



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:04 AM UTC

PDB ID : 5H3U / pdb_00005h3u
Title : Sm RNA bound to GEMIN5-WD
Authors : Bharath, S.R.; Tang, X.; Song, H.
Deposited on : 2016-10-27
Resolution : 2.50 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
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

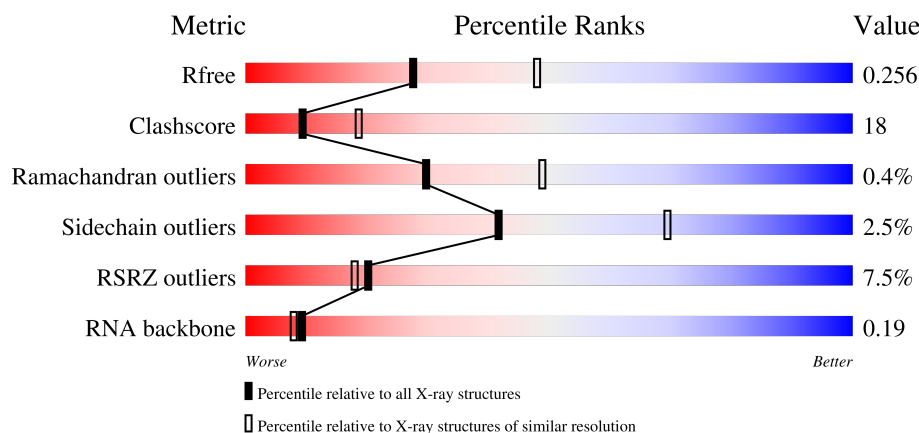
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	740	
1	B	740	
2	C	10	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	801	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10548 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.

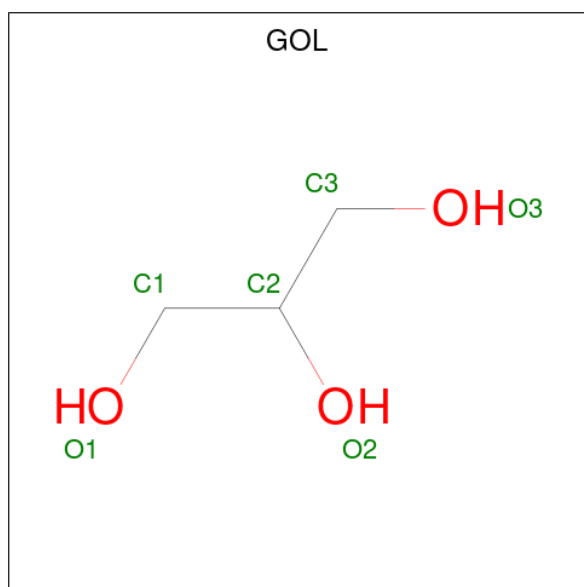
- Molecule 1 is a protein called Gem-associated protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5171	3296	890	957	28			
1	B	662	Total	C	N	O	S	0	0	0
			5117	3261	883	945	28			

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*UP*UP*UP*UP*UP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	0	0	0
			141	65	20	50	6			

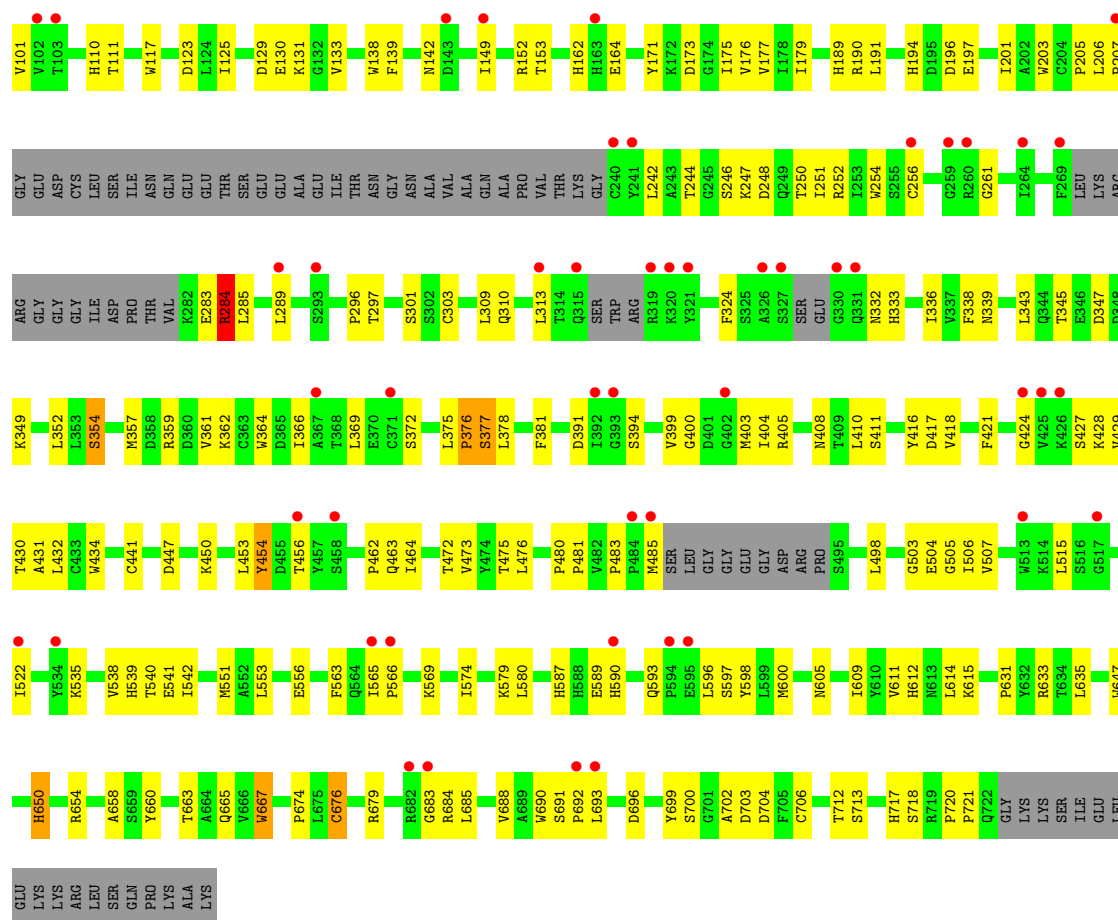
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

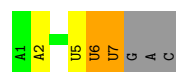
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total 84	O 84	0	0
4	B	23	Total 23	O 23	0	0
4	C	6	Total 6	O 6	0	0



- Molecule 2: RNA (5'-R(*AP*AP*UP*UP*UP*UP*UP*GP*AP*C)-3')

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.84Å 92.08Å 110.80Å 90.00° 99.99° 90.00°	Depositor
Resolution (Å)	48.88 – 2.50 48.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.88-2.50) 97.7 (48.88-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.48Å)	Xtriage
Refinement program	PHENIX (dev_2386: ???)	Depositor
R, R_{free}	0.202 , 0.256 0.208 , 0.256	Depositor DCC
R_{free} test set	2585 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10548	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: GOL

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	2/5322 (0.0%)	0.65	5/7269 (0.1%)
1	B	0.38	1/5266 (0.0%)	0.64	3/7191 (0.0%)
2	C	0.32	0/156	0.66	0/240
All	All	0.41	3/10744 (0.0%)	0.65	8/14700 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	377	SER	C-N	-8.76	1.21	1.33
1	A	309	LEU	C-N	-6.80	1.24	1.33
1	A	308	LEU	C-N	-5.21	1.26	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	PRO	O-C-N	-12.54	108.00	123.04
1	B	376	PRO	CA-C-N	10.02	140.87	121.63
1	B	376	PRO	C-N-CA	10.02	140.87	121.63
1	A	309	LEU	O-C-N	-7.94	113.67	123.36
1	A	511	ASN	CA-C-N	-6.79	111.82	119.28
1	A	511	ASN	C-N-CA	-6.79	111.82	119.28
1	A	308	LEU	CA-C-N	6.76	133.68	122.33
1	A	308	LEU	C-N-CA	6.76	133.68	122.33

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	5171	0	4942	188	0
1	B	5117	0	4903	180	0
2	C	141	0	74	4	0
3	A	6	0	8	6	0
4	A	84	0	0	4	0
4	B	23	0	0	1	0
4	C	6	0	0	0	0
All	All	10548	0	9927	367	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 18.

All (367) 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:110:HIS:CG	1:A:131:LYS:HG3	1.76	1.21
1:A:289:LEU:HD23	1:A:301:SER:HB3	1.22	1.10
1:A:482:VAL:H	1:A:509:GLN:HE22	1.08	1.01
1:A:110:HIS:CD2	1:A:131:LYS:HG3	1.98	0.97
1:A:576:GLN:HE21	1:A:612:HIS:HE1	1.06	0.95
1:A:289:LEU:HD23	1:A:301:SER:CB	2.01	0.90
1:B:13:ASN:HD21	1:B:33:ARG:H	1.20	0.89
1:A:110:HIS:CG	1:A:131:LYS:CG	2.56	0.89
1:B:58:GLY:HA3	1:B:99:LYS:HE2	1.53	0.88
1:B:289:LEU:CD2	1:B:301:SER:CB	2.51	0.88
1:A:116:HIS:HD2	1:A:159:CYS:H	1.21	0.87
1:B:665:GLN:NE2	1:B:674:PRO:HB3	1.91	0.84
1:B:88:ASP:HB3	1:B:90:THR:HG22	1.57	0.84
1:A:421:PHE:HD2	1:A:454:TYR:HH	1.26	0.82
1:A:149:ILE:HG22	1:A:150:GLU:HG2	1.63	0.80
1:B:289:LEU:HD23	1:B:301:SER:CB	2.13	0.79
1:A:576:GLN:HE21	1:A:612:HIS:CE1	1.97	0.79
1:B:289:LEU:CD2	1:B:301:SER:HB3	2.12	0.79
1:A:240:CYS:HB3	1:A:256:CYS:HB3	1.65	0.79
1:A:63:HIS:HE1	1:A:84:THR:OG1	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ILE:HG23	1:B:566:PRO:HD3	1.67	0.77
1:A:482:VAL:H	1:A:509:GLN:NE2	1.83	0.77
1:A:390:VAL:HG21	1:A:437:THR:O	1.85	0.77
1:B:289:LEU:CD2	1:B:301:SER:HB2	2.15	0.76
1:A:123:ASP:OD2	1:A:140:ASN:HB2	1.85	0.76
1:A:13:ASN:HD21	1:A:33:ARG:H	1.31	0.75
1:A:289:LEU:CD2	1:A:301:SER:HB3	2.12	0.74
1:B:6:ARG:NH2	1:B:47:GLU:OE2	2.21	0.74
1:A:22:ALA:HB1	1:A:343:LEU:HD23	1.70	0.74
1:A:297:THR:HG22	1:A:298:GLN:NE2	2.02	0.73
1:A:116:HIS:CD2	1:A:159:CYS:H	2.06	0.73
1:B:410:LEU:HG	1:B:693:LEU:HD21	1.72	0.72
3:A:801:GOL:O2	1:B:717:HIS:HD2	1.73	0.71
1:B:658:ALA:HB2	1:B:688:VAL:HG13	1.71	0.71
1:B:551:MET:HE3	1:B:553:LEU:HG	1.73	0.71
1:B:429:VAL:HG11	1:B:432:LEU:HD11	1.73	0.71
1:B:26:GLY:HA3	1:B:41:VAL:O	1.92	0.70
1:A:421:PHE:HD2	1:A:454:TYR:CZ	2.10	0.69
1:A:201:ILE:HG12	1:A:244:THR:HG22	1.75	0.69
1:B:92:LYS:HD2	1:B:101:VAL:HG21	1.75	0.69
1:B:194:HIS:CE1	1:B:252:ARG:HG3	2.29	0.68
1:A:421:PHE:CD2	1:A:454:TYR:CE1	2.82	0.68
1:A:26:GLY:HA2	1:A:343:LEU:HD11	1.75	0.67
1:A:665:GLN:NE2	1:A:674:PRO:HB3	2.09	0.67
1:A:392:ILE:HG12	1:A:693:LEU:HD21	1.77	0.67
1:A:392:ILE:HG12	1:A:693:LEU:CD2	2.24	0.67
1:A:421:PHE:CD2	1:A:454:TYR:CZ	2.83	0.66
1:A:593:GLN:HB2	1:A:596:LEU:HG	1.78	0.66
1:A:648:SER:OG	1:A:651:HIS:HD2	1.78	0.66
1:A:110:HIS:ND1	1:A:131:LYS:HE3	2.11	0.65
1:A:576:GLN:NE2	1:A:612:HIS:HE1	1.89	0.65
1:A:33:ARG:HD3	2:C:6:U:O2'	1.97	0.65
1:B:683:GLY:HA3	1:B:703:ASP:OD1	1.96	0.65
1:B:63:HIS:CE1	1:B:90:THR:HG23	2.32	0.65
1:B:289:LEU:HD23	1:B:301:SER:HB2	1.78	0.65
1:B:38:LEU:HD12	1:B:99:LYS:HE3	1.78	0.64
1:B:345:THR:OG1	1:B:349:LYS:HB2	1.96	0.64
3:A:801:GOL:H31	1:B:679:ARG:HH22	1.63	0.64
1:A:152:ARG:HB2	1:A:171:TYR:CD2	2.32	0.64
1:B:111:THR:HB	1:B:130:GLU:CD	2.23	0.64
1:B:352:LEU:HB2	1:B:366:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:HD21	1:B:301:SER:HB2	1.79	0.63
1:A:13:ASN:ND2	2:C:6:U:H3	1.96	0.63
1:B:431:ALA:O	1:B:432:LEU:HD12	1.98	0.63
1:A:611:VAL:HB	1:A:633:ARG:HB2	1.81	0.63
1:B:345:THR:HG21	1:B:349:LYS:HE2	1.81	0.63
1:B:696:ASP:OD1	1:B:712:THR:HB	1.99	0.62
1:B:475:THR:HG23	1:B:542:ILE:HG22	1.80	0.62
1:B:574:ILE:HD11	1:B:614:LEU:HD11	1.81	0.62
1:A:141:ARG:HG3	1:A:141:ARG:O	1.98	0.62
1:A:189:HIS:NE2	1:A:256:CYS:O	2.32	0.62
1:A:696:ASP:OD1	1:A:712:THR:HB	2.00	0.62
1:B:447:ASP:HA	1:B:472:THR:HG23	1.80	0.62
1:A:149:ILE:HG12	1:A:179:ILE:HG21	1.82	0.62
1:B:142:ASN:O	1:B:142:ASN:ND2	2.33	0.62
1:A:638:HIS:HE1	1:A:657:SER:HB2	1.65	0.61
1:A:505:GLY:HA2	1:A:539:HIS:O	2.00	0.61
1:B:535:LYS:HD2	1:B:535:LYS:H	1.65	0.61
1:B:285:LEU:HA	1:B:336:ILE:HG21	1.83	0.60
1:A:421:PHE:HB3	1:A:454:TYR:CZ	2.36	0.60
1:A:110:HIS:ND1	1:A:131:LYS:HG3	2.15	0.60
1:B:450:LYS:HD3	1:B:464:ILE:HD12	1.83	0.60
1:B:692:PRO:HG2	1:B:693:LEU:HD12	1.83	0.60
1:A:33:ARG:HG2	2:C:6:U:O2	2.02	0.59
1:A:121:VAL:HB	1:A:124:LEU:HB3	1.85	0.59
1:A:13:ASN:ND2	1:A:33:ARG:H	1.99	0.59
1:A:287:LEU:HD13	1:A:302:SER:O	2.03	0.59
1:B:676:CYS:SG	1:B:712:THR:HG23	2.43	0.59
1:A:421:PHE:HD2	1:A:454:TYR:OH	1.84	0.59
1:A:605:ASN:HA	1:A:641:LYS:HB2	1.85	0.59
1:A:665:GLN:HE21	1:A:674:PRO:HB3	1.65	0.59
1:B:574:ILE:HD12	1:B:600:MET:HE1	1.85	0.59
1:B:289:LEU:HD21	1:B:301:SER:CB	2.29	0.58
1:B:587:HIS:HD2	1:B:647:TRP:CE3	2.21	0.58
1:B:63:HIS:HE1	1:B:90:THR:HG23	1.68	0.58
1:B:660:TYR:HA	1:B:684:ARG:HB3	1.85	0.58
1:B:189:HIS:NE2	1:B:256:CYS:O	2.36	0.58
1:B:251:ILE:HG12	1:B:289:LEU:HD11	1.84	0.58
1:A:554:GLY:HA3	1:A:581:VAL:CG2	2.34	0.58
1:A:421:PHE:HB3	1:A:454:TYR:CE2	2.39	0.58
1:A:638:HIS:CE1	1:A:657:SER:HB2	2.38	0.58
1:B:481:PRO:HB3	1:B:485:MET:HE2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:HG22	1:A:289:LEU:N	2.19	0.57
1:A:309:LEU:HD23	1:A:323:LEU:HD12	1.86	0.57
1:A:500:SER:OG	1:A:510:HIS:CE1	2.57	0.57
1:B:26:GLY:HA2	1:B:343:LEU:HD21	1.86	0.57
1:A:396:ALA:HB1	1:A:432:LEU:HD13	1.86	0.57
1:A:564:GLN:HB2	1:A:571:ILE:CD1	2.35	0.57
1:A:51:THR:HG21	1:A:415:ASN:HD21	1.70	0.57
1:A:564:GLN:HB2	1:A:571:ILE:HD11	1.86	0.57
1:B:333:HIS:CE1	1:B:362:LYS:HG3	2.40	0.57
1:A:668:ASP:OD2	1:A:671:ARG:HG3	2.06	0.56
1:A:267:LEU:HD11	1:A:287:LEU:HD22	1.88	0.56
1:A:612:HIS:HD2	4:A:963:HOH:O	1.87	0.56
1:A:699:TYR:OH	1:A:709:LYS:NZ	2.37	0.56
1:A:5:PRO:HG3	1:A:714:MET:HE1	1.88	0.56
1:A:425:VAL:C	1:A:427:SER:H	2.14	0.56
1:A:63:HIS:CE1	1:A:84:THR:OG1	2.54	0.55
1:A:347:ASP:OD1	1:A:347:ASP:O	2.24	0.55
1:B:427:SER:HB2	1:B:447:ASP:OD1	2.06	0.55
1:A:406:VAL:HB	1:A:419:LYS:CG	2.36	0.55
1:A:425:VAL:O	1:A:427:SER:N	2.40	0.55
1:B:441:CYS:SG	1:B:453:LEU:HD11	2.47	0.55
1:A:665:GLN:OE1	1:A:677:ASN:HB2	2.06	0.55
1:B:284:ARG:HG3	1:B:336:ILE:HD13	1.87	0.55
1:A:673:GLU:HG2	1:A:675:LEU:HD23	1.89	0.55
1:B:654:ARG:HG2	1:B:690:TRP:CH2	2.42	0.55
1:A:480:PRO:HD2	1:A:544:TRP:CH2	2.42	0.54
1:B:303:CYS:HB2	1:B:309:LEU:HD13	1.89	0.54
1:A:717:HIS:HD1	3:A:801:GOL:HO2	1.55	0.54
3:A:801:GOL:O2	1:B:717:HIS:CD2	2.56	0.54
1:A:406:VAL:HB	1:A:419:LYS:HG3	1.90	0.54
1:B:665:GLN:HE21	1:B:674:PRO:HB3	1.70	0.54
1:B:702:ALA:HB3	1:B:704:ASP:OD1	2.07	0.54
1:A:400:GLY:HA3	2:C:7:U:O4	2.07	0.54
1:B:347:ASP:OD2	1:B:349:LYS:HD3	2.08	0.54
1:A:554:GLY:HA3	1:A:581:VAL:HG21	1.90	0.54
1:B:429:VAL:CG1	1:B:432:LEU:HD11	2.37	0.54
1:A:475:THR:HG23	1:A:542:ILE:HG22	1.90	0.54
1:A:638:HIS:HD2	1:A:661:ASP:OD2	1.91	0.54
1:B:201:ILE:HG12	1:B:244:THR:HG22	1.89	0.54
1:B:504:GLU:HG2	1:B:506:ILE:H	1.72	0.53
1:B:19:CYS:HB2	1:B:31:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ALA:HB1	1:B:685:LEU:HB3	1.89	0.53
1:A:137:TYR:OH	1:A:142:ASN:OD1	2.22	0.53
1:A:251:ILE:HG12	1:A:289:LEU:HD21	1.91	0.53
1:A:665:GLN:HE22	1:A:720:PRO:HD3	1.74	0.53
1:B:333:HIS:NE2	1:B:354:SER:HB3	2.24	0.53
1:B:542:ILE:HD11	1:B:551:MET:SD	2.49	0.53
1:A:665:GLN:NE2	1:A:720:PRO:HD3	2.24	0.52
1:A:163:HIS:HB3	1:A:166:LEU:HB2	1.92	0.52
1:A:26:GLY:HA3	1:A:41:VAL:O	2.10	0.52
1:B:11:SER:HA	1:B:377:SER:HB2	1.92	0.52
1:B:13:ASN:ND2	1:B:33:ARG:H	2.00	0.52
1:A:450:LYS:HB2	1:A:468:TYR:CE2	2.45	0.52
1:A:157:LEU:HD12	1:A:169:ILE:HG12	1.91	0.51
1:A:171:TYR:HB2	1:A:175:ILE:HG22	1.91	0.51
1:B:505:GLY:HA2	1:B:539:HIS:O	2.10	0.51
1:A:297:THR:HG22	1:A:298:GLN:HE21	1.73	0.51
1:A:500:SER:OG	1:A:510:HIS:HE1	1.94	0.51
1:A:677:ASN:HD22	1:A:679:ARG:HE	1.58	0.51
1:B:196:ASP:HB2	1:B:248:ASP:HB3	1.91	0.51
1:A:110:HIS:CE1	1:A:131:LYS:HE3	2.46	0.51
1:B:10:PRO:HB2	1:B:32:ALA:HB1	1.92	0.51
1:A:59:GLU:HG2	1:A:61:VAL:HG22	1.93	0.50
1:B:579:LYS:HB3	1:B:605:ASN:HB2	1.91	0.50
1:A:191:LEU:HD13	1:A:254:TRP:CG	2.46	0.50
1:B:696:ASP:OD2	1:B:713:SER:OG	2.22	0.50
1:A:602:SER:HB2	4:A:963:HOH:O	2.11	0.50
1:A:163:HIS:CE1	1:A:165:ASP:HB2	2.47	0.50
1:B:424:GLY:HA3	1:B:462:PRO:HG2	1.93	0.50
1:A:665:GLN:HG3	1:A:666:VAL:N	2.26	0.50
1:B:391:ASP:HB3	1:B:394:SER:HB3	1.94	0.50
1:A:110:HIS:CB	1:A:131:LYS:HG2	2.43	0.49
1:A:719:ARG:NH2	1:B:720:PRO:O	2.45	0.49
1:B:424:GLY:HA3	1:B:462:PRO:CG	2.42	0.49
1:B:483:PRO:HA	1:B:485:MET:H	1.77	0.49
1:B:676:CYS:HA	1:B:718:SER:HA	1.95	0.49
1:A:633:ARG:HD2	1:A:672:GLU:HG3	1.93	0.49
1:B:130:GLU:O	1:B:153:THR:HA	2.10	0.49
1:B:191:LEU:HD13	1:B:254:TRP:CG	2.47	0.49
3:A:801:GOL:H12	1:B:717:HIS:HB3	1.93	0.49
1:A:505:GLY:HA3	1:A:538:VAL:HB	1.95	0.49
1:B:480:PRO:HG3	1:B:565:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TRP:HA	1:B:261:GLY:HA2	1.94	0.49
1:B:303:CYS:HB2	1:B:309:LEU:CD1	2.43	0.49
1:B:650:HIS:HE1	1:B:692:PRO:O	1.95	0.49
1:B:663:THR:HG21	1:B:721:PRO:CD	2.42	0.49
1:A:482:VAL:N	1:A:509:GLN:HE22	1.92	0.49
1:B:381:PHE:O	1:B:399:VAL:HA	2.13	0.49
1:A:541:GLU:HG2	1:A:584:ILE:HG13	1.94	0.48
1:A:333:HIS:CE1	1:A:362:LYS:HD2	2.48	0.48
1:A:565:ILE:HG23	1:A:566:PRO:HD3	1.95	0.48
1:B:63:HIS:CE1	1:B:92:LYS:HG3	2.47	0.48
1:A:175:ILE:CD1	1:A:192:ARG:HG2	2.43	0.48
1:A:425:VAL:C	1:A:427:SER:N	2.71	0.48
1:B:289:LEU:HD23	1:B:301:SER:HA	1.96	0.48
1:A:390:VAL:HG11	1:A:439:GLU:HB3	1.96	0.48
1:B:18:ARG:O	1:B:69:GLY:HA2	2.14	0.48
1:A:194:HIS:CE1	1:A:252:ARG:HD2	2.49	0.48
1:A:297:THR:O	1:A:313:LEU:HG	2.13	0.48
1:B:251:ILE:HD11	1:B:289:LEU:HD21	1.96	0.48
1:B:88:ASP:CB	1:B:90:THR:HG22	2.38	0.48
1:B:505:GLY:HA3	1:B:538:VAL:HB	1.96	0.48
1:A:440:GLY:HA2	1:A:456:THR:HB	1.95	0.48
1:A:194:HIS:NE2	1:A:252:ARG:HD2	2.29	0.48
1:A:545:LYS:HG3	1:A:586:TRP:CE3	2.48	0.48
1:A:621:SER:O	1:A:621:SER:OG	2.26	0.47
1:A:556:GLU:HG3	1:A:580:LEU:HD12	1.95	0.47
1:B:691:SER:HB2	1:B:699:TYR:HE1	1.78	0.47
1:A:421:PHE:HD2	1:A:454:TYR:CE1	2.24	0.47
1:A:665:GLN:HE22	1:A:719:ARG:HA	1.79	0.47
1:A:28:PHE:CD1	1:A:353:LEU:HD13	2.49	0.47
1:A:683:GLY:HA3	1:A:703:ASP:OD1	2.14	0.47
1:B:297:THR:O	1:B:313:LEU:HG	2.15	0.47
1:B:21:ASP:OD2	1:B:72:PHE:HB2	2.15	0.47
1:A:425:VAL:CG1	1:A:429:VAL:HG22	2.45	0.47
1:B:378:LEU:HA	1:B:405:ARG:HH22	1.79	0.47
1:B:540:THR:HG21	1:B:580:LEU:HG	1.96	0.47
1:B:667:TRP:HB3	1:B:674:PRO:HA	1.96	0.47
1:A:483:PRO:HD2	1:A:525:LEU:HD21	1.97	0.46
1:B:289:LEU:HD23	1:B:301:SER:CA	2.44	0.46
1:A:19:CYS:HB2	1:A:31:ALA:HB3	1.97	0.46
1:A:480:PRO:HB2	1:A:565:ILE:HD11	1.96	0.46
1:B:63:HIS:CE1	1:B:92:LYS:HE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ARG:HB2	1:B:171:TYR:CD1	2.50	0.46
1:A:70:PHE:HD1	1:A:84:THR:HG22	1.79	0.46
1:B:338:PHE:C	1:B:339:ASN:HD22	2.23	0.46
1:A:163:HIS:CG	1:A:166:LEU:HG	2.51	0.46
1:A:545:LYS:NZ	1:A:547:ASP:OD2	2.37	0.46
1:A:472:THR:HG23	1:A:474:TYR:CE1	2.51	0.46
1:B:173:ASP:OD1	1:B:173:ASP:N	2.48	0.46
1:B:164:GLU:CD	1:B:164:GLU:H	2.24	0.46
1:A:297:THR:CG2	1:A:298:GLN:HE21	2.30	0.46
1:A:51:THR:HG21	1:A:415:ASN:ND2	2.31	0.45
1:A:110:HIS:CB	1:A:131:LYS:CG	2.94	0.45
1:A:288:THR:CG2	1:A:289:LEU:N	2.79	0.45
1:A:458:SER:OG	1:A:460:LYS:HG3	2.15	0.45
1:A:59:GLU:H	1:A:99:LYS:HZ2	1.64	0.45
1:A:309:LEU:CD2	1:A:323:LEU:HD12	2.46	0.45
1:A:665:GLN:HG2	1:A:667:TRP:NE1	2.31	0.45
1:B:117:TRP:CD2	1:B:125:ILE:CD1	3.00	0.45
1:B:250:THR:HG21	1:B:252:ARG:NE	2.31	0.45
1:A:297:THR:CG2	1:A:298:GLN:NE2	2.74	0.45
1:B:248:ASP:OD1	1:B:250:THR:HB	2.17	0.45
1:B:429:VAL:CG1	1:B:432:LEU:CD1	2.95	0.45
1:B:84:THR:OG1	1:B:94:TRP:NE1	2.50	0.45
1:B:251:ILE:CD1	1:B:289:LEU:HD21	2.46	0.45
1:B:399:VAL:HG21	1:B:405:ARG:HH21	1.81	0.45
1:A:59:GLU:HG2	1:A:61:VAL:CG2	2.46	0.45
1:B:650:HIS:CD2	1:B:650:HIS:H	2.34	0.45
1:A:254:TRP:HA	1:A:261:GLY:HA2	1.99	0.45
1:A:485:MET:HG3	1:A:520:PHE:CE2	2.52	0.45
1:A:63:HIS:CD2	1:A:92:LYS:HE2	2.52	0.45
1:A:390:VAL:HG21	1:A:437:THR:C	2.42	0.44
1:A:560:ILE:HD11	1:A:602:SER:OG	2.17	0.44
1:A:393:GLY:O	1:A:409:THR:HB	2.17	0.44
1:A:634:THR:N	1:A:672:GLU:OE1	2.40	0.44
1:B:11:SER:OG	1:B:359:ARG:HD3	2.18	0.44
1:B:123:ASP:HA	1:B:139:PHE:CE1	2.53	0.44
1:B:123:ASP:O	1:B:138:TRP:HA	2.18	0.44
1:B:354:SER:O	1:B:361:VAL:HA	2.17	0.44
1:A:349:LYS:HD3	1:A:351:LEU:HD21	1.99	0.44
1:B:590:HIS:N	1:B:590:HIS:CD2	2.85	0.44
1:A:63:HIS:CD2	1:A:86:SER:CB	3.01	0.44
1:B:375:LEU:HD12	1:B:376:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:TRP:CD1	1:B:667:TRP:N	2.85	0.44
1:A:123:ASP:O	1:A:138:TRP:HA	2.18	0.44
1:A:374:THR:HG22	4:A:967:HOH:O	2.18	0.44
1:B:162:HIS:HE1	1:B:205:PRO:O	2.00	0.44
1:A:251:ILE:HD11	1:A:301:SER:OG	2.17	0.44
1:B:283:GLU:O	1:B:284:ARG:C	2.60	0.44
1:B:476:LEU:HD22	1:B:498:LEU:HD21	2.00	0.44
1:B:598:TYR:CD1	1:B:615:LYS:HA	2.53	0.44
1:A:717:HIS:HA	3:A:801:GOL:H32	2.00	0.44
1:B:475:THR:HG21	1:B:542:ILE:H	1.83	0.44
1:A:558:GLY:O	1:A:577:HIS:HB2	2.18	0.43
1:B:129:ASP:OD2	1:B:133:VAL:HB	2.18	0.43
1:B:246:SER:HB3	1:B:248:ASP:OD1	2.18	0.43
1:B:111:THR:O	1:B:130:GLU:HG3	2.17	0.43
1:A:174:GLY:HA2	1:A:196:ASP:O	2.19	0.43
1:A:366:ILE:HD13	1:A:366:ILE:HA	1.79	0.43
1:B:10:PRO:HD3	1:B:706:CYS:SG	2.58	0.43
1:B:176:VAL:HB	1:B:191:LEU:HB2	2.00	0.43
1:B:416:TYR:O	1:B:418:VAL:N	2.52	0.43
1:A:47:GLU:OE2	1:A:47:GLU:HA	2.18	0.43
1:A:200:SER:OG	1:A:288:THR:HA	2.19	0.43
1:A:540:THR:HG21	1:A:580:LEU:HG	2.01	0.43
1:B:71:THR:HG22	1:B:83:ALA:HB3	2.01	0.43
1:A:163:HIS:HE1	1:A:165:ASP:HB2	1.84	0.42
1:B:504:GLU:HG2	1:B:505:GLY:N	2.34	0.42
1:B:612:HIS:CD2	1:B:631:PRO:HA	2.53	0.42
1:B:357:MET:C	1:B:359:ARG:H	2.27	0.42
1:A:129:ASP:OD2	1:A:133:VAL:HB	2.19	0.42
1:A:428:LYS:HB2	1:A:447:ASP:HB2	2.01	0.42
1:B:454:TYR:CZ	1:B:462:PRO:HD3	2.54	0.42
1:B:665:GLN:NE2	1:B:720:PRO:HD3	2.34	0.42
1:B:539:HIS:ND1	1:B:553:LEU:HD13	2.34	0.42
1:B:593:GLN:HB2	1:B:596:LEU:HG	2.01	0.42
1:A:110:HIS:CE1	1:A:131:LYS:HG3	2.54	0.42
1:B:110:HIS:CD2	1:B:131:LYS:HB2	2.54	0.42
1:B:611:VAL:HB	1:B:633:ARG:HB2	2.01	0.42
1:A:481:PRO:HA	1:A:509:GLN:NE2	2.34	0.42
1:A:650:HIS:CD2	1:A:695:PRO:HA	2.55	0.42
1:B:8:LEU:HD23	1:B:8:LEU:HA	1.82	0.42
1:B:14:TRP:CZ3	1:B:357:MET:HE2	2.54	0.42
1:B:408:ASN:ND2	1:B:411:SER:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:TRP:HH2	1:B:456:THR:HG21	1.85	0.42
1:A:432:LEU:HA	1:A:432:LEU:HD23	1.81	0.42
1:B:403:MET:HB2	1:B:403:MET:HE2	1.87	0.42
1:B:405:ARG:N	1:B:405:ARG:HD3	2.34	0.42
1:B:354:SER:HB2	1:B:364:TRP:HE1	1.83	0.42
1:B:400:GLY:HA2	1:B:428:LYS:HB3	2.02	0.42
1:B:609:ILE:HB	1:B:635:LEU:HB2	2.02	0.42
1:A:88:ASP:OD1	1:A:90:THR:HG22	2.19	0.42
1:A:407:TRP:CD1	1:A:407:TRP:C	2.97	0.42
1:B:324:PHE:CD1	1:B:324:PHE:N	2.87	0.42
1:A:203:TRP:HA	1:A:242:LEU:HD12	2.02	0.41
1:A:255:SER:O	1:A:259:GLY:N	2.48	0.41
1:B:421:PHE:HB3	1:B:454:TYR:CZ	2.55	0.41
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.79	0.41
1:B:310:GLN:NE2	1:B:369:LEU:HD21	2.35	0.41
1:B:507:VAL:HB	1:B:522:ILE:HG21	2.01	0.41
1:A:16:CYS:HB2	1:A:19:CYS:SG	2.60	0.41
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.82	0.41
1:B:289:LEU:HD21	1:B:301:SER:HB3	1.97	0.41
1:A:164:GLU:H	1:A:164:GLU:HG3	1.59	0.41
1:A:349:LYS:HE2	1:A:365:ASP:OD1	2.21	0.41
1:B:463:GLN:OE1	1:B:515:LEU:HD12	2.20	0.41
1:B:539:HIS:CE1	1:B:553:LEU:HD13	2.56	0.41
1:B:206:LEU:HG	1:B:296:PRO:HG3	2.01	0.41
1:B:332:ASN:HA	1:B:364:TRP:HH2	1.85	0.41
1:B:404:ILE:C	1:B:405:ARG:HD3	2.46	0.41
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.59	0.41
1:A:457:TYR:N	1:A:457:TYR:CD1	2.88	0.41
1:A:573:THR:O	1:A:627:THR:HA	2.20	0.41
1:B:149:ILE:HG12	1:B:179:ILE:HG21	2.01	0.41
1:B:366:ILE:HD13	1:B:366:ILE:HA	1.79	0.41
1:B:430:THR:HG21	1:B:472:THR:CG2	2.51	0.41
1:B:574:ILE:CD1	1:B:600:MET:HE1	2.50	0.41
1:B:684:ARG:H	1:B:684:ARG:HG3	1.73	0.41
1:B:61:VAL:HG12	4:B:811:HOH:O	2.20	0.41
1:B:538:VAL:HG22	1:B:556:GLU:HB3	2.02	0.41
1:B:589:GLU:HA	1:B:597:SER:HB3	2.03	0.41
1:A:89:GLY:HA2	4:A:903:HOH:O	2.20	0.41
1:A:387:PHE:CE1	1:A:395:LEU:HB2	2.56	0.41
1:A:392:ILE:O	1:A:392:ILE:HG23	2.20	0.41
1:A:580:LEU:O	1:A:604:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ILE:HD13	1:B:175:ILE:HA	1.81	0.41
1:B:177:VAL:HG12	1:B:190:ARG:HG3	2.03	0.41
1:B:587:HIS:CD2	1:B:647:TRP:CE3	3.04	0.41
1:A:110:HIS:HB3	1:A:131:LYS:HG2	2.03	0.41
1:B:40:ARG:HE	1:B:40:ARG:HB2	1.67	0.41
1:B:197:GLU:HG3	1:B:247:LYS:CB	2.51	0.41
1:B:563:PHE:HA	1:B:569:LYS:O	2.21	0.41
1:B:472:THR:O	1:B:503:GLY:N	2.47	0.40
1:A:63:HIS:CD2	1:A:86:SER:HB3	2.56	0.40
1:A:194:HIS:CD2	1:A:252:ARG:HD2	2.56	0.40
1:B:5:PRO:O	1:B:6:ARG:HD3	2.21	0.40
1:B:206:LEU:HA	1:B:207:PRO:HD3	1.94	0.40
1:A:481:PRO:HA	1:A:509:GLN:HE21	1.86	0.40
1:A:532:ILE:HG23	1:A:534:TYR:CD2	2.56	0.40
1:A:636:SER:C	1:A:667:TRP:HH2	2.29	0.40
1:B:203:TRP:CD2	1:B:242:LEU:HD12	2.56	0.40
1:A:474:TYR:CE2	1:A:503:GLY:HA2	2.56	0.40
1:B:11:SER:HA	1:B:377:SER:CB	2.52	0.40
1:B:284:ARG:HD3	1:B:357:MET:SD	2.61	0.40

There are no symmetry-related clashes.

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	660/740 (89%)	642 (97%)	16 (2%)	2 (0%)	36	55
1	B	650/740 (88%)	627 (96%)	20 (3%)	3 (0%)	24	43
All	All	1310/1480 (88%)	1269 (97%)	36 (3%)	5 (0%)	30	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	LYS
1	B	26	GLY
1	B	417	ASP
1	B	284	ARG
1	A	425	VAL

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	563/642 (88%)	546 (97%)	17 (3%)	36	64
1	B	559/642 (87%)	548 (98%)	11 (2%)	48	75
All	All	1122/1284 (87%)	1094 (98%)	28 (2%)	42	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	141	ARG
1	A	177	VAL
1	A	266	LYS
1	A	289	LEU
1	A	355	THR
1	A	394	SER
1	A	510	HIS
1	A	516	SER
1	A	572	CYS
1	A	576	GLN
1	A	581	VAL
1	A	621	SER
1	A	639	THR
1	A	651	HIS
1	A	657	SER
1	A	688	VAL
1	B	59	GLU
1	B	284	ARG

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Mol	Chain	Res	Type
1	B	354	SER
1	B	372	SER
1	B	454	TYR
1	B	473	VAL
1	B	541	GLU
1	B	650	HIS
1	B	667	TRP
1	B	676	CYS
1	B	700	SER

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	63	HIS
1	A	78	GLN
1	A	116	HIS
1	A	145	GLN
1	A	146	HIS
1	A	162	HIS
1	A	189	HIS
1	A	290	HIS
1	A	298	GLN
1	A	310	GLN
1	A	344	GLN
1	A	415	ASN
1	A	423	GLN
1	A	509	GLN
1	A	582	ASN
1	A	588	HIS
1	A	612	HIS
1	A	638	HIS
1	A	651	HIS
1	A	677	ASN
1	A	681	HIS
1	B	13	ASN
1	B	74	HIS
1	B	78	GLN
1	B	142	ASN
1	B	145	GLN
1	B	298	GLN
1	B	310	GLN

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Mol	Chain	Res	Type
1	B	408	ASN
1	B	423	GLN
1	B	510	HIS
1	B	575	GLN
1	B	577	HIS
1	B	582	ASN
1	B	587	HIS
1	B	590	HIS
1	B	612	HIS
1	B	613	ASN
1	B	650	HIS
1	B	717	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	6/10 (60%)	4 (66%)	1 (16%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	A
2	C	5	U
2	C	6	U
2	C	7	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	6	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand 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	$\# Z > 2$
3	GOL	A	801	-	5,5,5	1.10	0	5,5,5	0.95	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
3	GOL	A	801	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	GOL	O1-C1-C2-C3
3	A	801	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GOL	6	0

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, 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	670/740 (90%)	0.46	48 (7%)	21	19	25, 49, 86, 121	0
1	B	662/740 (89%)	0.72	53 (8%)	18	16	38, 61, 99, 119	0
2	C	7/10 (70%)	0.65	0	100	100	68, 76, 87, 92	0
All	All	1339/1490 (89%)	0.59	101 (7%)	20	18	25, 56, 93, 121	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	565	ILE	5.2
1	B	392	ILE	5.0
1	A	302	SER	4.9
1	A	667	TRP	4.8
1	A	25	GLY	4.6
1	A	454	TYR	4.4
1	A	425	VAL	4.4
1	B	565	ILE	4.4
1	B	693	LEU	4.3
1	A	594	PRO	4.3
1	B	240	CYS	4.2
1	A	240	CYS	4.1
1	A	3	GLN	4.1
1	A	327	SER	3.8
1	B	393	GLY	3.8
1	A	330	GLY	3.7
1	A	208	GLY	3.7
1	A	272	ARG	3.6
1	B	425	VAL	3.5
1	A	317	TRP	3.4
1	A	513	TRP	3.4
1	A	595	GLU	3.3
1	B	313	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	269	PHE	3.2
1	B	88	ASP	3.2
1	A	4	GLU	3.1
1	A	347	ASP	3.1
1	A	326	ALA	3.1
1	B	326	ALA	3.1
1	B	207	PRO	3.0
1	B	319	ARG	3.0
1	B	456	THR	3.0
1	B	426	LYS	3.0
1	B	424	GLY	3.0
1	B	534	TYR	2.9
1	B	330	GLY	2.9
1	A	532	ILE	2.9
1	A	26	GLY	2.8
1	B	26	GLY	2.8
1	A	48	SER	2.8
1	A	518	GLU	2.8
1	B	522	ILE	2.7
1	B	484	PRO	2.7
1	B	595	GLU	2.7
1	A	269	PHE	2.7
1	B	241	TYR	2.7
1	B	327	SER	2.7
1	A	426	LYS	2.6
1	B	367	ALA	2.6
1	B	485	MET	2.6
1	A	256	CYS	2.6
1	B	331	GLN	2.6
1	B	320	LYS	2.6
1	A	281	VAL	2.6
1	A	447	ASP	2.5
1	B	517	GLY	2.5
1	A	412	ILE	2.5
1	B	289	LEU	2.5
1	B	458	SER	2.5
1	B	566	PRO	2.5
1	A	392	ILE	2.5
1	B	3	GLN	2.5
1	B	590	HIS	2.5
1	A	301	SER	2.4
1	B	594	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	485	MET	2.4
1	A	131	LYS	2.4
1	A	593	GLN	2.4
1	B	682	ARG	2.3
1	B	163	HIS	2.3
1	A	616	THR	2.3
1	B	315	GLN	2.3
1	A	419	LYS	2.3
1	B	102	VAL	2.3
1	B	49	PRO	2.3
1	A	258	ARG	2.3
1	A	438	LYS	2.3
1	B	143	ASP	2.2
1	B	692	PRO	2.2
1	A	566	PRO	2.2
1	B	371	CYS	2.1
1	A	575	GLN	2.1
1	A	402	GLY	2.1
1	B	402	GLY	2.1
1	B	683	GLY	2.1
1	B	513	TRP	2.1
1	B	260	ARG	2.1
1	A	270	LEU	2.1
1	A	567	ASN	2.1
1	A	456	THR	2.1
1	B	321	TYR	2.1
1	A	207	PRO	2.1
1	B	256	CYS	2.1
1	B	259	GLY	2.0
1	B	149	ILE	2.0
1	A	20	SER	2.0
1	A	394	SER	2.0
1	A	517	GLY	2.0
1	B	103	THR	2.0
1	B	264	ILE	2.0
1	B	293	SER	2.0

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

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

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
3	GOL	A	801	6/6	0.84	0.34	21,32,37,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.