



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:46 PM UTC

PDB ID : 4MGH / pdb_00004mgh
Title : Importance of Hydrophobic Cavities in Allosteric Regulation of Formylglycinamide Synthetase: Insight from Xenon Trapping and Statistical Coupling Analysis
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Deposited on : 2013-08-28
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

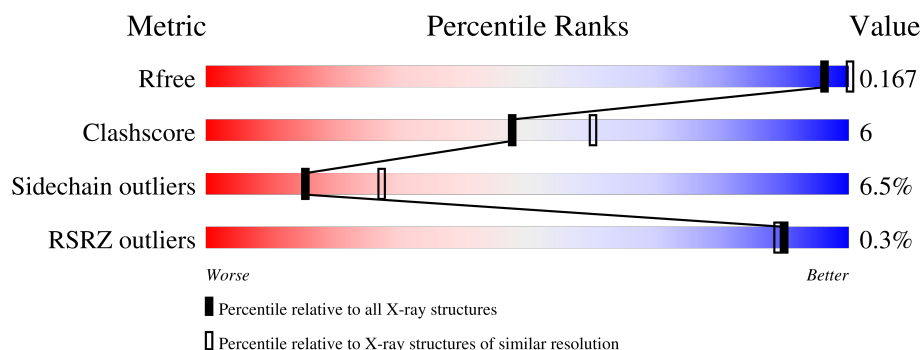
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1303	83% 13% ..

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	ACT	A	1320	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10514 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

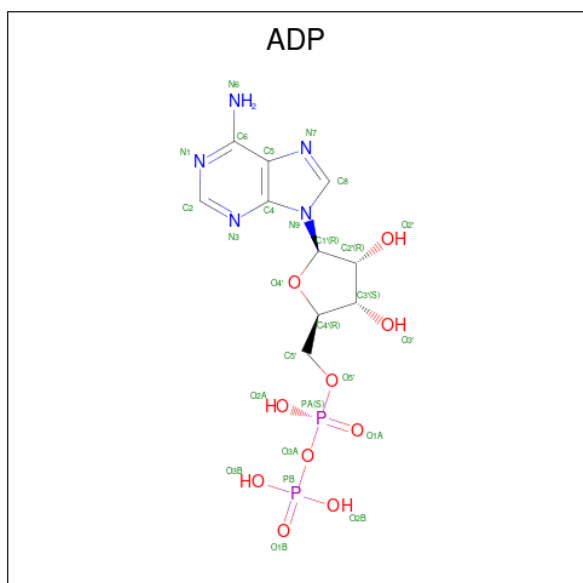
- Molecule 1 is a protein called Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1284	9879	6204	1757	1870	48	0	0	0

There are 8 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

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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		

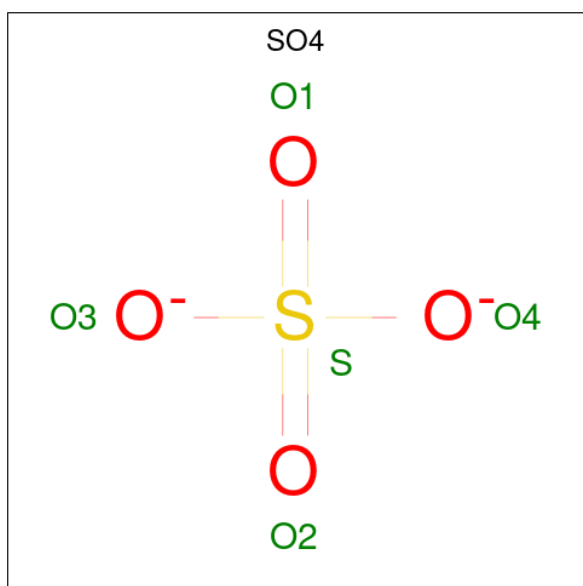
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



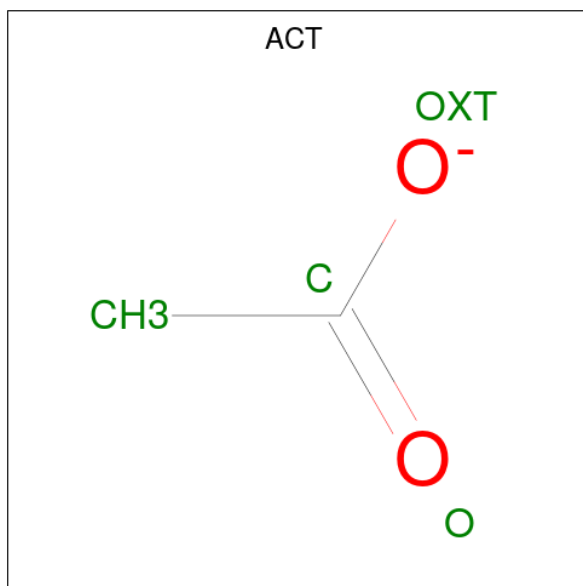
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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

- Molecule 7 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Xe	0	0
			4	4		

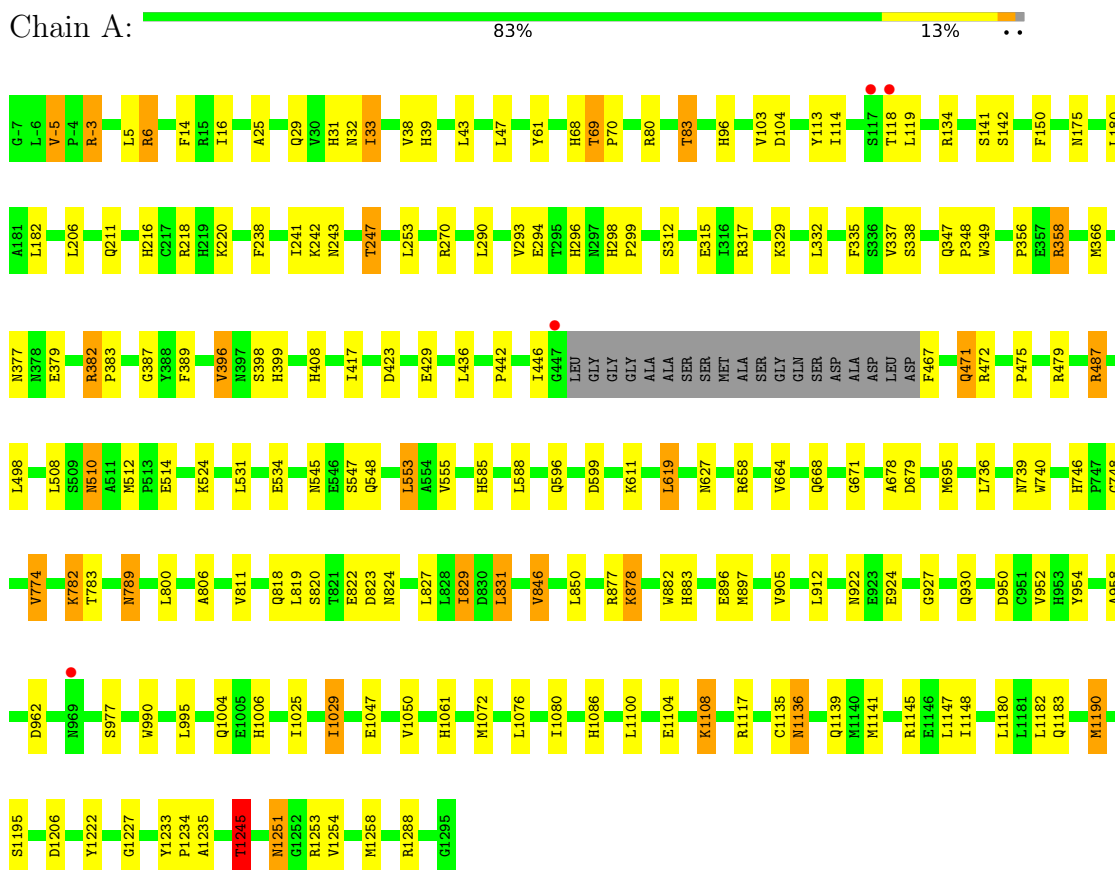
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	518	Total	O	0	0
			518	518		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoribosylformylglycinamide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	146.45Å 146.45Å 141.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.65 19.99 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.65) 99.7 (19.99-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.42 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.153 , 0.203 (Not available) , 0.167	Depositor DCC
R_{free} test set	1176 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10514	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 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CYG, ADP, MN, SO4, ACT, XE

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	1.06	5/10076 (0.0%)	1.07	19/13675 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1227	GLY	C-O	-6.06	1.16	1.24
1	A	952	VAL	C-O	-6.01	1.17	1.24
1	A	-5	VAL	CA-C	5.77	1.58	1.52
1	A	387	GLY	C-O	-5.21	1.18	1.24
1	A	627	ASN	CA-C	5.01	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ILE	N-CA-C	7.63	118.12	111.56
1	A	1190	MET	CA-C-N	-6.45	113.99	120.31
1	A	1190	MET	C-N-CA	-6.45	113.99	120.31
1	A	774	VAL	CB-CA-C	-6.33	99.09	110.48
1	A	-5	VAL	CB-CA-C	6.26	115.47	109.33
1	A	69	THR	CB-CA-C	5.87	117.83	109.38
1	A	789	ASN	N-CA-C	-5.83	105.48	112.59
1	A	746	HIS	CA-C-N	-5.69	113.69	119.83
1	A	746	HIS	C-N-CA	-5.69	113.69	119.83
1	A	312	SER	N-CA-C	5.66	117.13	111.07
1	A	1148	ILE	N-CA-C	5.52	114.03	107.73
1	A	1245	THR	CB-CA-C	-5.52	100.25	109.75
1	A	211	GLN	CB-CG-CD	5.43	121.83	112.60
1	A	25	ALA	N-CA-C	5.31	117.49	111.11
1	A	806	ALA	N-CA-C	5.25	117.06	108.55
1	A	-5	VAL	N-CA-CB	-5.10	106.18	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	GLY	CA-C-N	5.04	125.06	119.32
1	A	671	GLY	C-N-CA	5.04	125.06	119.32
1	A	487	ARG	NE-CZ-NH2	-5.00	114.69	119.20

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	9879	0	9656	110	0
2	A	27	0	12	0	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
5	A	65	0	0	4	0
6	A	16	0	12	5	0
7	A	4	0	0	1	0
8	A	518	0	0	18	0
All	All	10514	0	9680	111	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 6.

All (111) 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:782:LYS:NZ	8:A:1548:HOH:O	1.92	1.02
1:A:335:PHE:HB3	1:A:366:MET:HE1	1.47	0.93
1:A:80:ARG:CD	8:A:1716:HOH:O	2.19	0.88
1:A:820:SER:H	1:A:930:GLN:HE22	1.30	0.79
1:A:829:ILE:HD13	1:A:829:ILE:N	2.00	0.77
1:A:218:ARG:CZ	1:A:220:LYS:HE2	2.15	0.76
1:A:877:ARG:NH1	8:A:1852:HOH:O	2.19	0.75
1:A:175:ASN:HD21	1:A:182:LEU:H	1.36	0.73
1:A:1145:ARG:NH2	5:A:1317:SO4:O3	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.89	0.72
1:A:824:ASN:HD21	1:A:958:ALA:H	1.37	0.70
1:A:467:PHE:N	8:A:1618:HOH:O	2.24	0.69
1:A:358:ARG:NH2	8:A:1741:HOH:O	2.18	0.69
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.76	0.68
1:A:6:ARG:NH2	8:A:1831:HOH:O	2.21	0.67
1:A:243:ASN:O	1:A:247:THR:HG23	1.95	0.67
1:A:377:ASN:OD1	1:A:382:ARG:HD2	1.93	0.67
1:A:-3:ARG:HD2	1:A:150:PHE:HB2	1.81	0.63
1:A:358:ARG:NH1	8:A:1741:HOH:O	2.30	0.62
1:A:68:HIS:ND1	6:A:1323:ACT:H1	2.14	0.62
1:A:80:ARG:O	1:A:83:THR:HB	2.00	0.61
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.84	0.61
1:A:531:LEU:H	6:A:1320:ACT:H2	1.66	0.60
1:A:335:PHE:CB	1:A:366:MET:HE1	2.26	0.58
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.70	0.57
1:A:96:HIS:HE1	1:A:103:VAL:O	1.87	0.57
1:A:1251:ASN:ND2	1:A:1253:ARG:H	2.03	0.57
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.88	0.56
1:A:70:PRO:HB3	1:A:113:TYR:CE1	2.41	0.56
1:A:471:GLN:HE21	1:A:472:ARG:H	1.53	0.56
1:A:922:ASN:HD22	1:A:924:GLU:H	1.53	0.56
1:A:29:GLN:HE21	1:A:31:HIS:HE1	1.54	0.55
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.07	0.54
1:A:950:ASP:HB2	8:A:1421:HOH:O	2.08	0.54
1:A:396:VAL:HG22	1:A:850:LEU:HB2	1.89	0.54
1:A:829:ILE:N	1:A:829:ILE:CD1	2.71	0.54
1:A:337:VAL:HG13	1:A:366:MET:HE3	1.90	0.53
1:A:33:ILE:HG12	1:A:114:ILE:HD12	1.91	0.53
1:A:337:VAL:CG1	1:A:366:MET:HE3	2.40	0.52
1:A:238:PHE:CE2	1:A:242:LYS:HE2	2.45	0.52
1:A:349:TRP:CZ3	1:A:846:VAL:HG22	2.45	0.51
1:A:1086:HIS:HD2	5:A:1310:SO4:O4	1.93	0.51
1:A:16:ILE:HG23	1:A:33:ILE:HG22	1.93	0.51
1:A:1006:HIS:HD2	8:A:1517:HOH:O	1.92	0.51
1:A:298:HIS:HB3	1:A:299:PRO:HD3	1.93	0.51
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.59	0.51
1:A:995:LEU:C	1:A:995:LEU:HD12	2.35	0.50
1:A:442:PRO:HA	6:A:1320:ACT:O	2.12	0.50
1:A:829:ILE:HG22	1:A:831:LEU:HD13	1.93	0.50
1:A:349:TRP:CE3	1:A:846:VAL:HG22	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:HD3	8:A:1547:HOH:O	2.12	0.49
1:A:338:SER:OG	1:A:408:HIS:HD2	1.95	0.49
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.48	0.49
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.20	0.49
1:A:423:ASP:HB2	8:A:1783:HOH:O	2.12	0.49
1:A:290:LEU:C	1:A:290:LEU:HD12	2.37	0.48
1:A:619:LEU:HD23	1:A:619:LEU:N	2.27	0.48
1:A:545:ASN:HD22	1:A:547:SER:H	1.60	0.48
1:A:695:MET:HE2	7:A:1325:XE:XE	2.92	0.48
1:A:-3:ARG:CD	1:A:150:PHE:HB2	2.44	0.47
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.97	0.47
1:A:1061:HIS:HD2	8:A:1455:HOH:O	1.97	0.47
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.63	0.47
1:A:510:ASN:O	1:A:514:GLU:HB2	2.14	0.47
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.80	0.46
1:A:819:LEU:HG	1:A:897:MET:HB3	1.98	0.46
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.96	0.46
1:A:14:PHE:HB3	5:A:1315:SO4:O3	2.15	0.46
1:A:1100:LEU:O	1:A:1104:GLU:HG3	2.16	0.46
1:A:298:HIS:HB3	1:A:299:PRO:CD	2.46	0.46
1:A:1029:ILE:HD13	1:A:1288:ARG:HB3	1.98	0.45
1:A:329:LYS:O	1:A:383:PRO:HD2	2.16	0.45
1:A:358:ARG:HD3	1:A:358:ARG:H	1.81	0.45
1:A:356:PRO:HG2	1:A:783:THR:CG2	2.47	0.45
1:A:658:ARG:O	1:A:664:VAL:HG21	2.15	0.45
1:A:824:ASN:HD21	1:A:958:ALA:N	2.07	0.45
1:A:1234:PRO:O	1:A:1235:ALA:C	2.60	0.45
1:A:1108:LYS:HE2	8:A:1913:HOH:O	2.16	0.45
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.14	0.45
1:A:32:ASN:ND2	8:A:1663:HOH:O	2.50	0.45
1:A:882:TRP:CH2	1:A:927:GLY:HA3	2.52	0.44
1:A:1025:ILE:HD13	1:A:1025:ILE:HG21	1.65	0.44
1:A:820:SER:OG	1:A:822:GLU:HG2	2.17	0.44
1:A:1141:MET:HE1	1:A:1254:VAL:HG13	2.00	0.44
1:A:315:GLU:OE1	1:A:382:ARG:NH2	2.37	0.44
1:A:1047:GLU:H	1:A:1050:VAL:HG21	1.82	0.44
1:A:990:TRP:HB2	1:A:1006:HIS:CD2	2.54	0.43
1:A:436:LEU:HD13	1:A:512:MET:HE2	1.99	0.43
1:A:668:GLN:HA	1:A:678:ALA:HB3	2.01	0.43
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.17	0.43
1:A:347:GLN:HB3	1:A:348:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:GLN:NE2	8:A:1566:HOH:O	2.51	0.42
6:A:1320:ACT:H3	8:A:1615:HOH:O	2.19	0.42
1:A:531:LEU:O	6:A:1320:ACT:O	2.38	0.42
1:A:337:VAL:HG13	1:A:366:MET:CE	2.49	0.42
1:A:398:SER:OG	1:A:399:HIS:N	2.52	0.42
1:A:1076:LEU:HD11	8:A:1405:HOH:O	2.18	0.42
1:A:740:TRP:CH2	1:A:800:LEU:HD22	2.54	0.41
1:A:358:ARG:CZ	8:A:1741:HOH:O	2.56	0.41
1:A:479:ARG:HA	1:A:479:ARG:HD2	1.98	0.41
1:A:335:PHE:O	1:A:389:PHE:HA	2.19	0.41
1:A:553:LEU:HD12	1:A:555:VAL:HG23	2.02	0.41
1:A:216:HIS:HE1	5:A:1307:SO4:O3	2.04	0.41
1:A:962:ASP:OD2	1:A:977:SER:OG	2.30	0.41
1:A:379:GLU:HB3	1:A:475:PRO:HB2	2.03	0.41
1:A:878:LYS:HD2	1:A:878:LYS:HA	1.94	0.41
1:A:1072:MET:HE3	1:A:1072:MET:HB3	1.83	0.41
1:A:619:LEU:HG	1:A:748:GLY:CA	2.51	0.40
1:A:1222:TYR:CE2	1:A:1245:THR:HG23	2.56	0.40
1:A:471:GLN:NE2	1:A:472:ARG:H	2.19	0.40
1:A:1245:THR:HG22	1:A:1258:MET:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	1023/1040 (98%)	957 (94%)	66 (6%)	15 27

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	-3	ARG
1	A	5	LEU
1	A	6	ARG
1	A	33	ILE
1	A	38	VAL
1	A	43	LEU
1	A	47	LEU
1	A	69	THR
1	A	83	THR
1	A	104	ASP
1	A	118	THR
1	A	119	LEU
1	A	134	ARG
1	A	141	SER
1	A	142	SER
1	A	206	LEU
1	A	241	ILE
1	A	247	THR
1	A	253	LEU
1	A	294	GLU
1	A	296	HIS
1	A	332	LEU
1	A	358	ARG
1	A	382	ARG
1	A	396	VAL
1	A	417	ILE
1	A	429	GLU
1	A	471	GLN
1	A	487	ARG
1	A	498	LEU
1	A	508	LEU
1	A	510	ASN
1	A	524	LYS
1	A	534	GLU
1	A	553	LEU
1	A	588	LEU
1	A	596	GLN
1	A	611	LYS
1	A	619	LEU
1	A	736	LEU
1	A	774	VAL

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Mol	Chain	Res	Type
1	A	782	LYS
1	A	789	ASN
1	A	811	VAL
1	A	823	ASP
1	A	829	ILE
1	A	831	LEU
1	A	846	VAL
1	A	878	LYS
1	A	905	VAL
1	A	912	LEU
1	A	1029	ILE
1	A	1080	ILE
1	A	1108	LYS
1	A	1117	ARG
1	A	1136	ASN
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	1206	ASP
1	A	1245	THR
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	31	HIS
1	A	39	HIS
1	A	54	GLN
1	A	60	GLN
1	A	96	HIS
1	A	175	ASN
1	A	216	HIS
1	A	219	HIS
1	A	233	GLN
1	A	243	ASN
1	A	276	ASN
1	A	339	ASN
1	A	400	ASN

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Mol	Chain	Res	Type
1	A	408	HIS
1	A	419	ASN
1	A	426	GLN
1	A	445	ASN
1	A	471	GLN
1	A	545	ASN
1	A	548	GLN
1	A	584	GLN
1	A	585	HIS
1	A	592	HIS
1	A	739	ASN
1	A	786	GLN
1	A	791	GLN
1	A	818	GLN
1	A	824	ASN
1	A	883	HIS
1	A	916	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1026	ASN
1	A	1061	HIS
1	A	1086	HIS
1	A	1125	HIS
1	A	1251	ASN
1	A	1260	HIS
1	A	1293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.99	3 (25%)	10,17,19	4.09	5 (50%)

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	-	1/14/16/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	5.24	1.56	1.50
1	A	1135	CYG	OE2-CD1	3.64	1.26	1.21
1	A	1135	CYG	O2-C1	-2.09	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-CG1	-9.32	113.22	123.98
1	A	1135	CYG	CG1-CD1-SG	7.24	122.03	113.40
1	A	1135	CYG	CB-CA-C	3.06	119.10	110.80
1	A	1135	CYG	CB1-CG1-CD1	-3.04	105.56	112.27
1	A	1135	CYG	O2-C1-O1	-2.14	119.22	124.08

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 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	0.42	0	6,6,6	0.17	0
5	SO4	A	1309	-	4,4,4	0.56	0	6,6,6	0.59	0
5	SO4	A	1313	-	4,4,4	0.63	0	6,6,6	0.78	0
5	SO4	A	1318	-	4,4,4	0.54	0	6,6,6	0.97	0
5	SO4	A	1307	-	4,4,4	0.48	0	6,6,6	0.31	0
6	ACT	A	1320	-	3,3,3	0.88	0	3,3,3	1.70	1 (33%)
5	SO4	A	1319	-	4,4,4	0.56	0	6,6,6	0.83	0
5	SO4	A	1315	-	4,4,4	0.62	0	6,6,6	0.55	0
6	ACT	A	1322	-	3,3,3	1.57	0	3,3,3	0.75	0
5	SO4	A	1310	-	4,4,4	0.30	0	6,6,6	0.98	0
5	SO4	A	1308	-	4,4,4	0.66	0	6,6,6	0.54	0
5	SO4	A	1317	-	4,4,4	0.47	0	6,6,6	0.41	0
6	ACT	A	1323	-	3,3,3	0.99	0	3,3,3	1.94	1 (33%)
5	SO4	A	1312	-	4,4,4	0.58	0	6,6,6	0.33	0
5	SO4	A	1314	-	4,4,4	0.25	0	6,6,6	0.58	0
5	SO4	A	1311	-	4,4,4	0.28	0	6,6,6	0.37	0
2	ADP	A	1301	3	28,29,29	1.60	6 (21%)	43,45,45	1.55	6 (13%)
6	ACT	A	1321	-	3,3,3	1.34	0	3,3,3	1.24	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	-	1/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	C5-C4	3.94	1.46	1.39
2	A	1301	ADP	C5-N7	-3.86	1.32	1.39
2	A	1301	ADP	C4-N9	-3.75	1.29	1.37
2	A	1301	ADP	PB-O1B	2.50	1.58	1.50
2	A	1301	ADP	C8-N9	-2.05	1.34	1.37
2	A	1301	ADP	PA-O3A	2.05	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	ADP	N3-C4-N9	3.88	133.76	127.17
2	A	1301	ADP	C4-N9-C8	3.59	109.51	105.74
2	A	1301	ADP	C5-C4-N3	-3.50	121.90	126.72
2	A	1301	ADP	N6-C6-N1	3.47	126.11	118.38
6	A	1323	ACT	OXT-C-CH3	2.64	126.11	115.05
6	A	1320	ACT	OXT-C-CH3	2.37	125.00	115.05
2	A	1301	ADP	C5-C6-N6	-2.25	117.71	123.29
2	A	1301	ADP	N3-C2-N1	-2.04	125.49	128.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

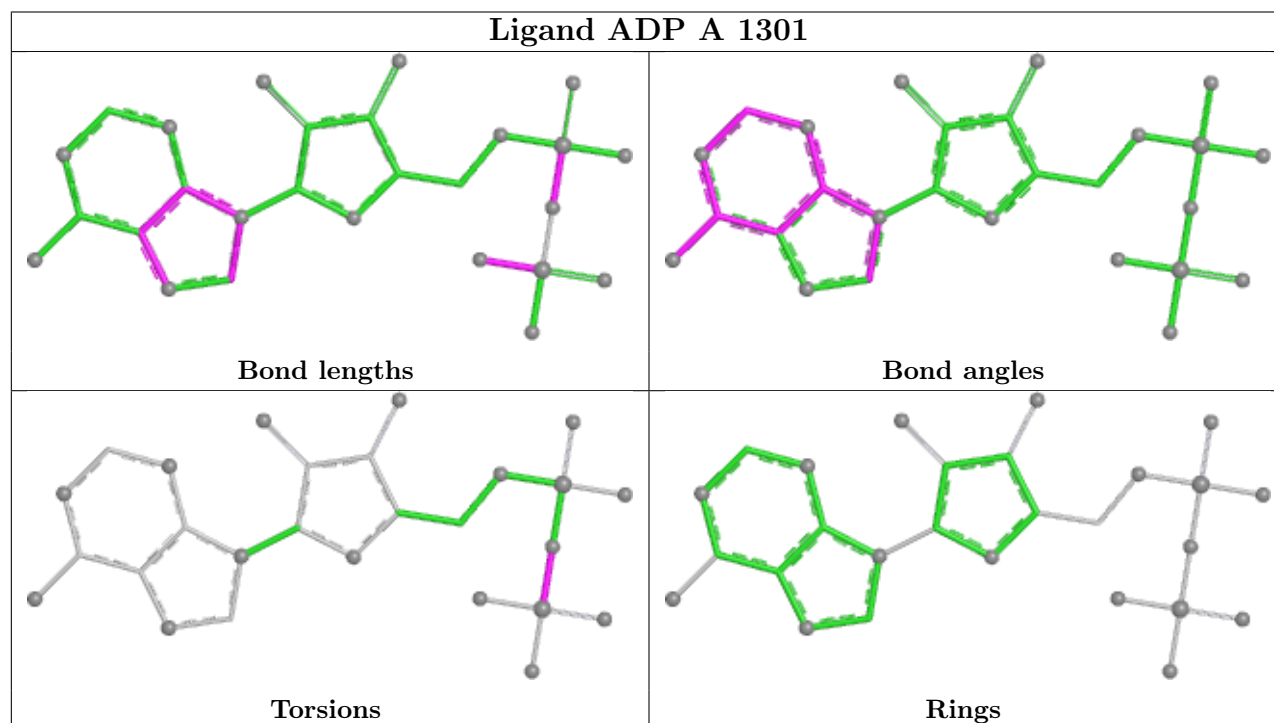
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1307	SO4	1	0
6	A	1320	ACT	4	0
5	A	1315	SO4	1	0
5	A	1310	SO4	1	0
5	A	1317	SO4	1	0
6	A	1323	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1283/1303 (98%)	-0.74	4 (0%) 90 89	9, 18, 37, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	SER	3.1
1	A	118	THR	2.7
1	A	447	GLY	2.1
1	A	969	ASN	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CYG	A	1135	15/16	0.97	0.06	11,13,14,15	0

6.3 Carbohydrates [i](#)

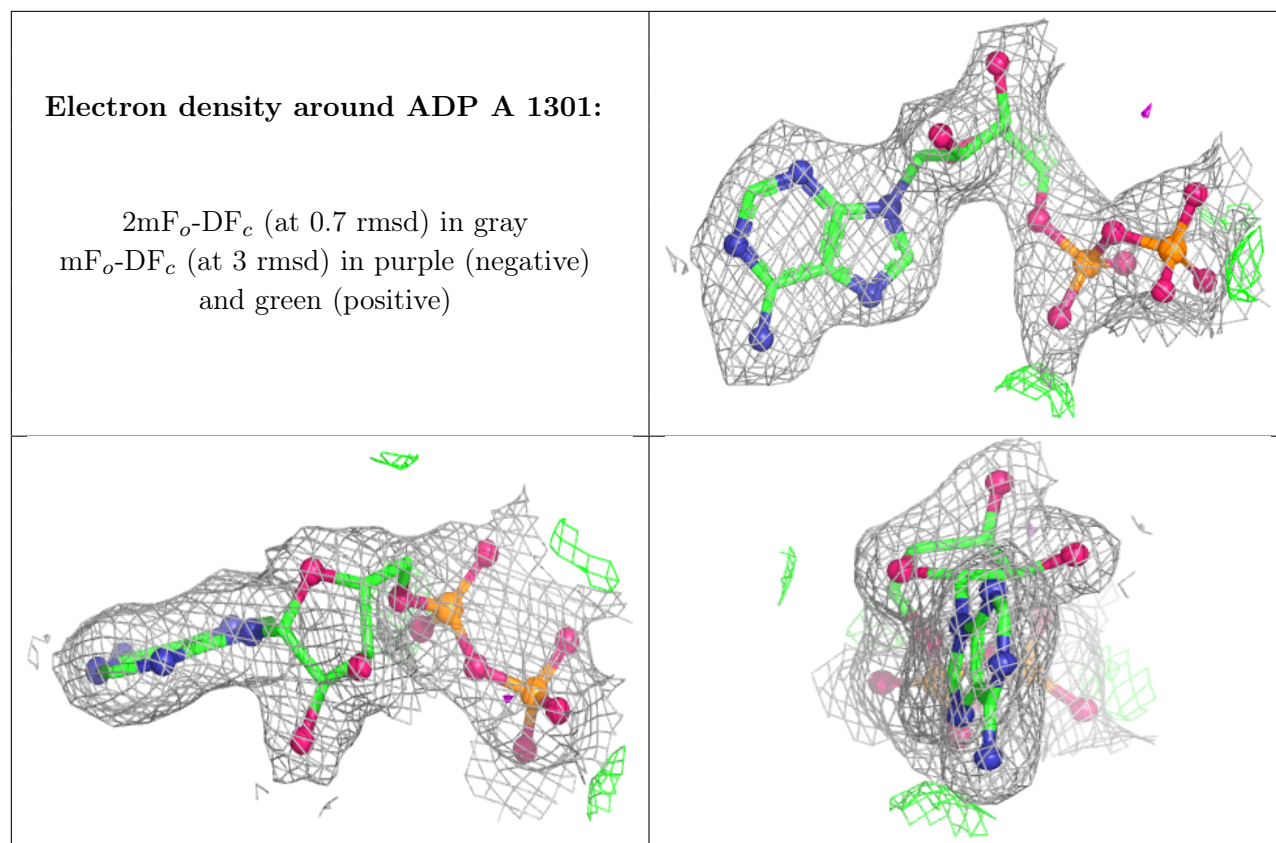
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	A	1320	4/4	0.74	0.27	47,50,52,53	0
6	ACT	A	1322	4/4	0.76	0.17	21,22,26,26	0
6	ACT	A	1323	4/4	0.78	0.17	33,33,36,40	0
5	SO4	A	1313	5/5	0.81	0.17	46,48,59,60	0
6	ACT	A	1321	4/4	0.89	0.12	18,20,21,22	0
5	SO4	A	1315	5/5	0.92	0.13	47,51,53,58	0
5	SO4	A	1312	5/5	0.94	0.12	46,46,50,51	0
5	SO4	A	1318	5/5	0.94	0.14	34,35,43,46	0
3	MG	A	1303	1/1	0.97	0.04	15,15,15,15	0
5	SO4	A	1316	5/5	0.97	0.10	14,14,15,15	5
5	SO4	A	1317	5/5	0.97	0.07	40,41,43,47	0
3	MG	A	1305	1/1	0.97	0.13	2,2,2,2	0
3	MG	A	1304	1/1	0.98	0.05	16,16,16,16	0
3	MG	A	1302	1/1	0.98	0.06	15,15,15,15	0
7	XE	A	1326	1/1	0.98	0.02	29,29,29,29	1
5	SO4	A	1308	5/5	0.99	0.05	20,20,23,24	0
5	SO4	A	1309	5/5	0.99	0.07	27,28,29,30	0
5	SO4	A	1310	5/5	0.99	0.06	23,25,26,28	0
5	SO4	A	1319	5/5	0.99	0.07	28,30,32,33	0
5	SO4	A	1311	5/5	0.99	0.04	26,29,31,31	0
2	ADP	A	1301	27/27	0.99	0.04	7,9,10,11	0
4	MN	A	1306	1/1	0.99	0.05	47,47,47,47	0
5	SO4	A	1314	5/5	0.99	0.04	25,25,26,27	0
5	SO4	A	1307	5/5	0.99	0.07	29,32,34,34	0
7	XE	A	1325	1/1	1.00	0.03	21,21,21,21	1
7	XE	A	1324	1/1	1.00	0.01	15,15,15,15	0
7	XE	A	1327	1/1	1.00	0.01	24,24,24,24	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.