Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:21 am BST

PDB ID	:	4L78
Title	:	Xenon Trapping and Statistical Coupling Analysis Uncover Regions Important for Structure and Function of Multidomain Protein StPurL
Authors	:	Tanwar, A.S.; Goyal, V.D.; Choudhary, D.; Panjikar, S.; Anand, R.
Deposited on	:	2013-06-13
Resolution	:	2.18 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 following versions of software and data (see references ⓘ) were used in the production of this report:

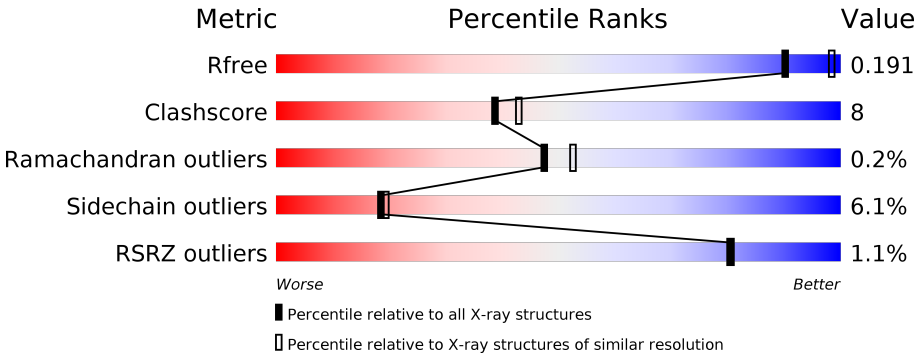
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on 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	% 81% 14%

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
6	XE	A	1320	-	-	X	-
6	XE	A	1323	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10897 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.

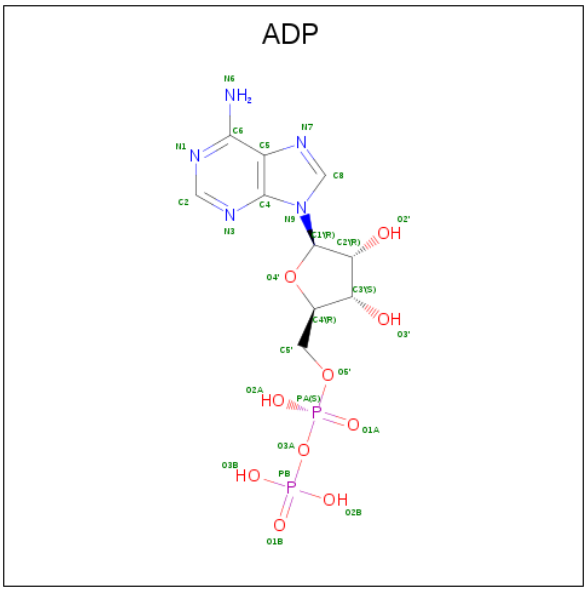
- Molecule 1 is a protein called Phosphoribosylformylglycinamidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1285	Total	C	N	O	S	0	1	0
			9897	6212	1764	1873	48			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P74881
A	-6	LEU	-	EXPRESSION TAG	UNP P74881
A	-5	VAL	-	EXPRESSION TAG	UNP P74881
A	-4	PRO	-	EXPRESSION TAG	UNP P74881
A	-3	ARG	-	EXPRESSION TAG	UNP P74881
A	-2	GLY	-	EXPRESSION TAG	UNP P74881
A	-1	SER	-	EXPRESSION TAG	UNP P74881
A	0	HIS	-	EXPRESSION TAG	UNP P74881
A	1263	ALA	ARG	ENGINEERED MUTATION	UNP P74881

- Molecule 2 is 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		

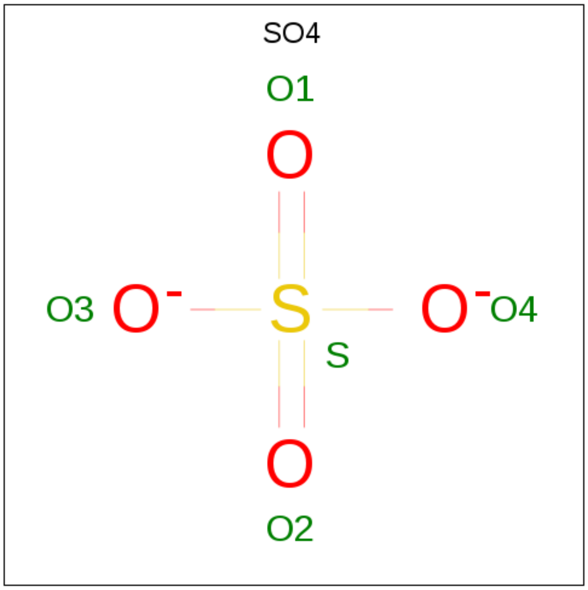
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

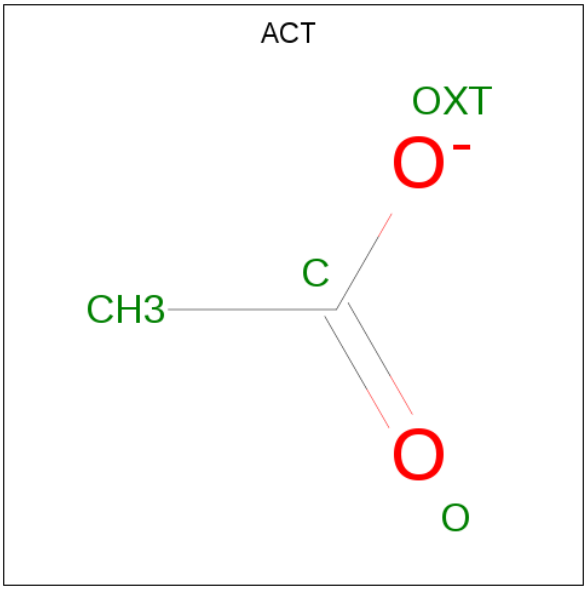
- Molecule 6 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total Xe 5 5	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

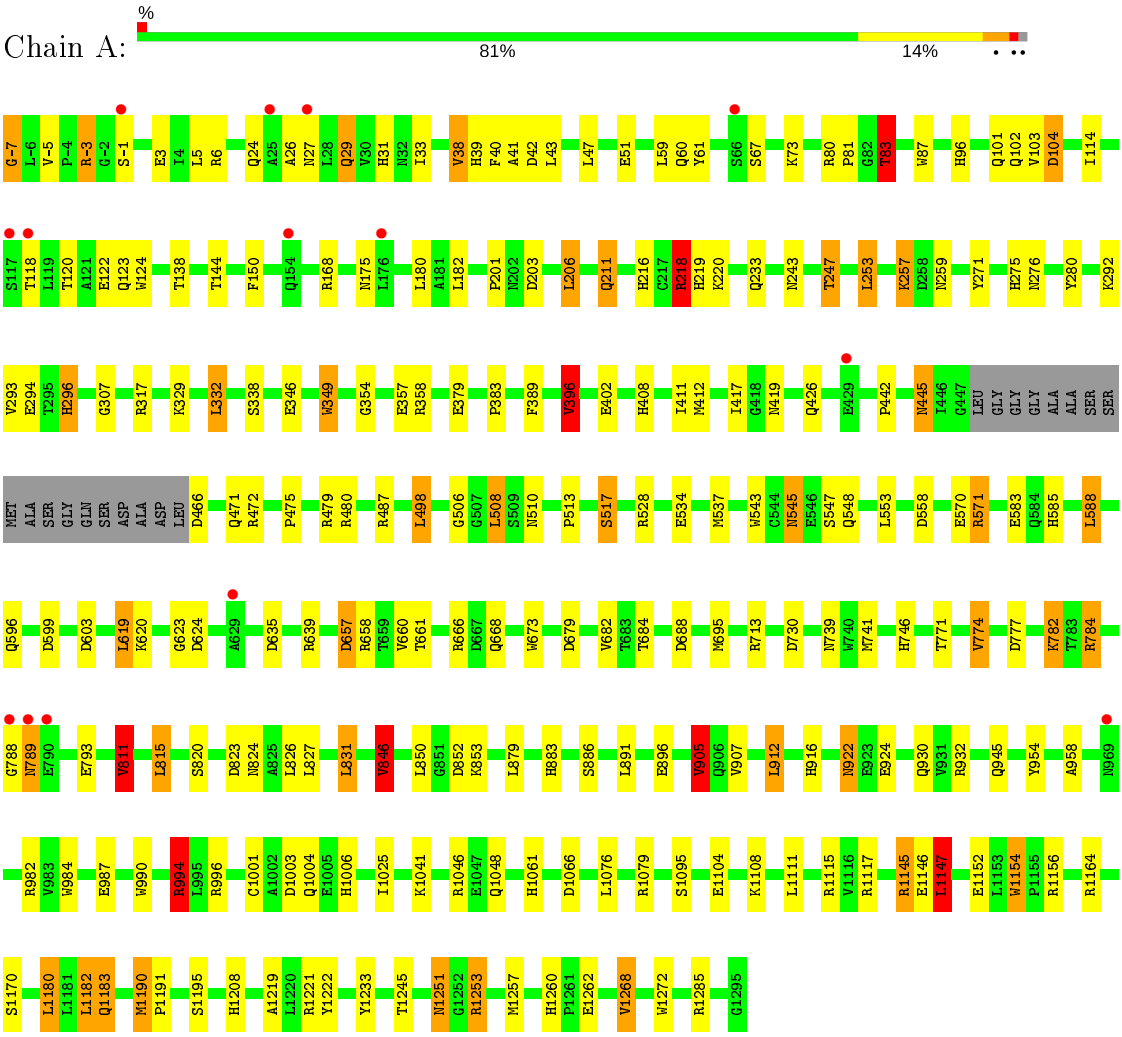
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	892	Total O 892 892	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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	146.68Å 146.68Å 141.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.57 – 2.18 19.57 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.57-2.18) 100.0 (19.57-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	5.80 (at 2.17Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.139 , 0.188 0.141 , 0.191	Depositor DCC
R_{free} test set	1068 reflections (1.19%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10897	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: MG, ADP, CL, MN, XE, CYG, SO4, ACT

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	17/10098 (0.2%)	1.16	71/13708 (0.5%)

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	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1156	ARG	CZ-NH1	9.07	1.44	1.33
1	A	349	TRP	CD2-CE2	7.61	1.50	1.41
1	A	673	TRP	CD2-CE2	6.77	1.49	1.41
1	A	1272	TRP	CD2-CE2	6.21	1.48	1.41
1	A	479	ARG	CD-NE	-6.20	1.35	1.46
1	A	570	GLU	CD-OE1	6.04	1.32	1.25
1	A	1253	ARG	CZ-NH1	5.92	1.40	1.33
1	A	984	TRP	CD2-CE2	5.83	1.48	1.41
1	A	994	ARG	CD-NE	-5.83	1.36	1.46
1	A	-7	GLY	N-CA	5.71	1.54	1.46
1	A	1152	GLU	CG-CD	5.60	1.60	1.51
1	A	124	TRP	CD2-CE2	5.52	1.48	1.41
1	A	543	TRP	CD2-CE2	5.34	1.47	1.41
1	A	87	TRP	CG-CD2	5.06	1.52	1.43
1	A	1154	TRP	CD2-CE2	5.06	1.47	1.41
1	A	990	TRP	CD2-CE2	5.04	1.47	1.41
1	A	987	GLU	CD-OE2	-5.04	1.20	1.25

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	479	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	479	ARG	NE-CZ-NH1	16.05	128.32	120.30
1	A	1156	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	A	932	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	480	ARG	NE-CZ-NH2	-13.37	113.61	120.30
1	A	994	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	480	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	A	1253	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	A	932	ARG	NE-CZ-NH2	-10.27	115.16	120.30
1	A	1156	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	A	994	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	571	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	994	ARG	CG-CD-NE	-8.84	93.24	111.80
1	A	218	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	A	218	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	1164	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	811	VAL	CG1-CB-CG2	7.99	123.68	110.90
1	A	332	LEU	CB-CG-CD2	7.92	124.46	111.00
1	A	1253	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	1147	LEU	CB-CG-CD1	7.88	124.39	111.00
1	A	1221	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	774	VAL	CB-CA-C	-7.54	97.06	111.40
1	A	846	VAL	CG1-CB-CG2	7.50	122.90	110.90
1	A	1025	ILE	CG1-CB-CG2	-7.50	94.91	111.40
1	A	1115	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	203	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	253	LEU	CB-CG-CD1	7.40	123.58	111.00
1	A	83	THR	CA-CB-CG2	7.39	122.74	112.40
1	A	635	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	657	ASP	CB-CG-OD1	7.35	124.92	118.30
1	A	815	LEU	CA-CB-CG	-7.34	98.42	115.30
1	A	571	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	1180	LEU	CB-CG-CD1	7.17	123.19	111.00
1	A	588	LEU	CB-CG-CD2	7.17	123.19	111.00
1	A	831	LEU	CB-CG-CD1	7.03	122.94	111.00
1	A	358	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	891	LEU	CA-CB-CG	-6.79	99.69	115.30
1	A	508	LEU	CB-CG-CD1	6.71	122.41	111.00
1	A	332	LEU	CA-CB-CG	6.63	130.54	115.30
1	A	1046	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	1079	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	A	1221	ARG	NE-CZ-NH2	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	905	VAL	CG1-CB-CG2	6.45	121.22	110.90
1	A	1268	VAL	CB-CA-C	-6.27	99.48	111.40
1	A	168	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	396	VAL	CG1-CB-CG2	6.25	120.89	110.90
1	A	479	ARG	CB-CG-CD	-6.24	95.37	111.60
1	A	730	ASP	CB-CG-OD1	6.21	123.88	118.30
1	A	83	THR	N-CA-CB	-6.12	98.68	110.30
1	A	846	VAL	CA-CB-CG1	6.09	120.03	110.90
1	A	713	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	826	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	688	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	104	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	815	LEU	CB-CG-CD1	5.53	120.39	111.00
1	A	466	ASP	N-CA-C	-5.52	96.09	111.00
1	A	487	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	639	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	619	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	1145	ARG	CB-CA-C	-5.33	99.74	110.40
1	A	945	GLN	CB-CA-C	-5.32	99.77	110.40
1	A	912	LEU	CB-CG-CD1	5.29	120.00	111.00
1	A	358	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	774	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	A	891	LEU	CB-CG-CD1	5.18	119.81	111.00
1	A	1152	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	A	603	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	558	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	1190	MET	CG-SD-CE	5.06	108.29	100.20
1	A	996	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	498	LEU	CB-CG-CD1	5.00	119.51	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ALA	Peptide
1	A	788	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	9897	0	9674	148	0
2	A	27	0	12	1	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	60	0	0	1	0
6	A	5	0	0	5	0
7	A	3	0	0	1	0
8	A	8	0	6	0	0
9	A	892	0	0	40	2
All	All	10897	0	9692	148	2

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 (148) 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:60:GLN:CB	9:A:1794:HOH:O	1.76	1.23
1:A:824:ASN:HD21	1:A:958:ALA:H	1.15	0.92
1:A:276:ASN:HB2	9:A:1837:HOH:O	1.73	0.88
1:A:1257:MET:HE1	9:A:1959:HOH:O	1.73	0.87
1:A:175:ASN:HD21	1:A:182:LEU:H	1.23	0.87
1:A:402:GLU:HG3	9:A:1601:HOH:O	1.76	0.86
1:A:782:LYS:HE2	1:A:784:ARG:NH2	1.92	0.85
1:A:820:SER:H	1:A:930:GLN:HE22	1.21	0.84
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.58	0.83
1:A:120:THR:H	1:A:123:GLN:NE2	1.76	0.82
1:A:746:HIS:HD2	9:A:2135:HOH:O	1.62	0.82
1:A:1257:MET:CE	9:A:1959:HOH:O	2.26	0.81
1:A:545:ASN:HD22	1:A:547:SER:H	1.25	0.81
1:A:823:ASP:HB3	9:A:1865:HOH:O	1.82	0.78
1:A:120:THR:H	1:A:123:GLN:HE21	1.27	0.78
1:A:96:HIS:HE1	1:A:103:VAL:O	1.68	0.77
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.34	0.76
1:A:695:MET:HG3	6:A:1320:XE:XE	2.65	0.75
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.52	0.75
1:A:73:LYS:HE3	9:A:1922:HOH:O	1.87	0.75
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.71	0.73
1:A:1117:ARG:HD3	1:A:1147:LEU:HD11	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.71	0.72
1:A:-3:ARG:HD3	1:A:42:ASP:OD1	1.88	0.72
1:A:1104:GLU:CD	9:A:1758:HOH:O	2.27	0.72
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.71	0.72
1:A:1251:ASN:ND2	1:A:1253:ARG:H	1.89	0.71
1:A:80:ARG:HA	1:A:138:THR:HG22	1.70	0.71
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.74	0.70
1:A:-3:ARG:HD2	1:A:150:PHE:HB2	1.73	0.70
1:A:1076:LEU:HD21	9:A:1442:HOH:O	1.91	0.70
1:A:346:GLU:OE1	9:A:2259:HOH:O	2.10	0.69
1:A:657:ASP:OD1	1:A:660:VAL:HG12	1.92	0.69
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.37	0.69
1:A:922:ASN:HD22	1:A:924:GLU:H	1.39	0.69
1:A:296:HIS:HE1	9:A:1995:HOH:O	1.76	0.68
1:A:5:LEU:HD22	1:A:59:LEU:HD12	1.76	0.68
1:A:402:GLU:CG	9:A:1601:HOH:O	2.39	0.68
1:A:275:HIS:HD2	9:A:2075:HOH:O	1.76	0.67
1:A:80:ARG:CB	9:A:2016:HOH:O	2.42	0.66
1:A:317:ARG:HH22	1:A:548:GLN:NE2	1.92	0.66
1:A:83:THR:HG21	9:A:1761:HOH:O	1.95	0.65
1:A:81:PRO:HD3	1:A:138:THR:CG2	2.26	0.64
1:A:1183:GLN:HE22	1:A:1285:ARG:HH21	1.44	0.64
1:A:1004:GLN:NE2	1:A:1233:TYR:H	1.95	0.64
1:A:211:GLN:NE2	9:A:1786:HOH:O	2.31	0.63
1:A:357:GLU:HB3	9:A:1625:HOH:O	1.99	0.63
1:A:-7:GLY:O	1:A:3:GLU:HG3	1.99	0.63
1:A:218:ARG:HD2	1:A:220:LYS:HG3	1.81	0.63
1:A:243:ASN:O	1:A:247:THR:HG23	1.99	0.63
1:A:80:ARG:O	1:A:83:THR:HB	1.99	0.62
1:A:471:GLN:HE21	1:A:472:ARG:H	1.47	0.62
1:A:905:VAL:HG13	1:A:907:VAL:HG13	1.80	0.62
1:A:33:ILE:HD12	1:A:114:ILE:HG12	1.83	0.61
1:A:789:ASN:H	1:A:789:ASN:ND2	1.99	0.61
1:A:571:ARG:HD3	9:A:2049:HOH:O	2.02	0.60
1:A:1076:LEU:HD11	9:A:1442:HOH:O	2.02	0.60
1:A:513:PRO:O	1:A:517:SER:HB2	2.00	0.60
1:A:211:GLN:OE1	7:A:1326:CL:CL	2.57	0.59
1:A:73:LYS:CE	9:A:1922:HOH:O	2.48	0.59
1:A:81:PRO:CD	1:A:138:THR:HG21	2.31	0.58
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.85	0.58
1:A:823:ASP:CB	9:A:1865:HOH:O	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.89	0.56
1:A:354:GLY:O	1:A:408:HIS:HE1	1.88	0.56
1:A:29:GLN:HE22	1:A:31[B]:HIS:CE1	2.24	0.56
1:A:1208:HIS:HB2	9:A:2206:HOH:O	2.06	0.56
1:A:1108:LYS:NZ	9:A:1758:HOH:O	2.37	0.55
1:A:101:GLN:HG3	9:A:1704:HOH:O	2.06	0.55
1:A:782:LYS:HE2	1:A:784:ARG:HH22	1.70	0.55
1:A:96:HIS:HD2	9:A:1559:HOH:O	1.89	0.55
1:A:402:GLU:CB	9:A:1601:HOH:O	2.55	0.54
1:A:585:HIS:HD2	9:A:2149:HOH:O	1.90	0.54
1:A:338:SER:OG	1:A:408:HIS:HD2	1.90	0.54
1:A:175:ASN:ND2	1:A:182:LEU:H	2.00	0.54
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	1.91	0.53
1:A:329:LYS:CE	1:A:419:ASN:HD21	2.22	0.52
1:A:6:ARG:HD3	9:A:2223:HOH:O	2.10	0.51
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.08	0.51
1:A:402:GLU:HB2	9:A:1601:HOH:O	2.11	0.51
1:A:41:ALA:HB2	6:A:1323:XE:XE	2.89	0.51
1:A:545:ASN:ND2	1:A:547:SER:H	2.01	0.51
1:A:682:VAL:CG1	1:A:811:VAL:HG22	2.41	0.51
1:A:39:HIS:CE1	1:A:61:TYR:OH	2.59	0.51
1:A:1004:GLN:HE21	1:A:1233:TYR:HB3	1.76	0.50
1:A:1006:HIS:HE1	9:A:1524:HOH:O	1.95	0.50
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.76	0.50
1:A:38:VAL:HG22	1:A:40:PHE:CZ	2.46	0.50
1:A:411:ILE:HG12	1:A:741:MET:HG2	1.93	0.50
1:A:257:LYS:NZ	1:A:426:GLN:OE1	2.45	0.50
1:A:1117:ARG:HG2	1:A:1147:LEU:HD21	1.93	0.50
1:A:668:GLN:HG2	2:A:1301:ADP:H1'	1.93	0.49
1:A:83:THR:CG2	9:A:1761:HOH:O	2.57	0.49
1:A:80:ARG:HA	1:A:138:THR:CG2	2.42	0.49
1:A:329:LYS:O	1:A:383:PRO:HD2	2.14	0.48
1:A:296:HIS:HD2	1:A:307:GLY:O	1.97	0.48
1:A:39:HIS:HD2	9:A:1522:HOH:O	1.97	0.48
1:A:120:THR:OG1	1:A:122:GLU:HB3	2.14	0.47
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.96	0.47
1:A:1170:SER:O	1:A:1191:PRO:HA	2.15	0.47
1:A:1260:HIS:CD2	1:A:1262:GLU:OE2	2.61	0.47
1:A:211:GLN:HG2	1:A:506:GLY:HA2	1.95	0.47
1:A:1041:LYS:HA	1:A:1066:ASP:O	2.14	0.47
1:A:96:HIS:CE1	1:A:103:VAL:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:GLN:O	1:A:1095:SER:HA	2.15	0.47
1:A:1006:HIS:HD2	9:A:2056:HOH:O	1.98	0.47
1:A:1182:LEU:HD23	1:A:1219:ALA:HB1	1.97	0.46
1:A:782:LYS:HD3	1:A:793:GLU:OE2	2.16	0.46
1:A:695:MET:CE	6:A:1320:XE:XE	3.42	0.46
1:A:233:GLN:NE2	9:A:1760:HOH:O	2.47	0.46
1:A:445:ASN:HD22	1:A:445:ASN:C	2.17	0.46
1:A:-7:GLY:O	1:A:3:GLU:HA	2.16	0.46
1:A:1145:ARG:HD3	1:A:1154:TRP:HB2	1.97	0.46
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.19	0.46
1:A:329:LYS:CE	1:A:419:ASN:ND2	2.79	0.45
1:A:534:GLU:HB3	1:A:537:MET:HG3	1.97	0.45
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	1.99	0.45
1:A:41:ALA:CB	6:A:1323:XE:XE	3.43	0.45
1:A:820:SER:N	1:A:930:GLN:HE22	2.01	0.45
1:A:994:ARG:HD2	1:A:1003:ASP:OD1	2.17	0.44
1:A:789:ASN:N	1:A:789:ASN:ND2	2.63	0.44
1:A:216:HIS:HE1	5:A:1307:SO4:O3	2.01	0.44
1:A:292:LYS:HD2	1:A:292:LYS:HA	1.84	0.44
1:A:51:GLU:CD	1:A:102:GLN:HE22	2.21	0.44
1:A:349:TRP:CZ3	1:A:846:VAL:HG22	2.53	0.43
1:A:211:GLN:HG2	1:A:506:GLY:CA	2.48	0.43
1:A:1001:CYS:HB3	1:A:1233:TYR:CD2	2.54	0.43
1:A:746:HIS:CD2	9:A:2135:HOH:O	2.50	0.43
1:A:219:HIS:CD2	1:A:777:ASP:OD1	2.70	0.43
1:A:1004:GLN:HE21	1:A:1233:TYR:H	1.65	0.42
1:A:1222:TYR:CE2	1:A:1245:THR:HB	2.54	0.42
1:A:379:GLU:HB3	1:A:475:PRO:HB2	2.01	0.42
1:A:916:HIS:HD2	9:A:1508:HOH:O	2.02	0.42
1:A:6:ARG:CD	9:A:2223:HOH:O	2.67	0.41
1:A:417:ILE:HD11	6:A:1320:XE:XE	2.98	0.41
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.56	0.41
1:A:3:GLU:OE1	1:A:5:LEU:HD11	2.21	0.41
1:A:815:LEU:HD13	1:A:879:LEU:HD12	2.01	0.41
1:A:1257:MET:HE3	9:A:1959:HOH:O	2.07	0.41
1:A:789:ASN:HD22	1:A:789:ASN:H	1.68	0.41
1:A:1117:ARG:HD2	1:A:1117:ARG:HH11	1.70	0.41
1:A:658:ARG:HD2	1:A:668:GLN:OE1	2.20	0.41
1:A:1061:HIS:HD2	9:A:1465:HOH:O	2.04	0.41
1:A:396:VAL:HG22	1:A:850:LEU:HB2	2.03	0.41
1:A:684:THR:HG22	1:A:811:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PRO:HB2	1:A:206:LEU:HD13	2.02	0.40
1:A:528:ARG:HD3	1:A:528:ARG:HA	1.90	0.40
1:A:623:GLY:HA3	1:A:852:ASP:HA	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1921:HOH:O	9:A:2288:HOH:O[5_555]	1.59	0.61
9:A:2101:HOH:O	9:A:2292:HOH:O[5_555]	1.92	0.28

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	1281/1303 (98%)	1242 (97%)	36 (3%)	3 (0%)	47 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	661	THR
1	A	886	SER

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	1027/1039 (99%)	964 (94%)	63 (6%)	18 19

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	-3	ARG
1	A	-1	SER
1	A	24	GLN
1	A	29	GLN
1	A	38	VAL
1	A	43	LEU
1	A	47	LEU
1	A	67	SER
1	A	83	THR
1	A	104	ASP
1	A	118	THR
1	A	144	THR
1	A	206	LEU
1	A	211	GLN
1	A	218	ARG
1	A	247	THR
1	A	253	LEU
1	A	257	LYS
1	A	259	ASN
1	A	294	GLU
1	A	296	HIS
1	A	332	LEU
1	A	389	PHE
1	A	396	VAL
1	A	412	MET
1	A	442	PRO
1	A	445	ASN
1	A	498	LEU
1	A	508	LEU
1	A	510	ASN
1	A	517	SER
1	A	545	ASN
1	A	553	LEU
1	A	583	GLU
1	A	588	LEU
1	A	596	GLN
1	A	619	LEU

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Mol	Chain	Res	Type
1	A	620	LYS
1	A	624	ASP
1	A	666	ARG
1	A	771	THR
1	A	774	VAL
1	A	782	LYS
1	A	784	ARG
1	A	789	ASN
1	A	811	VAL
1	A	831	LEU
1	A	846	VAL
1	A	853	LYS
1	A	905	VAL
1	A	912	LEU
1	A	922	ASN
1	A	982	ARG
1	A	994	ARG
1	A	1147	LEU
1	A	1180	LEU
1	A	1182	LEU
1	A	1183	GLN
1	A	1190	MET
1	A	1195	SER
1	A	1251	ASN
1	A	1268	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	39	HIS
1	A	96	HIS
1	A	123	GLN
1	A	126	GLN
1	A	152	HIS
1	A	175	ASN
1	A	216	HIS
1	A	219	HIS
1	A	233	GLN
1	A	275	HIS
1	A	296	HIS
1	A	408	HIS

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Mol	Chain	Res	Type
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	617	GLN
1	A	674	GLN
1	A	739	ASN
1	A	746	HIS
1	A	789	ASN
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	1026	ASN
1	A	1061	HIS
1	A	1114	HIS
1	A	1128	GLN
1	A	1183	GLN
1	A	1189	GLN
1	A	1251	ASN
1	A	1260	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	9,14,15	2.71	3 (33%)	6,17,19	5.12	4 (66%)

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	-	1/10/16/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	6.57	1.57	1.50
1	A	1135	CYG	OE2-CD1	3.37	1.26	1.21
1	A	1135	CYG	CD1-SG	2.82	1.83	1.76

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	CYG	OE2-CD1-CG1	-9.03	113.33	123.99
1	A	1135	CYG	CB1-CG1-CD1	-6.05	98.92	112.33
1	A	1135	CYG	CG1-CD1-SG	5.31	119.64	113.46
1	A	1135	CYG	OE2-CD1-SG	3.24	126.82	122.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
5	SO4	A	1316	-	4,4,4	0.46	0	6,6,6	1.27	1 (16%)
5	SO4	A	1314	-	4,4,4	0.20	0	6,6,6	0.97	0
5	SO4	A	1312	-	4,4,4	0.56	0	6,6,6	0.49	0
5	SO4	A	1318	-	4,4,4	0.18	0	6,6,6	0.91	0
5	SO4	A	1315	-	4,4,4	0.53	0	6,6,6	0.79	0
5	SO4	A	1311	-	4,4,4	0.49	0	6,6,6	0.55	0
8	ACT	A	1328	-	1,3,3	1.35	0	0,3,3	0.00	-
5	SO4	A	1310	-	4,4,4	0.94	0	6,6,6	0.59	0
5	SO4	A	1308	-	4,4,4	0.71	0	6,6,6	0.69	0
8	ACT	A	1327	-	1,3,3	1.38	0	0,3,3	0.00	-
5	SO4	A	1317	-	4,4,4	0.39	0	6,6,6	1.15	0
2	ADP	A	1301	3	24,29,29	1.01	2 (8%)	29,45,45	1.66	6 (20%)
5	SO4	A	1307	-	4,4,4	0.83	0	6,6,6	0.40	0
5	SO4	A	1309	-	4,4,4	0.50	0	6,6,6	0.69	0
5	SO4	A	1313	-	4,4,4	0.43	0	6,6,6	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1301	3	-	2/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	O3'-C3'	2.60	1.49	1.43
2	A	1301	ADP	O4'-C1'	2.13	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1301	ADP	N3-C2-N1	-4.33	121.92	128.68
2	A	1301	ADP	C2-N1-C6	3.97	125.55	118.75
5	A	1316	SO4	O3-S-O1	2.59	122.81	109.31
2	A	1301	ADP	O2A-PA-O1A	2.39	124.05	112.24
2	A	1301	ADP	C5-C6-N1	-2.33	115.07	120.35
2	A	1301	ADP	PA-O3A-PB	-2.20	125.27	132.83
2	A	1301	ADP	O3B-PB-O2B	2.03	115.41	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O3B
2	A	1301	ADP	PA-O3A-PB-O2B

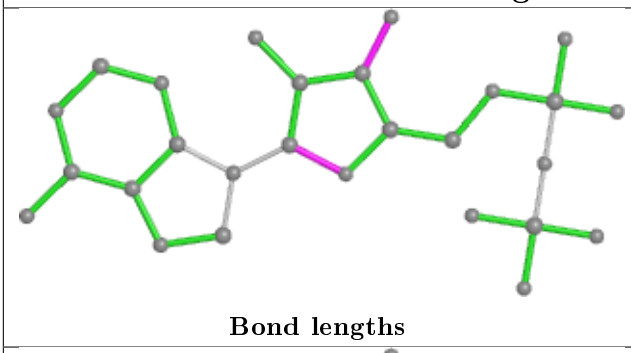
There are no ring outliers.

2 monomers are involved in 2 short contacts:

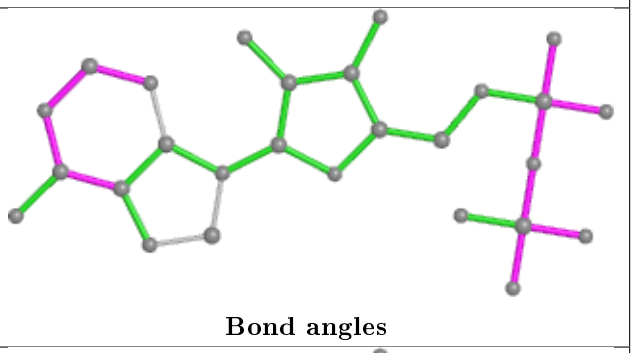
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	ADP	1	0
5	A	1307	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

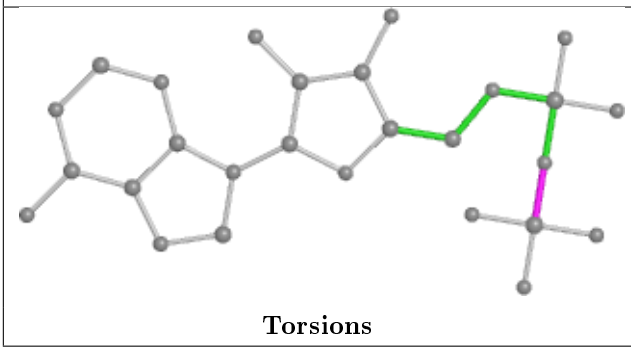
Ligand ADP A 1301



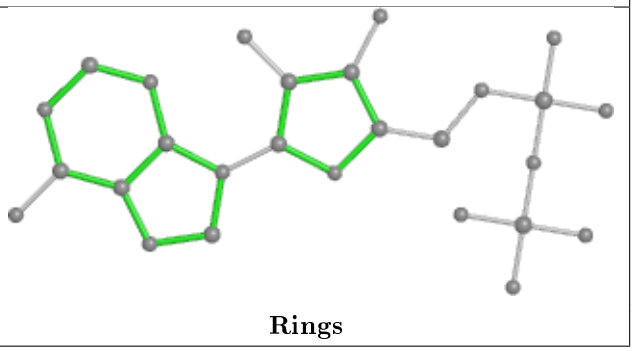
Bond lengths



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, 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	1284/1303 (98%)	-0.73	14 (1%)	80	80	10, 17, 37, 66	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	4.3
1	A	789	ASN	3.6
1	A	117	SER	3.5
1	A	25	ALA	3.3
1	A	-1	SER	3.2
1	A	788	GLY	2.9
1	A	429	GLU	2.9
1	A	66	SER	2.6
1	A	27	ASN	2.6
1	A	154	GLN	2.3
1	A	790	GLU	2.3
1	A	969	ASN	2.2
1	A	176	LEU	2.2
1	A	629	ALA	2.1

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

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	0.98	0.08	9,11,14,15	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.

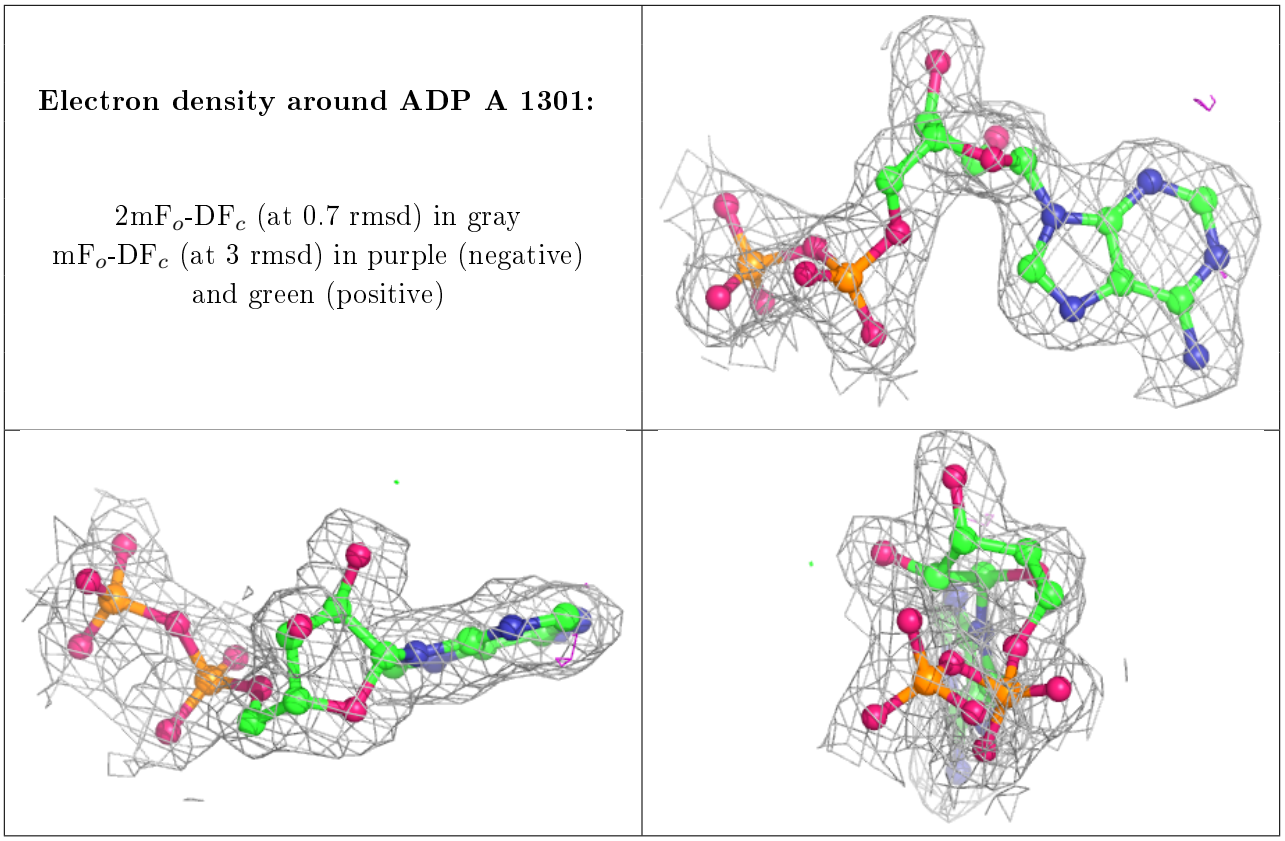
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MN	A	1306	1/1	0.91	0.10	56,56,56,56	0
8	ACT	A	1328	4/4	0.93	0.19	39,39,40,44	0
8	ACT	A	1327	4/4	0.94	0.16	34,34,35,36	0
5	SO4	A	1318	5/5	0.95	0.10	24,24,25,28	5
7	CL	A	1325	1/1	0.95	0.05	44,44,44,44	0
6	XE	A	1321	1/1	0.95	0.07	33,33,33,33	1
5	SO4	A	1316	5/5	0.96	0.13	33,39,47,51	0
5	SO4	A	1315	5/5	0.97	0.14	37,42,43,44	0
5	SO4	A	1310	5/5	0.97	0.18	29,35,40,42	0
5	SO4	A	1307	5/5	0.97	0.13	39,40,43,45	0
6	XE	A	1323	1/1	0.98	0.03	31,31,31,31	1
5	SO4	A	1309	5/5	0.98	0.18	34,36,39,40	0
5	SO4	A	1317	5/5	0.98	0.09	19,20,21,22	5
7	CL	A	1326	1/1	0.98	0.07	32,32,32,32	0
2	ADP	A	1301	27/27	0.99	0.05	10,11,13,14	0
3	MG	A	1302	1/1	0.99	0.02	12,12,12,12	0
3	MG	A	1303	1/1	0.99	0.03	14,14,14,14	0
5	SO4	A	1311	5/5	0.99	0.17	35,36,40,47	0
3	MG	A	1305	1/1	0.99	0.16	4,4,4,4	0
7	CL	A	1324	1/1	0.99	0.03	29,29,29,29	0
5	SO4	A	1308	5/5	0.99	0.06	22,25,29,31	0
5	SO4	A	1312	5/5	0.99	0.10	28,28,31,31	0
5	SO4	A	1313	5/5	0.99	0.24	42,46,50,53	0
5	SO4	A	1314	5/5	0.99	0.12	26,27,33,34	0
3	MG	A	1304	1/1	0.99	0.02	10,10,10,10	0
6	XE	A	1322	1/1	1.00	0.02	26,26,26,26	1
6	XE	A	1319	1/1	1.00	0.03	15,15,15,15	0
6	XE	A	1320	1/1	1.00	0.02	21,21,21,21	1

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.