



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:07 PM UTC

PDB ID : 4R7G / pdb_00004r7g
Title : Determination of the formylglycinamide ribonucleotide amidotransferase ammonia pathway by combining 3D-RISM theory with experiment
Authors : Tanwar, A.S.; Sindhikara, D.J.; Hirata, F.; Anand, R.
Deposited on : 2014-08-27
Resolution : 2.90 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

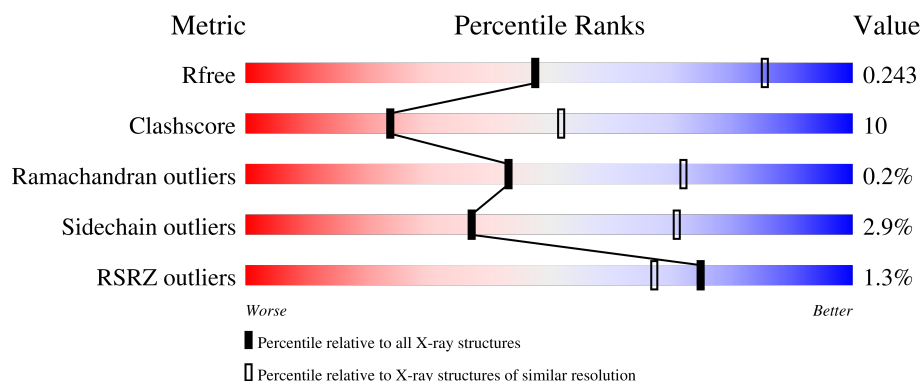
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10182 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
1	A	1284	Total	C	N	O	S	0	0	0
			9902	6213	1768	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	333	ILE	VAL	engineered mutation	UNP P74881

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

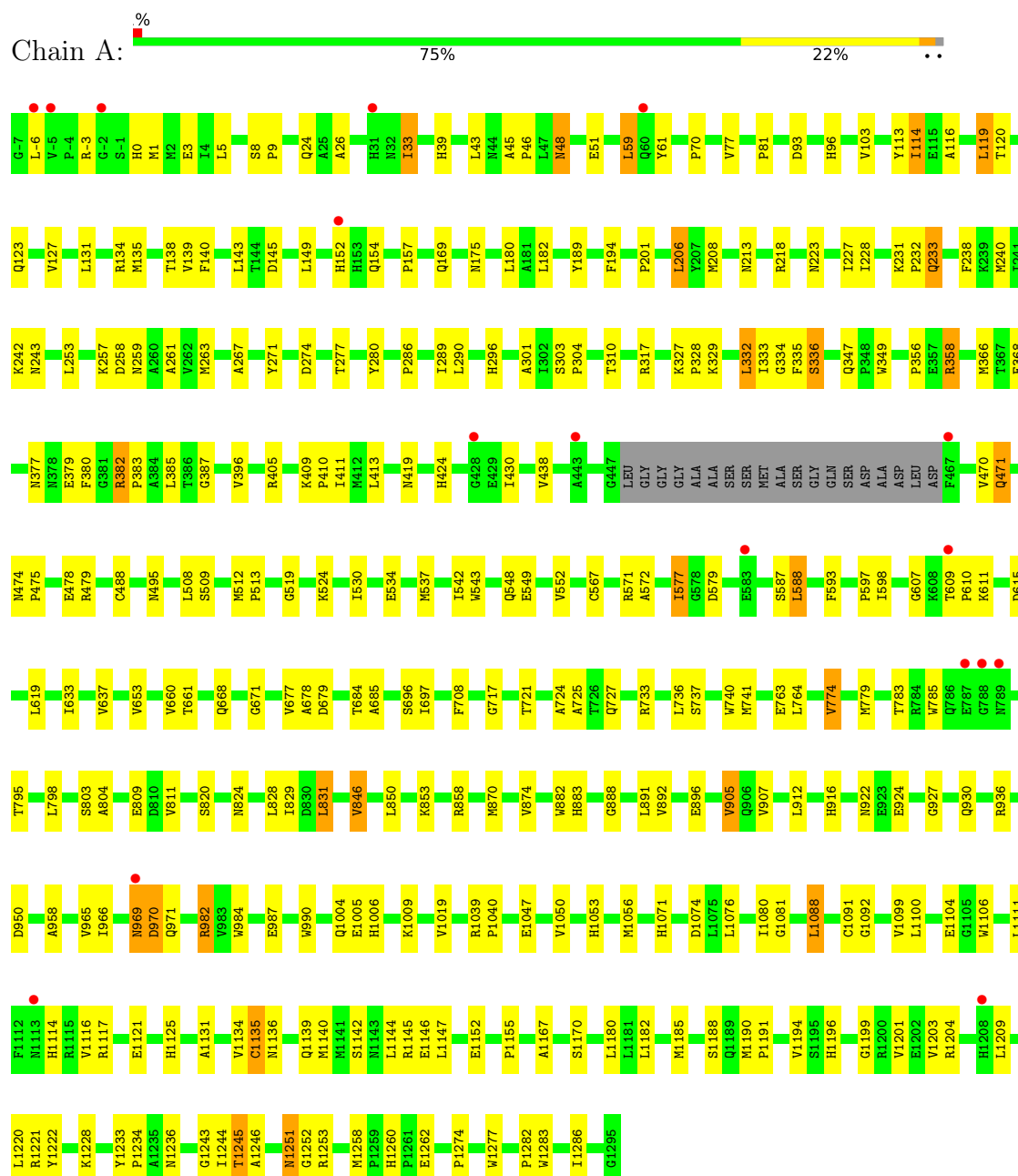
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	220	Total	O	0	0
			220	220		

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	146.57Å 146.57Å 141.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 92.2 (30.00-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.179 , 0.237 0.185 , 0.243	Depositor DCC
R_{free} test set	3769 reflections (8.13%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10182	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: CYG, SO4, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/10099	0.96	37/13706 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	SER	CA-C-N	8.72	130.74	119.84
1	A	303	SER	C-N-CA	8.72	130.74	119.84
1	A	534	GLU	CA-C-N	8.52	129.03	119.32
1	A	534	GLU	C-N-CA	8.52	129.03	119.32
1	A	779	MET	N-CA-C	8.38	123.08	113.02
1	A	409	LYS	N-CA-C	-7.68	94.43	109.10
1	A	1244	ILE	N-CA-C	7.53	118.72	109.30
1	A	385	LEU	N-CA-C	7.20	122.06	113.28
1	A	474	ASN	CA-C-N	6.39	126.61	119.32
1	A	474	ASN	C-N-CA	6.39	126.61	119.32
1	A	233	GLN	CA-C-N	6.34	125.76	118.85
1	A	233	GLN	C-N-CA	6.34	125.76	118.85
1	A	347	GLN	CA-C-N	6.29	126.49	119.32
1	A	347	GLN	C-N-CA	6.29	126.49	119.32
1	A	763	GLU	N-CA-C	6.16	120.52	111.34
1	A	671	GLY	CA-C-N	5.96	125.84	119.28
1	A	671	GLY	C-N-CA	5.96	125.84	119.28
1	A	114	ILE	N-CA-C	5.88	116.32	107.80
1	A	858	ARG	N-CA-C	5.75	118.49	111.82
1	A	965	VAL	N-CA-C	5.64	115.98	107.80
1	A	653	VAL	N-CA-C	5.61	116.39	111.56
1	A	764	LEU	N-CA-C	5.57	117.04	110.97
1	A	119	LEU	N-CA-C	5.53	118.37	110.24
1	A	936	ARG	N-CA-C	5.49	117.71	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1053	HIS	N-CA-C	5.45	119.10	112.23
1	A	59	LEU	N-CA-C	5.40	119.73	113.20
1	A	1104	GLU	N-CA-C	5.37	117.22	111.36
1	A	1019	VAL	N-CA-C	5.37	117.11	108.85
1	A	1236	ASN	N-CA-C	-5.36	97.04	108.93
1	A	333	ILE	CA-C-N	-5.34	118.02	121.65
1	A	333	ILE	C-N-CA	-5.34	118.02	121.65
1	A	1091	CYS	N-CA-C	5.27	118.32	110.52
1	A	289	ILE	N-CA-C	5.22	115.48	108.17
1	A	143	LEU	N-CA-C	-5.21	106.19	112.54
1	A	724	ALA	N-CA-C	5.20	118.41	111.75
1	A	93	ASP	N-CA-C	-5.02	105.69	111.07
1	A	740	TRP	N-CA-C	5.01	116.69	108.52

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	9902	0	9692	199	0
2	A	3	0	0	0	0
3	A	30	0	0	1	0
4	A	27	0	12	1	0
5	A	220	0	0	3	0
All	All	10182	0	9704	199	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 10.

All (199) 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:335:PHE:HB3	1:A:366:MET:HE1	1.42	1.00
1:A:512:MET:HE3	1:A:577:ILE:HD11	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ASN:HD21	1:A:958:ALA:H	1.19	0.89
1:A:336:SER:HB2	1:A:411:ILE:HB	1.54	0.86
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.25	0.81
1:A:5:LEU:HD12	1:A:59:LEU:HD12	1.63	0.81
1:A:175:ASN:HD21	1:A:182:LEU:H	1.26	0.81
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.66	0.78
1:A:1251:ASN:ND2	1:A:1253:ARG:H	1.82	0.77
1:A:727:GLN:HG2	1:A:809:GLU:HB3	1.69	0.75
1:A:120:THR:HG23	1:A:123:GLN:HE21	1.54	0.73
1:A:396:VAL:HG21	1:A:850:LEU:HB2	1.73	0.70
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.91	0.69
1:A:213:ASN:HA	1:A:218:ARG:HG3	1.75	0.68
1:A:228:ILE:HD13	1:A:233:GLN:HG3	1.76	0.68
1:A:396:VAL:CG2	1:A:850:LEU:HB2	2.24	0.67
1:A:-3:ARG:HH12	1:A:0:HIS:HB2	1.58	0.67
1:A:96:HIS:HE1	1:A:103:VAL:O	1.78	0.66
1:A:820:SER:H	1:A:930:GLN:HE22	1.44	0.65
1:A:335:PHE:CB	1:A:366:MET:HE1	2.22	0.65
1:A:1190:MET:HE3	1:A:1282:PRO:HB2	1.79	0.65
1:A:33:ILE:HG12	1:A:114:ILE:HG12	1.80	0.64
1:A:824:ASN:HD21	1:A:958:ALA:N	1.94	0.64
1:A:154:GLN:HE21	1:A:154:GLN:HA	1.63	0.63
1:A:1190:MET:HG2	1:A:1282:PRO:HG2	1.80	0.63
1:A:1076:LEU:HD23	1:A:1116:VAL:HG21	1.81	0.63
1:A:-3:ARG:NH1	1:A:0:HIS:HB2	2.14	0.62
1:A:261:ALA:HB2	1:A:774:VAL:HG13	1.83	0.60
1:A:537:MET:HE3	1:A:542:ILE:HG12	1.84	0.59
1:A:356:PRO:HG3	1:A:785:TRP:HB3	1.84	0.59
1:A:637:VAL:HG13	1:A:891:LEU:HD21	1.83	0.59
1:A:1167:ALA:HA	1:A:1194:VAL:O	2.02	0.59
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.02	0.57
1:A:227:ILE:HB	1:A:615:ASP:HA	1.87	0.57
1:A:588:LEU:O	1:A:597:PRO:HD2	2.04	0.57
1:A:1121:GLU:HG3	1:A:1125:HIS:CD2	2.40	0.57
1:A:1056:MET:HE1	1:A:1134:VAL:HG21	1.86	0.56
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.14	0.56
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.02	0.56
1:A:824:ASN:ND2	1:A:958:ALA:H	1.97	0.56
1:A:1145:ARG:NH2	1:A:1204:ARG:HH21	2.03	0.56
1:A:1099:VAL:HG12	1:A:1100:LEU:HG	1.87	0.56
1:A:530:ILE:HD13	1:A:577:ILE:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:HD22	1:A:51:GLU:HG3	1.70	0.55
1:A:828:LEU:HD12	1:A:927:GLY:O	2.07	0.55
1:A:1203:VAL:HG21	1:A:1209:LEU:HB2	1.87	0.55
1:A:1145:ARG:HH21	1:A:1204:ARG:HH21	1.55	0.55
1:A:888:GLY:HA3	1:A:892:VAL:HG21	1.87	0.54
1:A:5:LEU:HD12	1:A:59:LEU:CD1	2.37	0.54
1:A:317:ARG:NH1	1:A:549:GLU:H	2.05	0.53
1:A:438:VAL:HG23	1:A:577:ILE:HD12	1.91	0.53
1:A:405:ARG:HA	1:A:795:THR:O	2.09	0.52
1:A:301:ALA:HB2	1:A:410:PRO:HD2	1.91	0.52
1:A:1106:TRP:CD2	1:A:1140:MET:HG3	2.45	0.52
1:A:77:VAL:HG22	1:A:139:VAL:HG22	1.90	0.52
1:A:332:LEU:HG	1:A:697:ILE:HD11	1.91	0.52
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.92	0.52
1:A:114:ILE:HD11	1:A:131:LEU:HD11	1.92	0.52
1:A:488:CYS:HB3	1:A:495:ASN:OD1	2.09	0.52
1:A:238:PHE:CE2	1:A:242:LYS:HE3	2.45	0.52
1:A:717:GLY:O	1:A:721:THR:HG23	2.10	0.52
1:A:116:ALA:HB1	1:A:119:LEU:HD13	1.91	0.51
1:A:916:HIS:HD2	5:A:1408:HOH:O	1.94	0.51
1:A:380:PHE:O	1:A:479:ARG:HD3	2.10	0.51
1:A:820:SER:N	1:A:930:GLN:HE22	2.07	0.51
1:A:725:ALA:HB2	1:A:882:TRP:CD1	2.46	0.50
1:A:1222:TYR:CZ	1:A:1245:THR:HG21	2.46	0.50
1:A:1144:LEU:HD22	1:A:1147:LEU:HD22	1.93	0.50
1:A:668:GLN:HG2	4:A:1310:ADP:HI'	1.92	0.50
1:A:310:THR:HG21	1:A:471:GLN:HB3	1.93	0.50
1:A:524:LYS:HA	1:A:587:SER:HB3	1.92	0.50
1:A:509:SER:HB3	1:A:543:TRP:CD1	2.47	0.50
1:A:905:VAL:HG13	1:A:907:VAL:HG13	1.92	0.50
1:A:633:ILE:O	1:A:637:VAL:HG23	2.12	0.49
1:A:982:ARG:NH2	1:A:1009:LYS:HD3	2.27	0.49
1:A:1050:VAL:HG13	1:A:1092:GLY:O	2.12	0.49
1:A:1142:SER:O	1:A:1145:ARG:HG3	2.13	0.49
1:A:-3:ARG:HH11	1:A:-3:ARG:HB3	1.77	0.49
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.96	0.49
1:A:430:ILE:HD13	1:A:519:GLY:HA3	1.95	0.49
1:A:349:TRP:CZ3	1:A:846:VAL:HG22	2.47	0.49
1:A:984:TRP:O	1:A:987:GLU:HG3	2.13	0.48
1:A:1155:PRO:HB2	1:A:1201:VAL:HG13	1.95	0.48
1:A:81:PRO:HD3	1:A:138:THR:CG2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:GLU:HB2	1:A:1234:PRO:HD3	1.95	0.48
1:A:-3:ARG:NH1	1:A:-3:ARG:HB3	2.28	0.48
1:A:1071:HIS:O	1:A:1074:ASP:HB2	2.14	0.48
1:A:377:ASN:OD1	1:A:382:ARG:HD2	2.13	0.48
1:A:1121:GLU:HG3	1:A:1125:HIS:HD2	1.78	0.48
1:A:263:MET:HE1	1:A:733:ARG:O	2.14	0.47
1:A:356:PRO:HG2	1:A:783:THR:CG2	2.43	0.47
1:A:984:TRP:HA	1:A:987:GLU:HG3	1.94	0.47
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.14	0.47
1:A:227:ILE:HD13	1:A:232:PRO:HA	1.95	0.47
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.49	0.47
1:A:424:HIS:CD2	1:A:495:ASN:HD22	2.32	0.47
1:A:274:ASP:HB3	1:A:277:THR:OG1	2.14	0.47
1:A:588:LEU:HB2	1:A:598:ILE:HB	1.97	0.47
1:A:189:TYR:OH	1:A:607:GLY:HA3	2.14	0.47
1:A:201:PRO:HB2	1:A:206:LEU:HD13	1.97	0.47
1:A:696:SER:OG	1:A:804:ALA:HB3	2.14	0.47
1:A:1221:ARG:HA	1:A:1243:GLY:O	2.14	0.47
1:A:157:PRO:HA	1:A:593:PHE:CE2	2.50	0.47
1:A:512:MET:HE2	1:A:552:VAL:HG12	1.96	0.47
1:A:81:PRO:HA	1:A:149:LEU:HD23	1.97	0.47
1:A:411:ILE:HG12	1:A:741:MET:HG2	1.96	0.47
1:A:982:ARG:NH1	1:A:982:ARG:HG3	2.31	0.46
1:A:677:VAL:HG11	1:A:896:GLU:HB3	1.96	0.46
1:A:194:PHE:CE2	1:A:201:PRO:HB3	2.50	0.46
1:A:524:LYS:HE3	1:A:579:ASP:HB2	1.97	0.46
1:A:1080:ILE:HG22	1:A:1081:GLY:N	2.30	0.46
1:A:45:ALA:HB1	1:A:46:PRO:HD2	1.97	0.46
1:A:1088:LEU:C	1:A:1088:LEU:HD23	2.40	0.46
1:A:1185:MET:HE1	1:A:1286:ILE:CD1	2.45	0.46
1:A:238:PHE:HE2	1:A:242:LYS:HE3	1.80	0.46
1:A:922:ASN:HD22	1:A:924:GLU:H	1.63	0.46
1:A:1170:SER:O	1:A:1191:PRO:HA	2.16	0.46
1:A:267:ALA:HA	1:A:286:PRO:HA	1.99	0.45
1:A:1146:GLU:HG3	1:A:1147:LEU:HD13	1.98	0.45
1:A:135:MET:HB3	1:A:470:VAL:HG21	1.97	0.45
1:A:1088:LEU:O	1:A:1131:ALA:HA	2.16	0.45
1:A:1135:CYG:HB2	1:A:1136:ASN:H	1.48	0.45
1:A:990:TRP:HB2	1:A:1006:HIS:CD2	2.51	0.45
1:A:1:MET:HB2	1:A:43:LEU:HD12	1.97	0.45
1:A:335:PHE:CG	1:A:366:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ARG:HH21	1:A:1204:ARG:NH2	2.14	0.45
1:A:8:SER:HB2	1:A:9:PRO:CD	2.47	0.45
1:A:240:MET:O	1:A:243:ASN:HB3	2.17	0.45
1:A:8:SER:HB2	1:A:9:PRO:HD2	2.00	0.44
1:A:387:GLY:HA2	1:A:697:ILE:CD1	2.48	0.44
1:A:-6:LEU:HG	1:A:1:MET:HE3	1.98	0.44
1:A:70:PRO:HB3	1:A:113:TYR:CE1	2.52	0.44
1:A:379:GLU:HB3	1:A:475:PRO:HB2	1.98	0.44
1:A:1251:ASN:HD22	1:A:1252:GLY:N	2.16	0.44
1:A:478:GLU:HB2	1:A:549:GLU:HG3	2.00	0.44
1:A:1047:GLU:H	1:A:1050:VAL:CG2	2.30	0.44
1:A:1194:VAL:HG13	1:A:1196:HIS:CE1	2.53	0.44
1:A:684:THR:HG22	1:A:811:VAL:HG21	2.00	0.43
1:A:24:GLN:C	1:A:26:ALA:H	2.25	0.43
1:A:383:PRO:HD3	1:A:660:VAL:HG12	2.00	0.43
1:A:-3:ARG:HH22	1:A:152:HIS:CE1	2.36	0.43
1:A:228:ILE:HD13	1:A:233:GLN:CG	2.47	0.43
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.16	0.43
1:A:479:ARG:HA	1:A:479:ARG:HD2	1.84	0.43
1:A:1190:MET:HE3	1:A:1282:PRO:CB	2.48	0.43
1:A:3:GLU:OE1	1:A:5:LEU:HD21	2.18	0.43
1:A:39:HIS:HE1	1:A:61:TYR:OH	2.01	0.43
1:A:140:PHE:CD1	1:A:145:ASP:HB3	2.53	0.43
1:A:358:ARG:HD3	1:A:358:ARG:H	1.84	0.43
1:A:708:PHE:HD1	1:A:798:LEU:HD22	1.84	0.43
1:A:223:ASN:O	1:A:611:LYS:HE2	2.19	0.43
1:A:335:PHE:HB3	1:A:366:MET:CE	2.30	0.43
1:A:304:PRO:HB2	1:A:368:GLU:HB2	2.00	0.43
1:A:853:LYS:HE2	1:A:853:LYS:HB3	1.76	0.43
1:A:1220:LEU:HB2	1:A:1246:ALA:HB3	2.01	0.43
1:A:609:THR:HB	1:A:610:PRO:HD2	2.01	0.42
1:A:1114:HIS:CD2	1:A:1117:ARG:HH21	2.37	0.42
1:A:982:ARG:HG3	1:A:982:ARG:HH11	1.83	0.42
1:A:194:PHE:CD2	1:A:201:PRO:HB3	2.54	0.42
1:A:387:GLY:HA2	1:A:697:ILE:HD12	2.02	0.42
1:A:829:ILE:HG22	1:A:831:LEU:HD13	2.01	0.42
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	2.02	0.42
1:A:257:LYS:HB3	1:A:257:LYS:HE2	1.87	0.42
1:A:512:MET:HB2	1:A:513:PRO:HD3	2.02	0.42
1:A:123:GLN:O	1:A:127:VAL:HG23	2.19	0.42
1:A:334:GLY:HA3	1:A:413:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:GLY:CA	1:A:1258:MET:HE2	2.50	0.42
1:A:208:MET:HG3	1:A:509:SER:HB2	2.01	0.42
1:A:950:ASP:HB2	5:A:1419:HOH:O	2.18	0.42
1:A:1199:GLY:HA2	1:A:1258:MET:HE2	2.02	0.42
1:A:1274:PRO:HD2	1:A:1277:TRP:CE2	2.54	0.42
1:A:290:LEU:C	1:A:290:LEU:HD12	2.45	0.42
1:A:259:ASN:HB2	5:A:1577:HOH:O	2.19	0.41
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.85	0.41
1:A:134:ARG:HG3	1:A:135:MET:HE2	2.02	0.41
1:A:588:LEU:HD12	1:A:598:ILE:HD12	2.01	0.41
1:A:1:MET:HB2	1:A:43:LEU:CD1	2.50	0.41
1:A:329:LYS:O	1:A:383:PRO:HD2	2.20	0.41
1:A:567:CYS:HB3	1:A:572:ALA:O	2.21	0.41
1:A:1190:MET:HE2	1:A:1283:TRP:CZ2	2.56	0.41
1:A:1277:TRP:CZ3	1:A:1282:PRO:HD3	2.55	0.41
1:A:571:ARG:NH2	1:A:1076:LEU:HD12	2.36	0.41
1:A:660:VAL:HG13	1:A:661:THR:HG23	2.02	0.41
1:A:668:GLN:HA	1:A:678:ALA:HB3	2.02	0.41
1:A:1039:ARG:HA	1:A:1040:PRO:HD2	1.89	0.41
1:A:310:THR:HG22	1:A:548:GLN:HG3	2.03	0.41
1:A:969:ASN:O	1:A:970:ASP:HB2	2.20	0.41
1:A:231:LYS:HA	1:A:232:PRO:HD3	1.93	0.41
1:A:907:VAL:CG2	1:A:966:ILE:HG12	2.51	0.40
1:A:120:THR:H	1:A:123:GLN:HE21	1.68	0.40
1:A:1188:SER:HB3	1:A:1190:MET:SD	2.60	0.40
1:A:1228:LYS:HA	3:A:1306:SO4:O1	2.21	0.40
1:A:471:GLN:HE21	1:A:471:GLN:HA	1.85	0.40
1:A:329:LYS:HZ3	1:A:685:ALA:HA	1.86	0.40
1:A:43:LEU:HD12	1:A:43:LEU:O	2.22	0.40
1:A:261:ALA:O	1:A:290:LEU:HA	2.22	0.40
1:A:327:LYS:HA	1:A:328:PRO:HD3	1.96	0.40
1:A:737:SER:HB3	1:A:803:SER:HB2	2.02	0.40
1:A:870:MET:O	1:A:874:VAL:HG23	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	1279/1303 (98%)	1205 (94%)	72 (6%)	2 (0%)	43 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	970	ASP
1	A	969	ASN

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	1029/1040 (99%)	999 (97%)	30 (3%)	37 71

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ILE
1	A	48	ASN
1	A	169	GLN
1	A	206	LEU
1	A	253	LEU
1	A	258	ASP
1	A	296	HIS
1	A	332	LEU
1	A	336	SER

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Mol	Chain	Res	Type
1	A	358	ARG
1	A	382	ARG
1	A	471	GLN
1	A	508	LEU
1	A	577	ILE
1	A	588	LEU
1	A	619	LEU
1	A	736	LEU
1	A	774	VAL
1	A	831	LEU
1	A	846	VAL
1	A	905	VAL
1	A	912	LEU
1	A	971	GLN
1	A	982	ARG
1	A	1088	LEU
1	A	1152	GLU
1	A	1180	LEU
1	A	1182	LEU
1	A	1245	THR
1	A	1251	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	29	GLN
1	A	32	ASN
1	A	39	HIS
1	A	48	ASN
1	A	54	GLN
1	A	96	HIS
1	A	123	GLN
1	A	126	GLN
1	A	152	HIS
1	A	154	GLN
1	A	175	ASN
1	A	276	ASN
1	A	298	HIS
1	A	339	ASN
1	A	408	HIS
1	A	419	ASN

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Mol	Chain	Res	Type
1	A	426	GLN
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	786	GLN
1	A	824	ASN
1	A	835	HIS
1	A	862	GLN
1	A	883	HIS
1	A	916	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1000	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1026	ASN
1	A	1061	HIS
1	A	1084	ASN
1	A	1086	HIS
1	A	1113	ASN
1	A	1114	HIS
1	A	1125	HIS
1	A	1208	HIS
1	A	1251	ASN
1	A	1260	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.01	0	10,17,19	7.70	3 (30%)

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	-	7/14/16/18	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-SG	-18.47	99.19	122.68
1	A	1135	CYG	CG1-CD1-SG	15.13	131.43	113.40
1	A	1135	CYG	OE2-CD1-CG1	4.32	128.97	123.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	N-CA-CB-SG
1	A	1135	CYG	C-CA-CB-SG
1	A	1135	CYG	CG1-CD1-SG-CB
1	A	1135	CYG	OE2-CD1-SG-CB
1	A	1135	CYG	SG-CD1-CG1-CB1
1	A	1135	CYG	CA-CB-SG-CD1
1	A	1135	CYG	OE2-CD1-CG1-CB1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1135	CYG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1304	-	4,4,4	0.42	0	6,6,6	0.07	0
3	SO4	A	1307	-	4,4,4	0.40	0	6,6,6	0.15	0
3	SO4	A	1308	-	4,4,4	0.45	0	6,6,6	0.14	0
3	SO4	A	1306	-	4,4,4	0.42	0	6,6,6	0.14	0
3	SO4	A	1309	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	A	1305	-	4,4,4	0.40	0	6,6,6	0.12	0
4	ADP	A	1310	2	28,29,29	1.48	4 (14%)	43,45,45	1.34	5 (11%)

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
4	ADP	A	1310	2	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1310	ADP	PA-O3A	-4.50	1.54	1.59
4	A	1310	ADP	PB-O2B	-2.58	1.45	1.54
4	A	1310	ADP	C6-N6	-2.39	1.28	1.34
4	A	1310	ADP	PA-O1A	-2.15	1.43	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1310	ADP	C2-N1-C6	3.54	124.54	118.73
4	A	1310	ADP	N3-C2-N1	-3.25	123.67	128.58
4	A	1310	ADP	C5-C4-N3	2.82	130.60	126.72
4	A	1310	ADP	O2B-PB-O3A	2.32	112.43	104.64
4	A	1310	ADP	O2A-PA-O1A	2.04	121.93	112.44

There are no chirality outliers.

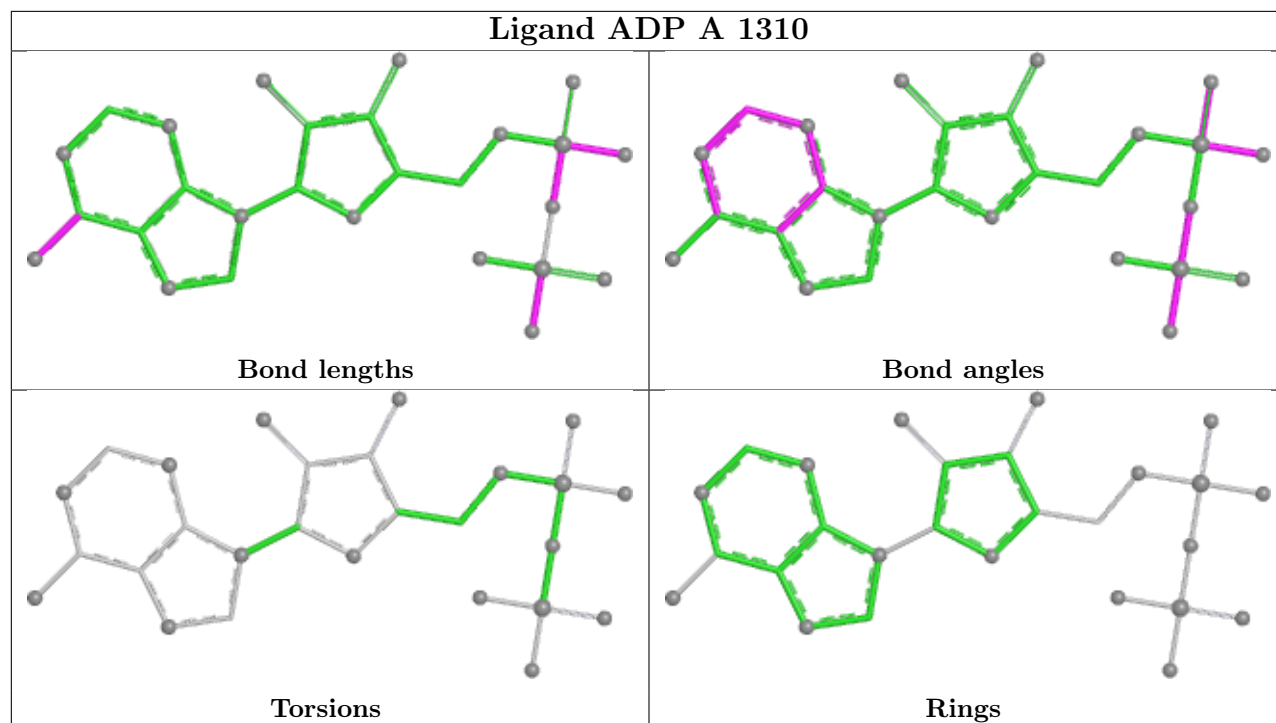
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1306	SO4	1	0
4	A	1310	ADP	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%)	-0.41	17 (1%) 75 67	3, 24, 63, 116	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1208	HIS	4.2
1	A	467	PHE	3.5
1	A	787	GLU	3.2
1	A	428	GLY	3.2
1	A	443	ALA	3.0
1	A	-6	LEU	2.7
1	A	-5	VAL	2.6
1	A	789	ASN	2.5
1	A	788	GLY	2.4
1	A	31	HIS	2.4
1	A	152	HIS	2.4
1	A	583	GLU	2.3
1	A	1113	ASN	2.2
1	A	609	THR	2.2
1	A	969	ASN	2.1
1	A	-2	GLY	2.1
1	A	60	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	CYG	A	1135	15/16	0.94	0.09	15,20,25,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

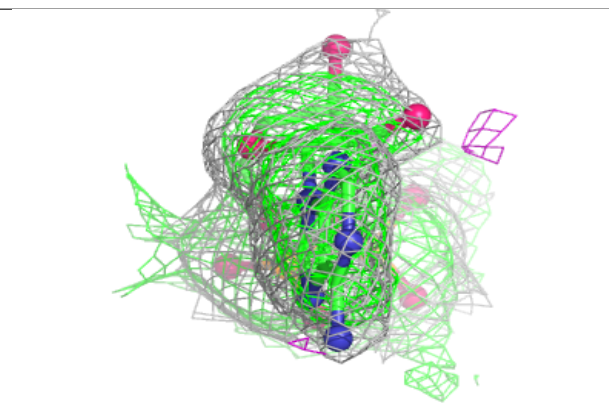
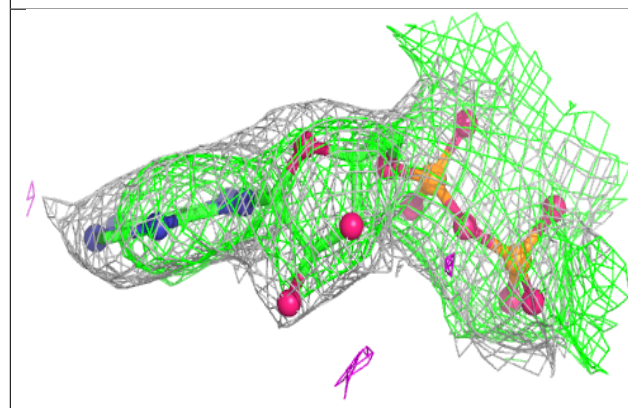
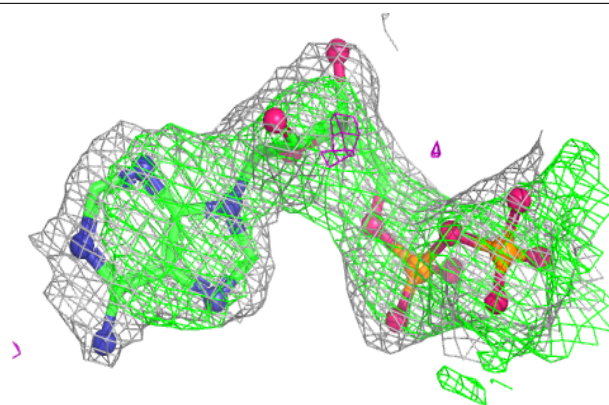
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	A	1301	1/1	0.94	0.19	18,18,18,18	0
3	SO4	A	1304	5/5	0.94	0.10	48,49,53,54	0
3	SO4	A	1307	5/5	0.95	0.07	33,36,38,38	0
3	SO4	A	1308	5/5	0.95	0.12	40,42,46,52	0
2	MG	A	1303	1/1	0.96	0.21	18,18,18,18	0
3	SO4	A	1305	5/5	0.96	0.07	28,30,35,35	0
4	ADP	A	1310	27/27	0.96	0.19	1,1,1,1	27
3	SO4	A	1306	5/5	0.97	0.06	30,32,33,40	0
2	MG	A	1302	1/1	0.97	0.15	28,28,28,28	0
3	SO4	A	1309	5/5	0.98	0.05	29,31,31,34	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 1310:

$2mF_o-DF_c$ (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.