	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	877[B]	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	666	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	521	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	18	LYS	CD-CE-NZ	5.59	124.56	111.70
1	A	1014	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	345	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	A	1062	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	1088[A]	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	1088[B]	LEU	CA-CB-CG	5.36	127.64	115.30
1	A	1224	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	148[A]	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	A	148[B]	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	A	203	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	466	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	6[A]	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	6[B]	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	1204	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	571	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	994	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	173	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	487	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	218	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	1024	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	199	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052[B]	SER	Mainchain
1	A	1091[B]	CYS	Peptide
1	A	1092[B]	GLY	Peptide

5.2 Too-close contacts (i)

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	10135	0	10034	136	0
2	A	27	0	12	0	0
3	A	246	0	325	47	0
4	A	95	0	0	2	0
5	A	3	0	0	0	0
6	A	1203	0	0	33	0
All	All	11709	0	10371	147	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 (147) 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:-2:GLY:HA3	4:A:1360:SO4:O2	1.65	0.96
1:A:787:GLU:CB	1:A:792[B]:ARG:HG3	2.01	0.89
1:A:824:ASN:HD21	1:A:958:ALA:H	1.21	0.86
1:A:-2:GLY:CA	4:A:1360:SO4:O2	2.23	0.86
1:A:493:ASP:HA	3:A:1339:GOL:H31	1.56	0.85
1:A:747:PRO:HA	3:A:1323:GOL:H31	1.59	0.84
3:A:1320:GOL:C3	6:A:1818:HOH:O	2.25	0.84
1:A:787:GLU:HB2	1:A:792[B]:ARG:HG3	1.61	0.81
3:A:1321:GOL:H31	6:A:2169:HOH:O	1.80	0.80
1:A:1055:GLU:HB2	6:A:1429:HOH:O	1.80	0.80
1:A:820:SER:H	1:A:930:GLN:HE22	1.28	0.79
1:A:175:ASN:HD21	1:A:182:LEU:H	1.32	0.77
1:A:936:ARG:HH22	3:A:1321:GOL:H32	1.50	0.75
1:A:791:GLN:HG2	6:A:2269:HOH:O	1.87	0.74
3:A:1320:GOL:H32	6:A:1818:HOH:O	1.85	0.74
1:A:787:GLU:HB3	1:A:792[B]:ARG:HG3	1.70	0.73
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.74	0.71
1:A:1052[B]:SER:HB3	1:A:1092[B]:GLY:HA3	1.72	0.70
1:A:96:HIS:HE1	1:A:103:VAL:O	1.74	0.69
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.55	0.69
1:A:324:ARG:NH1	3:A:1339:GOL:O2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1316:GOL:H32	6:A:2491:HOH:O	1.93	0.68
1:A:545:ASN:HD22	1:A:547:SER:H	1.41	0.67
1:A:922:ASN:HD22	1:A:924:GLU:H	1.42	0.67
1:A:1051[B]:ALA:O	1:A:1052[B]:SER:HB2	1.93	0.67
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.78	0.67
1:A:873:LEU:HD21	1:A:942[B]:LEU:HD23	1.77	0.66
3:A:1330:GOL:H32	6:A:1526:HOH:O	1.94	0.66
1:A:873:LEU:CD2	1:A:942[B]:LEU:HD23	2.25	0.66
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.79	0.65
1:A:984:TRP:HE1	3:A:1330:GOL:H2	1.62	0.65
1:A:1164:ARG:HH22	3:A:1324:GOL:C1	2.10	0.65
1:A:776:LYS:HE3	3:A:1316:GOL:O2	1.97	0.64
1:A:1251:ASN:HD22	1:A:1253[A]:ARG:H	1.45	0.64
1:A:1251:ASN:HD22	1:A:1253[B]:ARG:H	1.45	0.64
1:A:626:LEU:HB2	3:A:1319:GOL:H31	1.79	0.62
1:A:329:LYS:HG3	6:A:1424:HOH:O	1.99	0.62
1:A:275:HIS:HD2	6:A:2492:HOH:O	1.81	0.62
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.83	0.62
1:A:1251:ASN:ND2	1:A:1253[B]:ARG:H	1.98	0.61
1:A:1251:ASN:ND2	1:A:1253[A]:ARG:H	1.98	0.61
1:A:335:PHE:CE1	1:A:412[B]:MET:SD	2.94	0.61
1:A:471:GLN:HE21	1:A:472:ARG:H	1.47	0.61
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.48	0.60
1:A:747:PRO:HA	3:A:1323:GOL:C3	2.30	0.60
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.85	0.59
1:A:1164:ARG:HH22	3:A:1324:GOL:H12	1.67	0.59
1:A:6[A]:ARG:HD3	1:A:36:GLU:OE1	2.03	0.58
1:A:746:HIS:HD2	1:A:782:LYS:NZ	2.02	0.58
1:A:-3:ARG:HD3	1:A:150:PHE:HB2	1.88	0.56
1:A:368:GLU:HG3	3:A:1327:GOL:H31	1.88	0.56
1:A:1054:VAL:HG23	3:A:1310:GOL:H31	1.87	0.56
1:A:748:GLY:H	3:A:1323:GOL:H31	1.71	0.56
1:A:626:LEU:HB2	3:A:1319:GOL:C3	2.35	0.56
1:A:412[A]:MET:SD	6:A:2279:HOH:O	2.58	0.56
1:A:787:GLU:HB3	1:A:792[B]:ARG:CG	2.35	0.55
1:A:1180:LEU:HD12	1:A:1253[B]:ARG:HG2	1.88	0.55
1:A:1175:THR:HB	3:A:1309:GOL:H2	1.90	0.54
1:A:368:GLU:HG3	3:A:1327:GOL:C3	2.37	0.54
1:A:625:ALA:HA	3:A:1319:GOL:O2	2.07	0.54
1:A:585:HIS:HD2	6:A:2359:HOH:O	1.92	0.52
1:A:1197:GLY:H	3:A:1302:GOL:H11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1316:GOL:H2	6:A:1432:HOH:O	2.09	0.52
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.93	0.52
1:A:357:GLU:HB3	6:A:2273:HOH:O	2.10	0.52
1:A:877[B]:ARG:HH11	1:A:877[B]:ARG:HG3	1.75	0.52
1:A:1183:GLN:HE22	3:A:1315:GOL:H12	1.74	0.52
1:A:514:GLU:HG3	6:A:2367:HOH:O	2.10	0.52
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.13	0.52
1:A:1006:HIS:HE1	6:A:1783:HOH:O	1.92	0.52
1:A:296:HIS:HD2	1:A:307:GLY:O	1.93	0.51
1:A:120:THR:H	1:A:123:GLN:HE21	1.59	0.51
1:A:31:HIS:HB2	3:A:1325:GOL:C2	2.41	0.50
1:A:447:GLY:HA2	1:A:468:ALA:O	2.10	0.50
1:A:96:HIS:HD2	6:A:2099:HOH:O	1.94	0.50
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.08	0.50
3:A:1311:GOL:H12	6:A:1774:HOH:O	2.11	0.50
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.12	0.49
1:A:6[B]:ARG:NH1	1:A:36:GLU:OE2	2.46	0.49
1:A:31:HIS:HB2	3:A:1325:GOL:H2	1.92	0.49
1:A:1054:VAL:HG23	3:A:1310:GOL:H12	1.94	0.49
1:A:423:ASP:HB3	3:A:1339:GOL:H2	1.94	0.49
1:A:465:LEU:HA	6:A:2442:HOH:O	2.13	0.49
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.95	0.49
3:A:1320:GOL:H31	6:A:1818:HOH:O	2.05	0.49
3:A:1330:GOL:C3	6:A:1526:HOH:O	2.57	0.49
1:A:1180:LEU:HD12	1:A:1253[A]:ARG:HG2	1.94	0.48
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.12	0.48
3:A:1311:GOL:H11	6:A:2422:HOH:O	2.13	0.48
1:A:305:TRP:CD1	1:A:305:TRP:C	2.86	0.48
1:A:784:ARG:HG2	1:A:793:GLU:HG3	1.96	0.48
1:A:329:LYS:CG	6:A:1424:HOH:O	2.61	0.47
1:A:329:LYS:O	1:A:383:PRO:HD2	2.14	0.47
1:A:1164:ARG:HH22	3:A:1324:GOL:H11	1.80	0.47
3:A:1330:GOL:O1	3:A:1338:GOL:O2	2.27	0.47
1:A:984:TRP:NE1	3:A:1330:GOL:H2	2.28	0.47
1:A:1265:PHE:HE2	6:A:1429:HOH:O	1.97	0.47
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.96	0.47
1:A:936:ARG:HH22	3:A:1321:GOL:C3	2.25	0.47
1:A:1019[A]:VAL:HG12	1:A:1021:LEU:HG	1.97	0.47
1:A:298:HIS:HE1	1:A:469:SER:OG	1.98	0.47
1:A:1279:GLU:HG3	6:A:1457:HOH:O	2.15	0.47
1:A:782:LYS:CE	1:A:793:GLU:CD	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:TRP:HE1	3:A:1330:GOL:C2	2.26	0.46
1:A:748:GLY:H	3:A:1323:GOL:C3	2.28	0.46
1:A:1006:HIS:HD2	6:A:1813:HOH:O	1.98	0.46
1:A:782:LYS:HE2	1:A:793:GLU:CD	2.36	0.46
1:A:70:PRO:HB3	1:A:113:TYR:CE1	2.51	0.46
1:A:1156[B]:ARG:HH11	1:A:1156[B]:ARG:HG2	1.81	0.46
1:A:275:HIS:HE1	6:A:2459:HOH:O	1.99	0.45
1:A:354:GLY:O	1:A:408:HIS:HE1	1.99	0.45
1:A:585:HIS:CE1	1:A:599:ASP:OD1	2.66	0.45
1:A:-8:SER:N	6:A:1407:HOH:O	2.39	0.45
1:A:623:GLY:HA3	1:A:852[B]:ASP:HA	1.99	0.45
1:A:1051[B]:ALA:O	1:A:1052[B]:SER:CB	2.62	0.45
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.82	0.45
1:A:515:LEU:HD23	1:A:515:LEU:C	2.36	0.45
1:A:1051[A]:ALA:O	3:A:1310:GOL:H32	2.17	0.45
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.35	0.44
1:A:73:LYS:HE2	6:A:2481:HOH:O	2.17	0.44
1:A:338:SER:OG	1:A:408:HIS:HD2	1.99	0.44
1:A:626:LEU:H	3:A:1319:GOL:H31	1.83	0.44
1:A:545:ASN:ND2	1:A:547:SER:H	2.13	0.44
1:A:-7:GLY:O	1:A:3:GLU:HA	2.18	0.43
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.53	0.43
1:A:1197:GLY:H	3:A:1302:GOL:C1	2.30	0.43
1:A:877[B]:ARG:HG3	1:A:877[B]:ARG:NH1	2.33	0.43
1:A:1052[A]:SER:HB3	6:A:1527:HOH:O	2.18	0.43
1:A:424:HIS:NE2	3:A:1339:GOL:H32	2.33	0.43
1:A:1183:GLN:CG	3:A:1317:GOL:H32	2.48	0.43
1:A:294:GLU:HB3	6:A:2104:HOH:O	2.18	0.42
1:A:368:GLU:HG3	3:A:1327:GOL:O3	2.20	0.42
1:A:448:LEU:HD23	1:A:448:LEU:HA	1.89	0.42
1:A:763:GLU:O	1:A:767[B]:GLN:HG3	2.20	0.41
1:A:298:HIS:CE1	1:A:469:SER:OG	2.74	0.41
1:A:216:HIS:HD2	6:A:1469:HOH:O	2.04	0.41
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.19	0.41
1:A:379:GLU:HG2	6:A:2308:HOH:O	2.21	0.40
1:A:39:HIS:HD2	6:A:1615:HOH:O	2.05	0.40
1:A:324:ARG:HH12	3:A:1339:GOL:HO2	1.58	0.40
1:A:1051[A]:ALA:O	3:A:1310:GOL:C3	2.69	0.40
1:A:1234:PRO:O	1:A:1235:ALA:C	2.60	0.40
1:A:288:HIS:O	1:A:419:ASN:HA	2.22	0.40
1:A:1041:LYS:HA	1:A:1066:ASP:O	2.22	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	1324/1304 (102%)	1281 (97%)	39 (3%)	4 (0%)	41 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1052[A]	SER
1	A	1052[B]	SER
1	A	886	SER
1	A	661	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1068/1041 (103%)	1039 (97%)	29 (3%)	44 31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	24	GLN
1	A	67	SER
1	A	104	ASP

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Mol	Chain	Res	Type
1	A	144[A]	THR
1	A	144[B]	THR
1	A	196	LYS
1	A	294	GLU
1	A	296	HIS
1	A	448	LEU
1	A	471	GLN
1	A	545	ASN
1	A	560	LEU
1	A	571	ARG
1	A	596[A]	GLN
1	A	596[B]	GLN
1	A	611	LYS
1	A	622	LYS
1	A	666	ARG
1	A	791	GLN
1	A	922	ASN
1	A	982	ARG
1	A	1088[A]	LEU
1	A	1088[B]	LEU
1	A	1144	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1251	ASN
1	A	1276	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	29	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	233	GLN
1	A	243	ASN
1	A	275	HIS

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Mol	Chain	Res	Type
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	791	GLN
1	A	824	ASN
1	A	883	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1061	HIS
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS
1	A	1276	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 3 are monoatomic - leaving 61 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	GOL	A	1321	-	5,5,5	0.44	0	5,5,5	1.76	1 (20%)
3	GOL	A	1302	-	5,5,5	1.11	0	5,5,5	2.82	3 (60%)
3	GOL	A	1309	-	5,5,5	1.81	2 (40%)	5,5,5	2.93	3 (60%)
3	GOL	A	1314	-	5,5,5	0.62	0	5,5,5	1.06	0
3	GOL	A	1305	-	5,5,5	1.09	0	5,5,5	0.86	0
3	GOL	A	1325	-	5,5,5	0.49	0	5,5,5	0.92	0
3	GOL	A	1304[B]	-	5,5,5	0.70	0	5,5,5	0.66	0
3	GOL	A	1337	-	5,5,5	0.50	0	5,5,5	1.53	1 (20%)
4	SO4	A	1355	-	4,4,4	0.68	0	6,6,6	0.76	0
4	SO4	A	1360	-	4,4,4	0.37	0	6,6,6	0.97	0
4	SO4	A	1350	-	4,4,4	0.65	0	6,6,6	0.71	0
3	GOL	A	1317	-	5,5,5	0.89	0	5,5,5	1.41	1 (20%)
3	GOL	A	1307	-	5,5,5	0.78	0	5,5,5	0.73	0
3	GOL	A	1311	-	5,5,5	0.75	0	5,5,5	1.02	0
3	GOL	A	1341	-	5,5,5	0.87	0	5,5,5	0.81	0
4	SO4	A	1356	-	4,4,4	0.47	0	6,6,6	0.28	0
3	GOL	A	1330	-	5,5,5	0.80	0	5,5,5	0.90	0
4	SO4	A	1352	-	4,4,4	1.03	0	6,6,6	0.84	0
3	GOL	A	1320	-	5,5,5	0.67	0	5,5,5	1.26	1 (20%)
3	GOL	A	1315	-	5,5,5	0.55	0	5,5,5	0.96	0
4	SO4	A	1347	-	4,4,4	0.53	0	6,6,6	0.82	0
3	GOL	A	1312	-	5,5,5	0.91	0	5,5,5	1.24	0
4	SO4	A	1348	-	4,4,4	0.80	0	6,6,6	1.13	1 (16%)
4	SO4	A	1358	-	4,4,4	0.42	0	6,6,6	0.61	0
3	GOL	A	1318	-	5,5,5	0.98	0	5,5,5	0.93	0
3	GOL	A	1308	-	5,5,5	1.48	2 (40%)	5,5,5	1.82	2 (40%)
3	GOL	A	1322	-	5,5,5	0.75	0	5,5,5	0.92	0
4	SO4	A	1344	-	4,4,4	0.41	0	6,6,6	0.88	0
3	GOL	A	1306	-	5,5,5	0.27	0	5,5,5	0.82	0
4	SO4	A	1353	-	4,4,4	0.92	0	6,6,6	1.17	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	1332	-	5,5,5	0.40	0	5,5,5	1.22	0
3	GOL	A	1313	-	5,5,5	0.97	0	5,5,5	1.04	0
4	SO4	A	1342	-	4,4,4	0.33	0	6,6,6	0.61	0
4	SO4	A	1343	-	4,4,4	0.72	0	6,6,6	1.46	2 (33%)
3	GOL	A	1338	-	5,5,5	0.46	0	5,5,5	1.35	1 (20%)
3	GOL	A	1334	-	5,5,5	0.66	0	5,5,5	0.79	0
3	GOL	A	1304[A]	-	5,5,5	0.99	0	5,5,5	1.71	2 (40%)
3	GOL	A	1310	-	5,5,5	1.76	2 (40%)	5,5,5	1.85	1 (20%)
4	SO4	A	1346	-	4,4,4	0.61	0	6,6,6	1.04	0
3	GOL	A	1335	-	5,5,5	0.51	0	5,5,5	0.84	0
3	GOL	A	1316	-	5,5,5	0.42	0	5,5,5	0.72	0
4	SO4	A	1351	-	4,4,4	0.57	0	6,6,6	1.61	2 (33%)
4	SO4	A	1354	-	4,4,4	0.45	0	6,6,6	1.02	0
4	SO4	A	1345	-	4,4,4	1.57	1 (25%)	6,6,6	0.97	0
3	GOL	A	1333	-	5,5,5	0.60	0	5,5,5	1.44	1 (20%)
3	GOL	A	1340	-	5,5,5	0.52	0	5,5,5	1.27	1 (20%)
3	GOL	A	1324	-	5,5,5	1.20	0	5,5,5	1.15	1 (20%)
4	SO4	A	1357	-	4,4,4	0.57	0	6,6,6	0.50	0
3	GOL	A	1319	-	5,5,5	0.56	0	5,5,5	1.69	1 (20%)
3	GOL	A	1323	-	5,5,5	1.89	2 (40%)	5,5,5	2.71	3 (60%)
4	SO4	A	1359	-	4,4,4	0.91	0	6,6,6	0.71	0
4	SO4	A	1349	-	4,4,4	0.46	0	6,6,6	1.10	1 (16%)
3	GOL	A	1303	-	5,5,5	0.73	0	5,5,5	1.35	0
3	GOL	A	1339	-	5,5,5	0.60	0	5,5,5	2.50	3 (60%)
3	GOL	A	1331	-	5,5,5	0.66	0	5,5,5	0.73	0
3	GOL	A	1326	-	5,5,5	0.58	0	5,5,5	1.25	1 (20%)
3	GOL	A	1336	-	5,5,5	2.42	1 (20%)	5,5,5	2.45	3 (60%)
3	GOL	A	1329	-	5,5,5	0.74	0	5,5,5	1.41	0
2	ADP	A	1301	5	24,29,29	1.20	3 (12%)	29,45,45	0.91	1 (3%)
3	GOL	A	1328	-	5,5,5	0.24	0	5,5,5	0.95	0
3	GOL	A	1327	-	5,5,5	0.44	0	5,5,5	1.68	2 (40%)

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	GOL	A	1321	-	-	3/4/4/4	-
3	GOL	A	1302	-	-	4/4/4/4	-
3	GOL	A	1309	-	-	4/4/4/4	-
3	GOL	A	1314	-	-	0/4/4/4	-
3	GOL	A	1305	-	-	0/4/4/4	-
3	GOL	A	1325	-	-	0/4/4/4	-
3	GOL	A	1304[B]	-	-	0/4/4/4	-
3	GOL	A	1337	-	-	2/4/4/4	-
3	GOL	A	1317	-	-	2/4/4/4	-
3	GOL	A	1307	-	-	0/4/4/4	-
3	GOL	A	1311	-	-	2/4/4/4	-
3	GOL	A	1341	-	-	0/4/4/4	-
3	GOL	A	1330	-	-	3/4/4/4	-
3	GOL	A	1320	-	-	3/4/4/4	-
3	GOL	A	1315	-	-	2/4/4/4	-
3	GOL	A	1312	-	-	4/4/4/4	-
3	GOL	A	1318	-	-	2/4/4/4	-
3	GOL	A	1308	-	-	0/4/4/4	-
3	GOL	A	1322	-	-	0/4/4/4	-
3	GOL	A	1306	-	-	2/4/4/4	-
3	GOL	A	1332	-	-	2/4/4/4	-
3	GOL	A	1313	-	-	4/4/4/4	-
3	GOL	A	1338	-	-	0/4/4/4	-
3	GOL	A	1334	-	-	2/4/4/4	-
3	GOL	A	1304[A]	-	-	1/4/4/4	-
3	GOL	A	1310	-	-	4/4/4/4	-
3	GOL	A	1335	-	-	4/4/4/4	-
3	GOL	A	1316	-	-	0/4/4/4	-
3	GOL	A	1333	-	-	2/4/4/4	-
3	GOL	A	1340	-	-	2/4/4/4	-
3	GOL	A	1324	-	-	0/4/4/4	-
3	GOL	A	1319	-	-	4/4/4/4	-
3	GOL	A	1323	-	-	2/4/4/4	-
3	GOL	A	1303	-	-	2/4/4/4	-
3	GOL	A	1339	-	-	2/4/4/4	-
3	GOL	A	1331	-	-	0/4/4/4	-
3	GOL	A	1326	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1336	-	-	3/4/4/4	-
3	GOL	A	1329	-	-	2/4/4/4	-
2	ADP	A	1301	5	-	2/12/32/32	0/3/3/3
3	GOL	A	1328	-	-	2/4/4/4	-
3	GOL	A	1327	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1336	GOL	O2-C2	5.21	1.58	1.43
3	A	1310	GOL	O1-C1	-3.13	1.29	1.42
2	A	1301	ADP	C2-N3	2.91	1.36	1.32
3	A	1323	GOL	O1-C1	-2.84	1.30	1.42
3	A	1309	GOL	O1-C1	2.79	1.54	1.42
3	A	1308	GOL	O2-C2	2.42	1.50	1.43
4	A	1345	SO4	O2-S	2.35	1.58	1.46
2	A	1301	ADP	C2'-C1'	2.31	1.57	1.53
2	A	1301	ADP	O4'-C1'	2.28	1.44	1.41
3	A	1309	GOL	O2-C2	2.21	1.50	1.43
3	A	1323	GOL	C1-C2	-2.13	1.42	1.51
3	A	1310	GOL	O3-C3	2.12	1.51	1.42
3	A	1308	GOL	C1-C2	2.04	1.60	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1323	GOL	C3-C2-C1	-4.58	93.91	111.70
3	A	1339	GOL	O3-C3-C2	4.42	131.40	110.20
3	A	1302	GOL	O2-C2-C1	4.29	128.01	109.12
3	A	1336	GOL	O1-C1-C2	3.97	129.26	110.20
3	A	1309	GOL	O2-C2-C1	3.97	126.60	109.12
3	A	1309	GOL	O3-C3-C2	-3.81	91.94	110.20
3	A	1302	GOL	O3-C3-C2	-3.37	94.03	110.20
3	A	1319	GOL	O3-C3-C2	3.14	125.23	110.20
3	A	1309	GOL	O1-C1-C2	3.07	124.94	110.20
3	A	1327	GOL	O2-C2-C3	-2.94	96.19	109.12
4	A	1343	SO4	O4-S-O3	-2.74	97.35	109.06
3	A	1336	GOL	O2-C2-C1	-2.69	97.29	109.12
3	A	1323	GOL	O3-C3-C2	2.69	123.08	110.20
4	A	1351	SO4	O4-S-O3	2.68	120.51	109.06
3	A	1320	GOL	O1-C1-C2	-2.52	98.14	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1337	GOL	O1-C1-C2	-2.50	98.20	110.20
4	A	1353	SO4	O4-S-O2	2.47	122.19	109.31
4	A	1348	SO4	O4-S-O3	-2.41	98.76	109.06
3	A	1323	GOL	O2-C2-C3	2.39	119.65	109.12
3	A	1308	GOL	O1-C1-C2	-2.38	98.78	110.20
3	A	1333	GOL	O2-C2-C3	-2.36	98.73	109.12
3	A	1340	GOL	O1-C1-C2	2.35	121.46	110.20
3	A	1317	GOL	O3-C3-C2	2.33	121.39	110.20
3	A	1304[A]	GOL	C3-C2-C1	2.33	120.77	111.70
3	A	1339	GOL	C3-C2-C1	2.30	120.65	111.70
3	A	1339	GOL	O2-C2-C3	-2.29	99.05	109.12
3	A	1308	GOL	C3-C2-C1	-2.28	102.84	111.70
4	A	1343	SO4	O4-S-O1	2.27	121.15	109.31
3	A	1324	GOL	O1-C1-C2	2.27	121.08	110.20
4	A	1351	SO4	O4-S-O1	-2.25	97.56	109.31
4	A	1349	SO4	O4-S-O3	-2.22	99.60	109.06
3	A	1304[A]	GOL	O1-C1-C2	-2.21	99.62	110.20
3	A	1336	GOL	O2-C2-C3	2.18	118.71	109.12
3	A	1326	GOL	O3-C3-C2	-2.12	100.04	110.20
3	A	1327	GOL	O2-C2-C1	2.12	118.44	109.12
3	A	1321	GOL	O2-C2-C3	-2.10	99.89	109.12
3	A	1302	GOL	O2-C2-C3	-2.07	99.99	109.12
2	A	1301	ADP	PA-O3A-PB	-2.06	125.74	132.83
3	A	1310	GOL	C3-C2-C1	-2.04	103.78	111.70
3	A	1338	GOL	O1-C1-C2	-2.01	100.57	110.20

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O2B
3	A	1306	GOL	C1-C2-C3-O3
3	A	1309	GOL	C1-C2-C3-O3
3	A	1310	GOL	O1-C1-C2-C3
3	A	1310	GOL	C1-C2-C3-O3
3	A	1311	GOL	C1-C2-C3-O3
3	A	1311	GOL	O2-C2-C3-O3
3	A	1315	GOL	C1-C2-C3-O3
3	A	1318	GOL	C1-C2-C3-O3
3	A	1319	GOL	O1-C1-C2-C3
3	A	1319	GOL	C1-C2-C3-O3
3	A	1323	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	1326	GOL	O1-C1-C2-O2
3	A	1326	GOL	O1-C1-C2-C3
3	A	1328	GOL	C1-C2-C3-O3
3	A	1329	GOL	O1-C1-C2-C3
3	A	1332	GOL	O1-C1-C2-C3
3	A	1333	GOL	O1-C1-C2-C3
3	A	1334	GOL	C1-C2-C3-O3
3	A	1335	GOL	O1-C1-C2-O2
3	A	1335	GOL	O1-C1-C2-C3
3	A	1337	GOL	O1-C1-C2-C3
3	A	1306	GOL	O2-C2-C3-O3
3	A	1310	GOL	O1-C1-C2-O2
3	A	1330	GOL	O1-C1-C2-O2
3	A	1302	GOL	O1-C1-C2-C3
3	A	1303	GOL	O1-C1-C2-C3
3	A	1309	GOL	O1-C1-C2-C3
3	A	1312	GOL	O1-C1-C2-C3
3	A	1312	GOL	C1-C2-C3-O3
3	A	1313	GOL	O1-C1-C2-C3
3	A	1313	GOL	C1-C2-C3-O3
3	A	1317	GOL	O1-C1-C2-C3
3	A	1320	GOL	O1-C1-C2-C3
3	A	1320	GOL	C1-C2-C3-O3
3	A	1321	GOL	C1-C2-C3-O3
3	A	1330	GOL	O1-C1-C2-C3
3	A	1336	GOL	O1-C1-C2-C3
3	A	1340	GOL	O1-C1-C2-C3
3	A	1302	GOL	O2-C2-C3-O3
3	A	1303	GOL	O1-C1-C2-O2
3	A	1309	GOL	O1-C1-C2-O2
3	A	1309	GOL	O2-C2-C3-O3
3	A	1313	GOL	O1-C1-C2-O2
3	A	1313	GOL	O2-C2-C3-O3
3	A	1317	GOL	O1-C1-C2-O2
3	A	1319	GOL	O2-C2-C3-O3
3	A	1321	GOL	O2-C2-C3-O3
3	A	1323	GOL	O1-C1-C2-O2
3	A	1333	GOL	O1-C1-C2-O2
3	A	1334	GOL	O2-C2-C3-O3
3	A	1302	GOL	O1-C1-C2-O2
3	A	1310	GOL	O2-C2-C3-O3
3	A	1312	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1315	GOL	O2-C2-C3-O3
3	A	1318	GOL	O2-C2-C3-O3
3	A	1328	GOL	O2-C2-C3-O3
3	A	1332	GOL	O1-C1-C2-O2
3	A	1340	GOL	O1-C1-C2-O2
2	A	1301	ADP	PA-O3A-PB-O1B
3	A	1336	GOL	O1-C1-C2-O2
3	A	1304[A]	GOL	O1-C1-C2-O2
3	A	1319	GOL	O1-C1-C2-O2
3	A	1339	GOL	O1-C1-C2-O2
3	A	1335	GOL	O2-C2-C3-O3
3	A	1302	GOL	C1-C2-C3-O3
3	A	1312	GOL	O1-C1-C2-O2
3	A	1320	GOL	O1-C1-C2-O2
3	A	1339	GOL	O1-C1-C2-C3
3	A	1321	GOL	O1-C1-C2-O2
3	A	1329	GOL	O1-C1-C2-O2
3	A	1337	GOL	O1-C1-C2-O2
3	A	1335	GOL	C1-C2-C3-O3
3	A	1330	GOL	O2-C2-C3-O3
3	A	1336	GOL	O2-C2-C3-O3

There are no ring outliers.

18 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1321	GOL	3	0
3	A	1302	GOL	2	0
3	A	1309	GOL	1	0
3	A	1325	GOL	2	0
4	A	1360	SO4	2	0
3	A	1317	GOL	1	0
3	A	1311	GOL	2	0
3	A	1330	GOL	6	0
3	A	1320	GOL	3	0
3	A	1315	GOL	1	0
3	A	1338	GOL	1	0
3	A	1310	GOL	4	0
3	A	1316	GOL	3	0
3	A	1324	GOL	3	0
3	A	1319	GOL	4	0
3	A	1323	GOL	4	0

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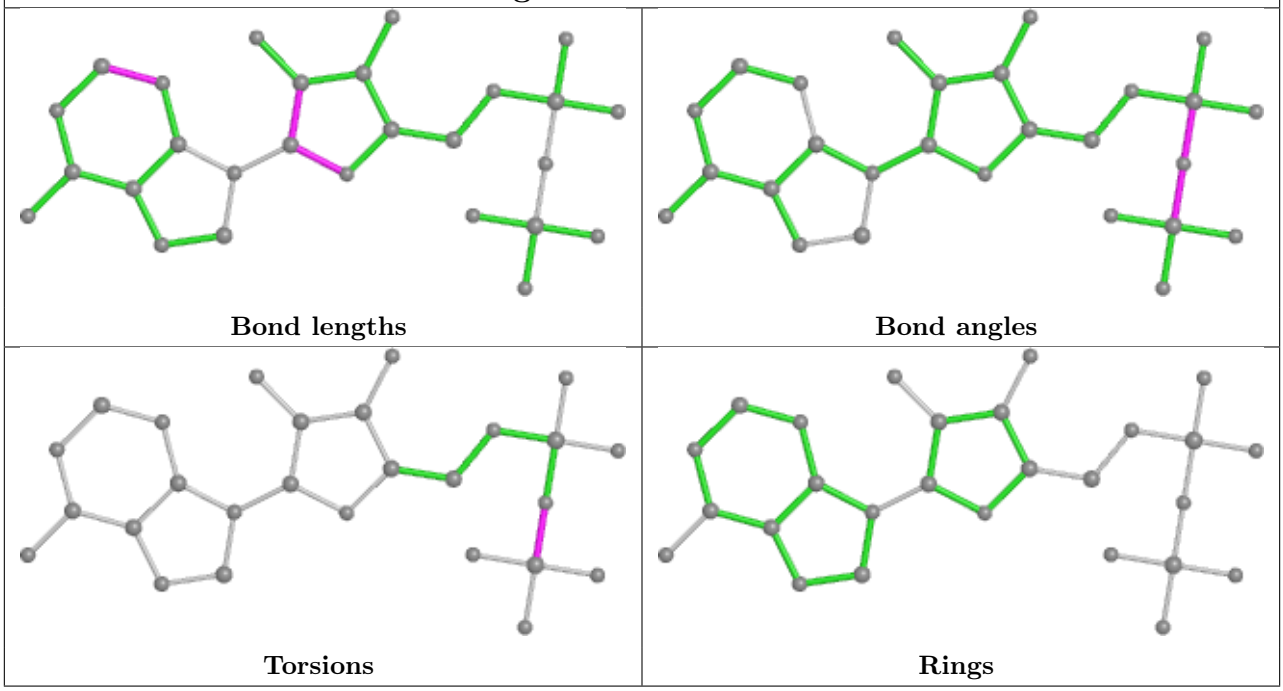
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1339	GOL	5	0
3	A	1327	GOL	3	0

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 1301



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	1290/1304 (98%)	-0.39	30 (2%) 60 56	13, 18, 37, 74	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	VAL	4.6
1	A	-4	PRO	4.5
1	A	-7	GLY	4.2
1	A	118	THR	3.9
1	A	-6	LEU	3.7
1	A	789	ASN	3.5
1	A	27	ASN	3.2
1	A	788	GLY	3.0
1	A	-8	SER	3.0
1	A	465	LEU	3.0
1	A	609	THR	2.7
1	A	176	LEU	2.7
1	A	117	SER	2.7
1	A	-1	SER	2.7
1	A	25	ALA	2.6
1	A	-2	GLY	2.6
1	A	29	GLN	2.6
1	A	122	GLU	2.6
1	A	121	ALA	2.5
1	A	120	THR	2.5
1	A	608	LYS	2.4
1	A	449	GLY	2.4
1	A	969	ASN	2.3
1	A	786	GLN	2.2
1	A	28	LEU	2.2
1	A	607	GLY	2.2
1	A	790	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	259[A]	ASN	2.1
1	A	119	LEU	2.1
1	A	0	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	GOL	A	1336	6/6	0.59	0.23	39,43,44,48	0
3	GOL	A	1324	6/6	0.61	0.27	45,52,58,59	0
3	GOL	A	1333	6/6	0.73	0.34	50,56,67,70	0
3	GOL	A	1330	6/6	0.74	0.35	52,55,61,64	0
3	GOL	A	1341	6/6	0.74	0.28	47,56,61,66	0
3	GOL	A	1337	6/6	0.78	0.18	57,59,61,62	0
3	GOL	A	1327	6/6	0.79	0.25	58,64,70,87	0
3	GOL	A	1313	6/6	0.79	0.32	32,54,69,74	0
3	GOL	A	1334	6/6	0.80	0.24	53,70,75,76	0
3	GOL	A	1318	6/6	0.81	0.28	33,46,50,50	0
3	GOL	A	1322	6/6	0.81	0.28	44,55,60,75	0
3	GOL	A	1317	6/6	0.83	0.36	47,55,63,68	0
3	GOL	A	1316	6/6	0.83	0.17	55,61,62,66	0
3	GOL	A	1321	6/6	0.83	0.38	42,50,57,58	0
3	GOL	A	1311	6/6	0.84	0.18	36,48,53,62	0
3	GOL	A	1338	6/6	0.84	0.31	51,60,64,67	0
3	GOL	A	1312	6/6	0.84	0.22	36,57,61,74	0
4	SO4	A	1357	5/5	0.84	0.33	66,73,87,100	0
3	GOL	A	1335	6/6	0.85	0.27	54,59,63,76	0
3	GOL	A	1328	6/6	0.85	0.23	55,62,63,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1325	6/6	0.86	0.16	52,59,63,76	0
3	GOL	A	1339	6/6	0.86	0.29	35,46,55,58	0
3	GOL	A	1340	6/6	0.88	0.22	34,46,52,55	0
4	SO4	A	1359	5/5	0.88	0.36	54,60,64,68	0
3	GOL	A	1308	6/6	0.89	0.14	25,29,30,33	0
3	GOL	A	1319	6/6	0.89	0.28	40,41,44,65	0
3	GOL	A	1326	6/6	0.89	0.14	31,45,62,64	0
3	GOL	A	1304[A]	6/6	0.89	0.16	21,26,27,29	6
3	GOL	A	1304[B]	6/6	0.89	0.16	21,28,28,29	6
3	GOL	A	1329	6/6	0.89	0.18	29,42,50,52	0
4	SO4	A	1360	5/5	0.89	0.32	76,82,100,107	0
3	GOL	A	1314	6/6	0.90	0.13	30,34,36,36	0
3	GOL	A	1331	6/6	0.90	0.26	27,49,55,56	0
3	GOL	A	1315	6/6	0.90	0.23	44,57,63,74	0
3	GOL	A	1320	6/6	0.90	0.35	35,42,44,63	0
3	GOL	A	1309	6/6	0.90	0.18	30,31,42,46	0
3	GOL	A	1306	6/6	0.90	0.27	25,48,49,50	0
3	GOL	A	1323	6/6	0.90	0.32	31,38,46,50	0
3	GOL	A	1310	6/6	0.91	0.14	23,28,35,38	0
3	GOL	A	1302	6/6	0.91	0.21	16,33,35,40	0
4	SO4	A	1354	5/5	0.92	0.21	61,69,71,83	0
4	SO4	A	1351	5/5	0.92	0.13	33,47,56,58	0
4	SO4	A	1352	5/5	0.93	0.27	33,39,46,48	0
3	GOL	A	1332	6/6	0.93	0.16	42,53,61,73	0
4	SO4	A	1355	5/5	0.93	0.25	53,67,70,76	0
4	SO4	A	1356	5/5	0.94	0.20	69,73,85,86	0
3	GOL	A	1307	6/6	0.94	0.10	26,30,32,33	0
4	SO4	A	1358	5/5	0.95	0.36	78,82,88,98	0
3	GOL	A	1305	6/6	0.95	0.08	17,20,24,26	0
4	SO4	A	1350	5/5	0.95	0.14	40,52,55,59	0
4	SO4	A	1345	5/5	0.96	0.17	19,28,32,33	0
3	GOL	A	1303	6/6	0.97	0.11	16,22,24,30	0
4	SO4	A	1349	5/5	0.97	0.23	40,40,47,50	0
4	SO4	A	1346	5/5	0.98	0.08	27,31,36,36	0
4	SO4	A	1348	5/5	0.98	0.21	37,39,46,47	0
4	SO4	A	1353	5/5	0.98	0.16	28,30,34,36	0
4	SO4	A	1344	5/5	0.98	0.09	28,34,41,46	0
4	SO4	A	1343	5/5	0.98	0.05	20,22,26,30	0
4	SO4	A	1342	5/5	0.99	0.07	23,24,26,29	0
4	SO4	A	1347	5/5	0.99	0.17	29,34,39,44	0
2	ADP	A	1301	27/27	0.99	0.08	12,12,14,14	0
5	MG	A	1361	1/1	1.00	0.04	13,13,13,13	0

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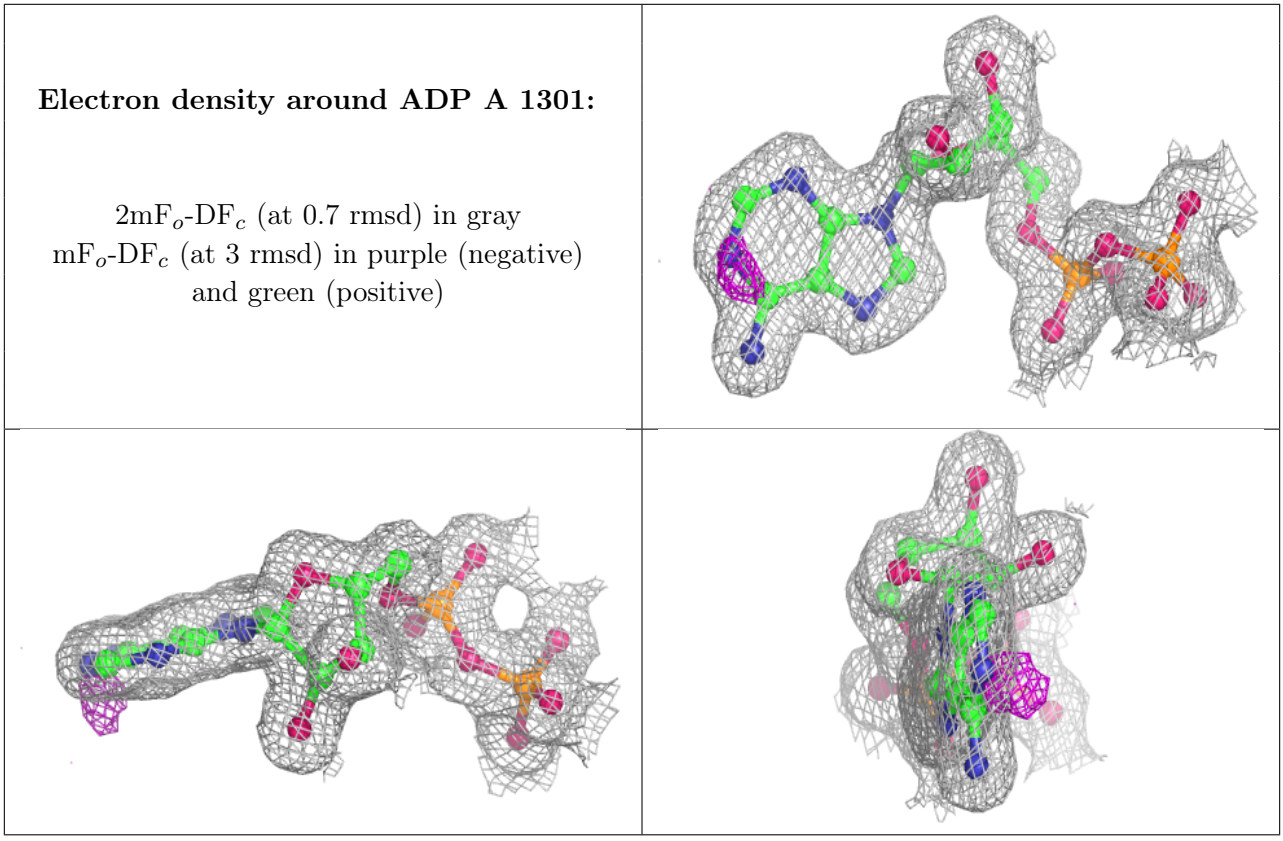
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1362	1/1	1.00	0.07	13,13,13,13	0
5	MG	A	1363	1/1	1.00	0.09	13,13,13,13	0

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 1301:

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



6.5 Other polymers (i)

There are no such residues in this entry.