



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 1E9L / pdb_00001e9l
Title : The crystal structure of novel mammalian lectin Ym1 suggests a saccharide binding site
Authors : Hsiao, C.D.; Sun, Y.J.
Deposited on : 2000-10-21
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

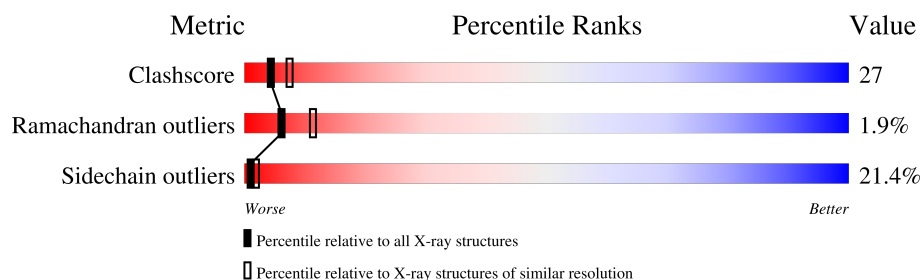
1 Overall quality at a glance

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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	

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
2	GCS	A	800	-	-	X	-

2 Entry composition [i](#)

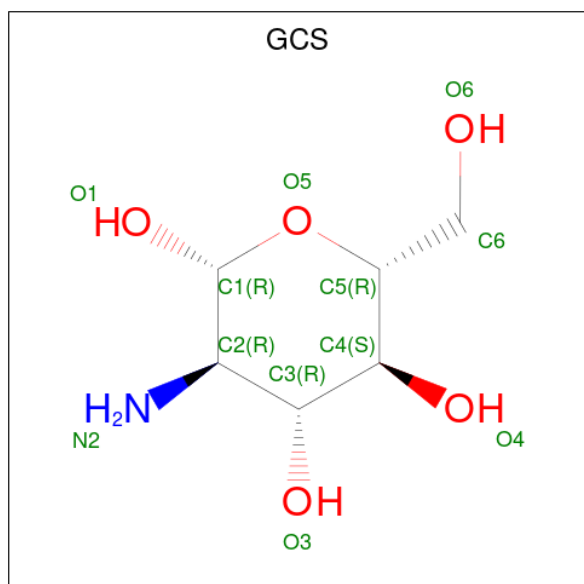
There are 3 unique types of molecules in this entry. The entry contains 4225 atoms, of which 1056 are hydrogens and 0 are deuteriums.

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 YM1 SECRETORY PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	372	3571	1889	628	481	562	11	0	0	0

- Molecule 2 is 2-amino-2-deoxy-beta-D-glucopyranose (CCD ID: GCS) (formula: $C_6H_{13}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	6	1	5	0	0

- Molecule 3 is water.

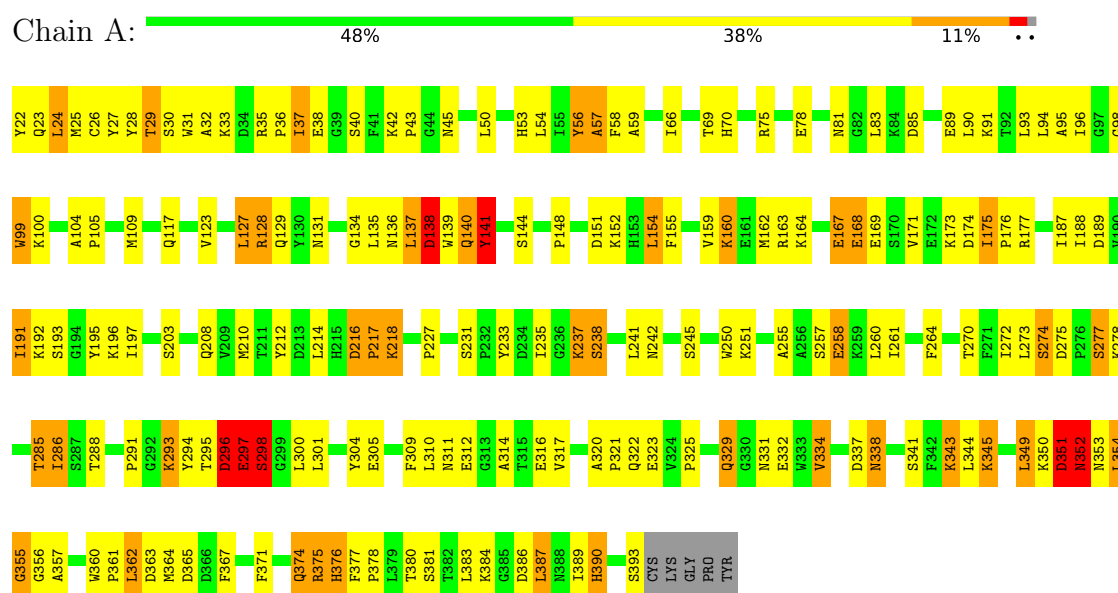
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	214	642	428	214	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: YM1 SECRETORY PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.34Å 60.66Å 60.76Å 90.00° 94.61° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	94.2 (20.00-2.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.198 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4225	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCS

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	0.57	1/3028 (0.0%)	1.03	18/4117 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ASP	N-CA	-13.90	1.26	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ASP	N-CA-C	-12.10	95.39	110.88
1	A	138	ASP	N-CA-C	11.18	123.85	110.44
1	A	355	GLY	N-CA-C	-9.36	91.00	113.18
1	A	141	TYR	CA-C-N	7.35	129.03	119.84
1	A	141	TYR	C-N-CA	7.35	129.03	119.84
1	A	297	GLU	N-CA-C	-7.17	98.33	108.23
1	A	298	SER	N-CA-C	-7.00	97.17	109.06
1	A	390	HIS	N-CA-C	6.70	119.50	109.25
1	A	286	ILE	CB-CA-C	-5.92	105.62	111.30
1	A	197	ILE	CB-CA-C	-5.81	108.19	114.35
1	A	152	LYS	N-CA-C	-5.75	105.09	111.36
1	A	357	ALA	N-CA-C	5.45	117.47	109.24
1	A	387	LEU	N-CA-C	-5.29	106.06	112.88
1	A	334	VAL	N-CA-C	5.24	115.52	107.77
1	A	352	ASN	N-CA-C	-5.23	105.00	111.90
1	A	59	ALA	N-CA-C	-5.21	102.75	110.46
1	A	56	TYR	N-CA-C	5.19	117.22	108.96
1	A	195	TYR	N-CA-C	5.05	117.13	108.90

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	2943	628	2825	155	0
2	A	12	0	12	22	0
3	A	214	428	0	3	0
All	All	3169	1056	2837	155	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 27.

All (155) 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:360:TRP:CH2	2:A:800:GCS:O3	1.91	1.23
1:A:360:TRP:CZ3	2:A:800:GCS:O3	2.00	1.13
1:A:210:MET:HG2	2:A:800:GCS:H61	1.21	1.12
1:A:98:GLY:HA2	2:A:800:GCS:O1	1.63	0.97
1:A:210:MET:HG2	2:A:800:GCS:C6	2.03	0.89
1:A:25:MET:HG2	1:A:53:HIS:HB2	1.54	0.87
1:A:138:ASP:CG	2:A:800:GCS:HN21	1.86	0.83
1:A:22:TYR:O	1:A:390:HIS:HE1	1.65	0.78
1:A:58:PHE:HZ	2:A:800:GCS:H2	1.50	0.77
1:A:29:THR:HB	1:A:363:ASP:OD2	1.85	0.76
1:A:297:GLU:OE1	1:A:300:LEU:CB	2.35	0.75
1:A:69:THR:HG22	1:A:70:HIS:CD2	2.21	0.75
1:A:360:TRP:CZ2	2:A:800:GCS:O3	2.33	0.74
1:A:164:LYS:O	1:A:168:GLU:HG2	1.87	0.72
1:A:297:GLU:CD	1:A:300:LEU:HB3	2.14	0.72
1:A:242:ASN:ND2	1:A:245:SER:H	1.87	0.72
1:A:374:GLN:C	1:A:375:ARG:HG3	2.15	0.72
1:A:309:PHE:CZ	1:A:329:GLN:HB2	2.26	0.71
1:A:169:GLU:HG2	1:A:173:LYS:HE3	1.73	0.71
1:A:297:GLU:OE2	1:A:300:LEU:HD22	1.91	0.70
1:A:297:GLU:OE1	1:A:300:LEU:HD13	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HG2	1:A:364:MET:HG3	1.77	0.66
1:A:155:PHE:O	1:A:159:VAL:HG23	1.95	0.66
1:A:275:ASP:OD1	1:A:277:SER:HB2	1.95	0.66
1:A:360:TRP:CE3	2:A:800:GCS:O3	2.49	0.66
1:A:361:PRO:HD2	1:A:364:MET:HB2	1.77	0.66
1:A:297:GLU:OE1	1:A:300:LEU:HB2	1.96	0.66
1:A:167:GLU:O	1:A:171:VAL:HG23	1.96	0.65
1:A:99:TRP:HD1	1:A:140:GLN:HG2	1.61	0.65
1:A:210:MET:HE3	2:A:800:GCS:H62	1.79	0.65
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.80	0.63
1:A:128:ARG:NH1	1:A:175:ILE:HD12	2.13	0.63
1:A:163:ARG:HD3	1:A:203:SER:O	1.99	0.62
1:A:255:ALA:HB1	1:A:260:LEU:HD21	1.82	0.62
1:A:127:LEU:HD21	1:A:135:LEU:HB2	1.82	0.62
1:A:217:PRO:HG2	1:A:288:THR:HG22	1.81	0.62
1:A:141:TYR:N	1:A:141:TYR:CD1	2.66	0.62
1:A:30:SER:N	1:A:57:ALA:HB2	2.15	0.61
1:A:28:TYR:CE1	1:A:43:PRO:HG3	2.36	0.61
1:A:353:ASN:O	1:A:354:LEU:O	2.19	0.60
1:A:349:LEU:HD21	1:A:356:GLY:HA2	1.83	0.60
1:A:301:LEU:HD22	1:A:305:GLU:HB3	1.84	0.60
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.84	0.60
1:A:270:THR:HG22	1:A:334:VAL:HG22	1.84	0.59
1:A:352:ASN:C	1:A:354:LEU:H	2.11	0.59
1:A:58:PHE:HZ	2:A:800:GCS:C2	2.16	0.58
1:A:349:LEU:O	1:A:353:ASN:HB2	2.02	0.58
1:A:297:GLU:OE1	1:A:300:LEU:HB3	2.02	0.58
1:A:338:ASN:ND2	1:A:341:SER:H	2.01	0.58
1:A:138:ASP:CG	2:A:800:GCS:N2	2.61	0.57
1:A:57:ALA:O	1:A:58:PHE:CD2	2.58	0.57
1:A:231:SER:HB2	1:A:322:GLN:CD	2.31	0.56
1:A:264:PHE:CE1	1:A:383:LEU:HD21	2.41	0.55
1:A:138:ASP:OD2	2:A:800:GCS:N2	2.39	0.55
1:A:325:PRO:HG3	1:A:338:ASN:CG	2.32	0.55
1:A:352:ASN:C	1:A:354:LEU:HD12	2.32	0.55
1:A:22:TYR:HA	1:A:355:GLY:O	2.07	0.55
1:A:257:SER:HB3	1:A:352:ASN:O	2.07	0.55
1:A:23:GLN:N	1:A:355:GLY:O	2.37	0.54
1:A:341:SER:O	1:A:345:LYS:HD3	2.07	0.54
1:A:353:ASN:C	1:A:354:LEU:O	2.50	0.53
1:A:56:TYR:O	1:A:57:ALA:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HG	1:A:90:LEU:HD11	1.91	0.53
1:A:189:ASP:OD2	1:A:237:LYS:HE3	2.09	0.53
1:A:99:TRP:CD1	1:A:140:GLN:HG2	2.42	0.52
1:A:212:TYR:OH	2:A:800:GCS:O4	1.71	0.52
1:A:297:GLU:HG2	1:A:298:SER:N	2.24	0.52
1:A:274:SER:HA	1:A:286:ILE:HD11	1.92	0.51
1:A:175:ILE:O	1:A:176:PRO:C	2.52	0.51
1:A:42:LYS:HG2	1:A:45:ASN:HD21	1.76	0.51
1:A:314:ALA:HA	1:A:329:GLN:HG2	1.91	0.51
1:A:216:ASP:OD1	1:A:218:LYS:HB2	2.11	0.50
1:A:285:THR:HG23	1:A:286:ILE:N	2.25	0.50
1:A:291:PRO:CB	1:A:297:GLU:O	2.59	0.50
1:A:78:GLU:HA	3:A:2048:HOH:O	2.11	0.50
1:A:231:SER:C	1:A:233:TYR:H	2.20	0.50
1:A:169:GLU:CG	1:A:173:LYS:HE3	2.42	0.49
1:A:160:LYS:HD3	3:A:2117:HOH:O	2.12	0.49
1:A:351:ASP:C	1:A:353:ASN:N	2.69	0.49
1:A:231:SER:HB2	1:A:322:GLN:NE2	2.27	0.49
1:A:297:GLU:OE1	1:A:300:LEU:CD1	2.60	0.49
1:A:365:ASP:OD1	1:A:378:PRO:HD2	2.13	0.49
1:A:214:LEU:HD12	1:A:227:PRO:HD2	1.95	0.48
1:A:272:ILE:HD13	1:A:331:ASN:O	2.13	0.48
1:A:141:TYR:CE1	1:A:210:MET:HE1	2.48	0.48
1:A:352:ASN:C	1:A:354:LEU:N	2.72	0.48
1:A:139:TRP:C	1:A:139:TRP:CD1	2.92	0.48
1:A:291:PRO:HG3	1:A:297:GLU:O	2.14	0.48
1:A:38:GLU:HG2	1:A:294:TYR:CE1	2.50	0.47
1:A:148:PRO:HD2	1:A:151:ASP:OD2	2.15	0.47
1:A:26:CYS:HB3	1:A:362:LEU:HG	1.97	0.47
1:A:83:LEU:C	1:A:85:ASP:H	2.21	0.47
1:A:212:TYR:CE1	2:A:800:GCS:H61	2.50	0.47
1:A:242:ASN:HD21	1:A:245:SER:H	1.59	0.47
1:A:28:TYR:OH	1:A:43:PRO:HD3	2.16	0.46
1:A:123:VAL:O	1:A:127:LEU:HB2	2.15	0.46
1:A:377:PHE:O	1:A:381:SER:HB2	2.16	0.46
1:A:187:ILE:O	1:A:191:ILE:HG13	2.16	0.45
1:A:29:THR:HG22	1:A:32:ALA:HB2	1.97	0.45
1:A:42:LYS:HG2	1:A:45:ASN:ND2	2.31	0.45
1:A:98:GLY:CA	2:A:800:GCS:O1	2.51	0.45
1:A:95:ALA:HA	1:A:136:ASN:O	2.16	0.45
1:A:99:TRP:CD1	1:A:140:GLN:HE21	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:HA	1:A:91:LYS:O	2.17	0.45
1:A:56:TYR:HB3	1:A:94:LEU:HD12	1.98	0.45
1:A:29:THR:HG23	1:A:31:TRP:CD2	2.52	0.44
1:A:261:ILE:HD13	1:A:356:GLY:N	2.32	0.44
1:A:304:TYR:HB2	1:A:371:PHE:CD1	2.52	0.44
1:A:167:GLU:OE1	1:A:177:ARG:HD3	2.17	0.44
1:A:151:ASP:HA	1:A:154:LEU:HB2	1.98	0.44
1:A:58:PHE:CZ	2:A:800:GCS:H2	2.41	0.44
1:A:360:TRP:CE2	2:A:800:GCS:O3	2.70	0.44
1:A:137:LEU:HD11	1:A:162:MET:HE1	2.00	0.44
1:A:360:TRP:CE2	2:A:800:GCS:H4	2.53	0.43
1:A:291:PRO:HB3	1:A:297:GLU:O	2.18	0.43
1:A:295:THR:O	1:A:296:ASP:C	2.61	0.43
1:A:173:LYS:O	1:A:174:ASP:HB3	2.18	0.43
1:A:42:LYS:H	1:A:45:ASN:ND2	2.17	0.43
1:A:365:ASP:O	1:A:367:PHE:N	2.51	0.43
1:A:109:MET:HB3	1:A:109:MET:HE3	1.73	0.43
1:A:343:LYS:HE3	1:A:386:ASP:OD2	2.19	0.43
1:A:30:SER:O	1:A:33:LYS:NZ	2.52	0.42
1:A:66:ILE:HG21	1:A:123:VAL:HA	2.01	0.42
1:A:27:TYR:O	1:A:362:LEU:HB2	2.18	0.42
1:A:22:TYR:CA	1:A:355:GLY:O	2.66	0.42
1:A:191:ILE:HD13	1:A:250:TRP:NE1	2.34	0.42
1:A:212:TYR:HE1	2:A:800:GCS:C6	2.33	0.42
1:A:297:GLU:CG	1:A:298:SER:N	2.82	0.42
1:A:135:LEU:HG	1:A:136:ASN:N	2.34	0.42
1:A:93:LEU:HD23	1:A:134:GLY:HA3	2.02	0.42
1:A:293:LYS:HD2	1:A:293:LYS:C	2.45	0.42
1:A:376:HIS:ND1	1:A:376:HIS:N	2.67	0.42
1:A:217:PRO:HB2	1:A:288:THR:HG22	2.02	0.41
1:A:141:TYR:HE1	1:A:210:MET:HE1	1.84	0.41
1:A:212:TYR:HE1	2:A:800:GCS:O6	2.04	0.41
1:A:238:SER:HA	1:A:241:LEU:HD12	2.01	0.41
1:A:30:SER:H	1:A:57:ALA:HB2	1.84	0.41
1:A:83:LEU:C	1:A:85:ASP:N	2.79	0.41
1:A:163:ARG:NH1	1:A:203:SER:O	2.45	0.41
1:A:258:GLU:CD	1:A:258:GLU:H	2.28	0.41
1:A:258:GLU:HA	1:A:354:LEU:HB2	2.03	0.41
1:A:291:PRO:HA	1:A:297:GLU:O	2.21	0.41
1:A:210:MET:CG	2:A:800:GCS:C6	2.87	0.41
1:A:231:SER:C	1:A:233:TYR:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TRP:HA	1:A:361:PRO:HA	1.91	0.41
1:A:217:PRO:CG	1:A:288:THR:HG22	2.48	0.40
1:A:81:ASN:HB2	3:A:2048:HOH:O	2.20	0.40
1:A:99:TRP:HD1	1:A:140:GLN:HE21	1.67	0.40
1:A:325:PRO:HD3	1:A:341:SER:HB3	2.02	0.40
1:A:24:LEU:HD12	1:A:389:ILE:HG13	2.03	0.40
1:A:338:ASN:C	1:A:338:ASN:HD22	2.29	0.40
1:A:35:ARG:O	1:A:36:PRO:C	2.65	0.40
1:A:261:ILE:HD13	1:A:356:GLY:H	1.87	0.40
1:A:38:GLU:HG2	1:A:294:TYR:HE1	1.85	0.40
1:A:50:LEU:HD21	1:A:380:THR:HG21	2.03	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	370/377 (98%)	333 (90%)	30 (8%)	7 (2%)	6 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ALA
1	A	354	LEU
1	A	296	ASP
1	A	37	ILE
1	A	141	TYR
1	A	217	PRO
1	A	188	ILE

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	318/324 (98%)	250 (79%)	68 (21%)	1 2

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	29	THR
1	A	37	ILE
1	A	40	SER
1	A	75	ARG
1	A	89	GLU
1	A	96	ILE
1	A	99	TRP
1	A	100	LYS
1	A	117	GLN
1	A	127	LEU
1	A	128	ARG
1	A	129	GLN
1	A	131	ASN
1	A	137	LEU
1	A	138	ASP
1	A	140	GLN
1	A	144	SER
1	A	154	LEU
1	A	160	LYS
1	A	167	GLU
1	A	168	GLU
1	A	175	ILE
1	A	191	ILE
1	A	192	LYS
1	A	193	SER
1	A	196	LYS
1	A	208	GLN
1	A	216	ASP
1	A	218	LYS

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Mol	Chain	Res	Type
1	A	235	ILE
1	A	237	LYS
1	A	238	SER
1	A	251	LYS
1	A	258	GLU
1	A	273	LEU
1	A	274	SER
1	A	277	SER
1	A	278	LYS
1	A	285	THR
1	A	293	LYS
1	A	296	ASP
1	A	297	GLU
1	A	298	SER
1	A	310	LEU
1	A	311	ASN
1	A	312	GLU
1	A	316	GLU
1	A	317	VAL
1	A	323	GLU
1	A	329	GLN
1	A	332	GLU
1	A	337	ASP
1	A	338	ASN
1	A	343	LYS
1	A	344	LEU
1	A	345	LYS
1	A	349	LEU
1	A	350	LYS
1	A	351	ASP
1	A	352	ASN
1	A	362	LEU
1	A	374	GLN
1	A	375	ARG
1	A	376	HIS
1	A	384	LYS
1	A	387	LEU
1	A	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	63	ASN
1	A	70	HIS
1	A	115	ASN
1	A	117	GLN
1	A	136	ASN
1	A	242	ASN
1	A	322	GLN
1	A	329	GLN
1	A	338	ASN
1	A	374	GLN
1	A	390	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	GCS	A	800	-	12,12,12	1.86	6 (50%)	16,17,17	2.44	6 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GCS	A	800	-	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	GCS	O3-C3	2.89	1.50	1.43
2	A	800	GCS	O4-C4	2.75	1.49	1.43
2	A	800	GCS	C3-C2	2.53	1.56	1.53
2	A	800	GCS	C1-C2	2.13	1.55	1.52
2	A	800	GCS	O5-C5	-2.07	1.39	1.44
2	A	800	GCS	C2-N2	2.02	1.50	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	GCS	O5-C1-C2	4.82	115.13	109.51
2	A	800	GCS	C4-C3-C2	4.77	118.91	110.99
2	A	800	GCS	O1-C1-O5	3.39	120.48	110.41
2	A	800	GCS	O4-C4-C3	-3.32	102.56	110.38
2	A	800	GCS	O6-C6-C5	-3.01	101.07	111.33
2	A	800	GCS	O5-C5-C4	-2.12	105.87	109.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	GCS	22	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.