

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4MGH
Title	:	Importance of Hydrophobic Cavities in Allosteric Regulation of Formylglyci-
		namide Synthetase: Insight from Xenon Trapping and Statistical Coupling Analysis
Authors	:	Tanwar, A.S.; Goyal, V.D.; Choudhary, D.; Panjikar, S.; Anand, R.
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 (i) symbol.

The following versions of software and data (see references (1)) 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	:	2.13.1
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)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374(2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	84%	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	-



$4 \mathrm{MGH}$

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 Phosphoribosylformylglycinamidine synthase.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	GLY	-	EXPRESSION TAG	UNP P74881
А	-6	LEU	-	EXPRESSION TAG	UNP P74881
А	-5	VAL	-	EXPRESSION TAG	UNP P74881
А	-4	PRO	-	EXPRESSION TAG	UNP P74881
А	-3	ARG	-	EXPRESSION TAG	UNP P74881
А	-2	GLY	-	EXPRESSION TAG	UNP P74881
А	-1	SER	-	EXPRESSION TAG	UNP P74881
А	0	HIS	-	EXPRESSION TAG	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	А	1	Total 27	C 10	N 5	O 10	Р 2	0	0

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

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

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

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

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Δ	1	Total O S	0	0
0	Л	T	$5 \ 4 \ 1$	0	0
5	Δ	1	Total O S	0	0
0	Л	T	5 4 1	0	0
5	Λ	1	Total O S	0	0
	Л	T	5 4 1	0	0
5	Δ	1	Total O S	0	0
	А		5 4 1	0	



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total O S	0	0
			5 4 1	_	_
5	Δ	1	Total O S	0	0
0	11	T	5 4 1	0	0
F	Δ	1	Total O S	0	0
5	А	L	5 4 1	0	0
F	Λ	1	Total O S	0	0
0	A	L	5 4 1	0	0
5	Λ	1	Total O S	0	0
0	А	L	5 4 1	0	0
5	Λ	1	Total O S	0	0
0	Л	I	5 4 1	0	0
5	Λ	1	Total O S	0	0
0	Л	I	5 4 1	0	0
5	Λ	1	Total O S	0	0
0	А		5 4 1		0
5	Λ	1	Total O S	0	0
0	A		5 4 1		U

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0

• Molecule 7 is XENON (three-letter code: XE) (formula: Xe).

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

• Molecule 8 is water.

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



3 Residue-property plots (i)

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



• Molecule 1: Phosphoribosylformylglycinamidine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	146.45Å 146.45 Å 141.69 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	19.99 - 2.65	Depositor
Resolution (A)	19.99 - 2.65	EDS
% Data completeness	99.7 (19.99-2.65)	Depositor
(in resolution range)	$100.0\ (19.99-2.65)$	EDS
R _{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$8.42 (at 2.67 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D	0.153 , 0.203	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.161 , 0.206	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 $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , 43.5	EDS
L-test for twinning ²	$< L >=0.52, < L^2>=0.35$	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	Bo	nd lengths	B	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.78	2/10076~(0.0%)	0.91	22/13675~(0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	1152	GLU	CG-CD	5.62	1.60	1.51
1	А	211	GLN	CG-CD	5.26	1.63	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	487	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	А	932	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	А	382	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	А	332	LEU	CA-CB-CG	7.30	132.09	115.30
1	А	1115	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	А	479	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	А	774	VAL	CB-CA-C	-6.48	99.09	111.40
1	А	487	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	А	730	ASP	CB-CG-OD1	6.07	123.76	118.30
1	А	188	ASP	CB-CG-OD1	5.97	123.67	118.30
1	А	332	LEU	CB-CG-CD2	5.84	120.92	111.00
1	А	932	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	А	713	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	А	1117	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	А	730	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	А	679	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	1145	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	695	MET	CG-SD-CE	5.21	108.53	100.20
1	A	473	ASP	CB-CG-OD2	5.21	122.98	118.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	184	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	А	1168	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	А	1062	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	А	9879	0	9656	107	0
2	А	27	0	12	0	0
3	А	4	0	0	0	0
4	А	1	0	0	0	0
5	А	65	0	0	4	0
6	А	16	0	12	5	0
7	А	4	0	0	0	0
8	А	518	0	0	18	0
All	All	10514	0	9680	108	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 5.

All (108) 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: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
1:A:1222:TYR:OH	1:A:1245:THR:HG21	1.89	0.72



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:HB3	1:A:366:MET:HE1	1.85	0.57
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.70	0.57
1:A:1251:ASN:ND2	1:A:1253:ARG:H	2.03	0.57
1:A:96:HIS:HE1	1:A:103:VAL:O	1.87	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:335:PHE:HB3	1:A:366:MET:CE	2.37	0.55
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.07	0.54
1:A:337:VAL:HG11	1:A:366:MET:HE2	1.90	0.54
1:A:950:ASP:HB2	8:A:1421:HOH:O	2.08	0.54
1:A:829:ILE:CD1	1:A:829:ILE:N	2.71	0.54
1:A:396:VAL:HG22	1:A:850:LEU:HB2	1.89	0.54
1:A:335:PHE:CD1	1:A:366:MET:HE1	2.43	0.53
1:A:33:ILE:HG12	1:A:114:ILE:HD12	1.91	0.53
1:A:238:PHE:CE2	1:A:242:LYS:HE2	2.45	0.52
1:A:1086:HIS:HD2	5:A:1310:SO4:O4	1.93	0.51
1:A:349:TRP:CZ3	1:A:846:VAL:HG22	2.45	0.51
1:A:1006:HIS:HD2	8:A:1517:HOH:O	1.92	0.51
1:A:16:ILE:HG23	1:A:33:ILE:HG22	1.93	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: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
1:A:270:ARG:HD3	8:A:1547:HOH:O	2.12	0.49



	• • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:423:ASP:HB2	8:A:1783:HOH:O	2.12	0.49
1:A:619:LEU:N	1:A:619:LEU:HD23	2.27	0.48
1:A:545:ASN:HD22	1:A:547:SER:H	1.60	0.48
1:A:337:VAL:CG1	1:A:366:MET:HE2	2.44	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:1100:LEU:O	1:A:1104:GLU:HG3	2.16	0.46
1:A:14:PHE:HB3	5:A:1315:SO4:O3	2.15	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:995:LEU:C	1:A:995:LEU:HD12	2.35	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:1025:ILE:HD13	1:A:1025:ILE:HG21	1.65	0.44
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.20	0.44
1:A:882:TRP:CH2	1:A:927:GLY:HA3	2.52	0.44
1:A:820:SER:OG	1:A:822:GLU:HG2	2.17	0.44
1:A:290:LEU:HD12	1:A:290:LEU:C	2.37	0.44
1:A:1047:GLU:H	1:A:1050:VAL:HG21	1.82	0.44
1:A:315:GLU:OE1	1:A:382:ARG:NH2	2.37	0.44
1:A:436:LEU:HD13	1:A:512:MET:HE2	1.99	0.43
1:A:990:TRP:HB2	1:A:1006:HIS:CD2	2.54	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:337:VAL:HG13	1:A:366:MET:CE	2.49	0.43
1:A:347:GLN:HB3	1:A:348:PRO:HD2	2.01	0.42
6:A:1320:ACT:H3	8:A:1615:HOH:O	2.19	0.42



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:A:818:GLN:NE2	8:A:1566:HOH:O	2.51	0.42
1:A:531:LEU:O	6:A:1320:ACT:O	2.38	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: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:1234:PRO:O	1:A:1235:ALA:C	2.60	0.40
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)

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	А	1279/1303~(98%)	1232~(96%)	44 (3%)	3~(0%)	47 64	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	623	GLY
1	А	969	ASN
1	А	594	ASP



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	Analysed Rotameric Outlie		Percentiles	
1	А	1023/1040~(98%)	960~(94%)	63~(6%)	18 29	

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

Mol	Chain	Res	Type
1	А	-5	VAL
1	А	-3	ARG
1	А	5	LEU
1	А	6	ARG
1	А	14	PHE
1	А	33	ILE
1	А	43	LEU
1	А	47	LEU
1	А	69	THR
1	А	83	THR
1	А	104	ASP
1	А	118	THR
1	А	119	LEU
1	А	134	ARG
1	А	141	SER
1	А	142	SER
1	А	206	LEU
1	А	247	THR
1	А	250	ASP
1	А	253	LEU
1	А	294	GLU
1	А	296	HIS
1	А	332	LEU
1	А	358	ARG
1	А	382	ARG
1	А	396	VAL
1	А	412	MET
1	А	417	ILE
1	А	429	GLU
1	А	445	ASN



Mol	Chain	Res	Type
1	А	487	ARG
1	А	508	LEU
1	А	510	ASN
1	А	553	LEU
1	А	588	LEU
1	А	596	GLN
1	А	611	LYS
1	А	619	LEU
1	А	774	VAL
1	А	782	LYS
1	А	789	ASN
1	А	811	VAL
1	А	823	ASP
1	А	829	ILE
1	А	831	LEU
1	А	846	VAL
1	А	866	PHE
1	А	878	LYS
1	А	912	LEU
1	А	922	ASN
1	А	982	ARG
1	А	1029	ILE
1	А	1108	LYS
1	А	1136	ASN
1	А	1147	LEU
1	А	1180	LEU
1	А	1182	LEU
1	А	1183	GLN
1	А	1190	MET
1	А	1195	SER
1	А	1206	ASP
1	А	1245	THR
1	А	1251	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	31	HIS
1	А	39	HIS
1	А	60	GLN
1	А	96	HIS
1	А	123	GLN



Mol	Chain	Res	Type
1	А	175	ASN
1	А	216	HIS
1	А	233	GLN
1	А	276	ASN
1	А	298	HIS
1	А	339	ASN
1	А	408	HIS
1	А	419	ASN
1	А	426	GLN
1	А	445	ASN
1	А	471	GLN
1	А	545	ASN
1	А	548	GLN
1	А	584	GLN
1	А	585	HIS
1	А	592	HIS
1	А	739	ASN
1	А	746	HIS
1	А	786	GLN
1	А	818	GLN
1	А	824	ASN
1	А	883	HIS
1	А	916	HIS
1	А	922	ASN
1	А	930	GLN
1	A	993	GLN
1	А	1004	GLN
1	А	1006	HIS
1	A	1018	ASN
1	А	1026	ASN
1	А	1061	HIS
1	А	1086	HIS
1	A	1125	HIS
1	А	1128	GLN
1	А	1251	ASN
1	А	1260	HIS

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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		B	ond leng	gths	B	Bond ang	gles
	туре	Chain	Talli Res Lin	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	CYG	А	1135	1	$9,\!14,\!15$	2.12	2 (22%)	6, 17, 19	<mark>5.02</mark>	3 (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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	CYG	А	1135	1	-	1/10/16/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	1135	CYG	CG1-CD1	5.14	1.56	1.50
1	А	1135	CYG	OE2-CD1	3.49	1.26	1.21

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	A	1135	CYG	OE2-CD1-CG1	-9.12	113.22	123.99
1	А	1135	CYG	CG1-CD1-SG	7.36	122.03	113.46
1	А	1135	CYG	CB1-CG1-CD1	-3.06	105.56	112.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	1135	CYG	N-CA-CB-SG

There are no ring outliers.



No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 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).

Mal	Tune	Chain	Pog	Tink	B	ond leng	gths	В	ond ang	les
WIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	SO4	А	1318	-	$4,\!4,\!4$	0.45	0	6,6,6	1.22	1(16%)
5	SO4	А	1313	-	4,4,4	0.56	0	$6,\!6,\!6$	0.80	0
5	SO4	А	1317	-	4, 4, 4	0.38	0	$6,\!6,\!6$	0.39	0
2	ADP	А	1301	3	24,29,29	1.12	3 (12%)	$29,\!45,\!45$	1.44	3 (10%)
5	SO4	А	1310	-	4,4,4	0.24	0	$6,\!6,\!6$	1.03	0
6	ACT	А	1323	-	$1,\!3,\!3$	0.30	0	$0,\!3,\!3$	0.00	-
5	SO4	А	1314	-	4,4,4	0.17	0	$6,\!6,\!6$	0.58	0
6	ACT	А	1320	-	$1,\!3,\!3$	4.24	1 (100%)	$_{0,3,3}$	0.00	-
5	SO4	А	1315	-	4,4,4	0.53	0	$6,\!6,\!6$	0.63	0
5	SO4	А	1319	-	4,4,4	0.50	0	$6,\!6,\!6$	0.81	0
5	SO4	А	1307	-	4,4,4	0.39	0	$6,\!6,\!6$	0.28	0
6	ACT	А	1322	-	$1,\!3,\!3$	6.09	1 (100%)	$_{0,3,3}$	0.00	-
5	SO4	А	1309	-	4,4,4	0.49	0	$6,\!6,\!6$	0.61	0
5	SO4	А	1312	-	4,4,4	0.50	0	$6,\!6,\!6$	0.36	0
5	SO4	А	1308	-	4, 4, 4	0.59	0	$6,\!6,\!6$	0.49	0
5	SO4	A	1316	-	4,4,4	0.32	0	$6,\!6,\!6$	0.20	0
5	SO4	A	1311	-	4,4,4	0.24	0	6, 6, 6	0.38	0
6	ACT	A	1321	_	1,3,3	3.66	1 (100%)	$0,\!3,\!3$	0.00	_

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	ADP	А	1301	3	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
6	А	1322	ACT	CH3-C	6.09	1.56	1.48
6	А	1320	ACT	CH3-C	4.24	1.54	1.48
6	А	1321	ACT	CH3-C	3.66	1.53	1.48
2	А	1301	ADP	PB-O1B	2.39	1.58	1.50
2	А	1301	ADP	O4'-C1'	2.36	1.44	1.41
2	А	1301	ADP	C5-N7	-2.12	1.32	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	1301	ADP	N6-C6-N1	3.63	126.11	118.57
2	А	1301	ADP	PA-O3A-PB	-3.48	120.87	132.83
5	А	1318	SO4	O4-S-O3	-2.59	98.02	109.06
2	А	1301	ADP	N3-C2-N1	-2.04	125.49	128.68

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	А	1317	SO4	1	0
5	А	1310	SO4	1	0
6	А	1323	ACT	1	0
6	А	1320	ACT	4	0
5	А	1315	SO4	1	0
5	А	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.



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	А	1283/1303~(98%)	-0.58	16 (1%)	79	77	9, 18, 37, 76	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	25	ALA	4.9
1	А	789	ASN	4.3
1	А	-1	SER	4.0
1	А	276	ASN	3.9
1	А	117	SER	3.8
1	А	969	ASN	3.7
1	А	624	ASP	2.8
1	А	914	ASP	2.8
1	А	152	HIS	2.5
1	А	21	ALA	2.4
1	А	27	ASN	2.4
1	А	970	ASP	2.4
1	А	121	ALA	2.3
1	А	-2	GLY	2.2
1	А	630	ASP	2.1
1	А	790	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	CYG	A	1135	15/16	0.97	0.10	11, 13, 14, 15	0



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	\mathbf{B} -factors (\mathbf{A}^2)	Q<0.9
6	ACT	А	1320	4/4	0.80	0.44	47,50,52,53	0
6	ACT	А	1322	4/4	0.84	0.26	21,22,26,26	0
5	SO4	А	1313	5/5	0.86	0.37	$46,\!48,\!59,\!60$	0
6	ACT	А	1323	4/4	0.91	0.19	$33,\!33,\!36,\!40$	0
5	SO4	А	1312	5/5	0.95	0.37	$46,\!46,\!50,\!51$	0
5	SO4	А	1315	5/5	0.95	0.29	$47,\!51,\!53,\!58$	0
3	MG	А	1302	1/1	0.95	0.07	$15,\!15,\!15,\!15$	0
5	SO4	А	1316	5/5	0.96	0.17	14,14,15,15	5
3	MG	А	1304	1/1	0.96	0.07	16, 16, 16, 16	0
6	ACT	А	1321	4/4	0.96	0.10	$18,\!20,\!21,\!22$	0
3	MG	А	1303	1/1	0.96	0.05	$15,\!15,\!15,\!15$	0
5	SO4	А	1318	5/5	0.97	0.31	$34,\!35,\!43,\!46$	0
3	MG	А	1305	1/1	0.98	0.20	2,2,2,2	0
2	ADP	А	1301	27/27	0.98	0.09	$7,\!9,\!10,\!11$	0
5	SO4	А	1317	5/5	0.98	0.22	$40,\!41,\!43,\!47$	0
5	SO4	А	1307	5/5	0.98	0.17	29,32,34,34	0
5	SO4	А	1309	5/5	0.98	0.22	27, 28, 29, 30	0
4	MN	А	1306	1/1	0.98	0.09	47,47,47,47	0
5	SO4	А	1314	5/5	0.99	0.12	$25,\!25,\!26,\!27$	0
5	SO4	А	1319	5/5	0.99	0.24	$28,\!30,\!32,\!33$	0
5	SO4	А	1311	5/5	0.99	0.15	26, 29, 31, 31	0
5	SO4	А	1310	5/5	0.99	0.17	$23,\!25,\!26,\!28$	0
7	XE	А	1326	1/1	0.99	0.10	29,29,29,29	1
5	SO4	А	1308	5/5	0.99	0.12	20,20,23,24	0
7	XE	А	1325	1/1	1.00	0.07	21,21,21,21	1
7	XE	А	1324	1/1	1.00	0.06	15, 15, 15, 15	0
7	XE	А	1327	1/1	1.00	0.03	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.

