



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:09 PM GMT

PDB ID : 1E9L  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

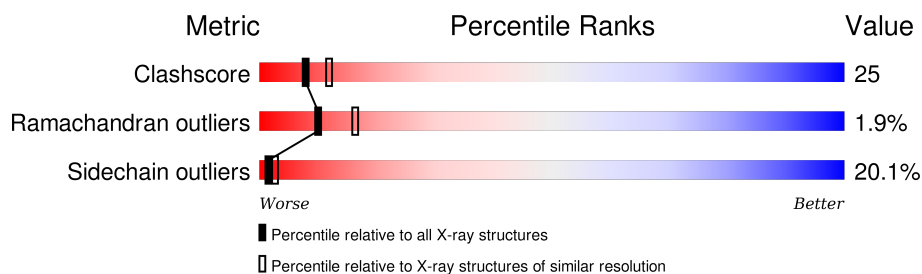
# 1 Overall quality at a glance ⓘ

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div></div> <div>50%</div> <div>38%</div> <div>10%</div> <div>..</div> </div>

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](#)

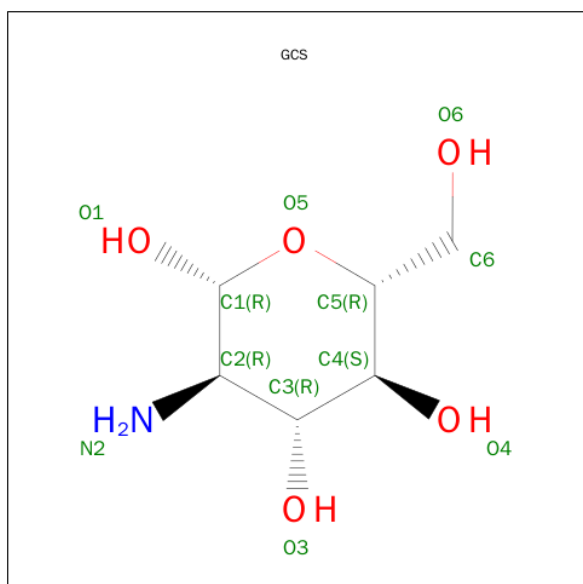
There are 3 unique types of molecules in this entry. The entry contains 4226 atoms, of which 1056 are hydrogens and 0 are deuteriums.

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
1	A	372	Total	C	H	N	O	S	0	0	0
			3572	1889	628	481	563	11			

- Molecule 2 is SUGAR (D-GLUCOSAMINE) (three-letter code: GCS) (formula:  $C_6H_{13}NO_5$ ).



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

- Molecule 3 is water.

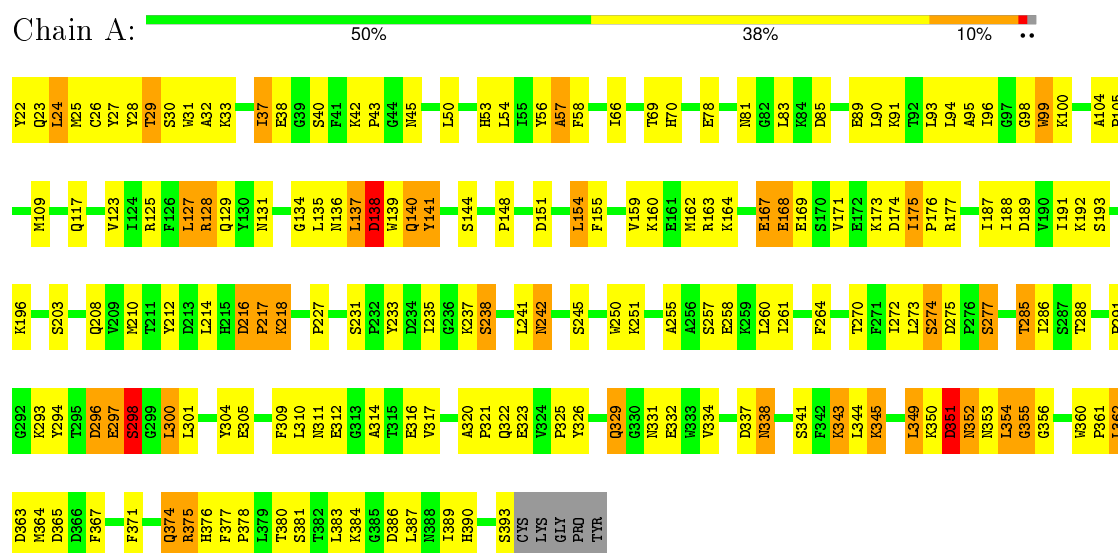
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	214	Total	H	O	0	0
			642	428	214		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: YM1 SECRETORY PROTEIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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	4226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

## 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: 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	0.45	1/3029 (0.0%)	0.68	4/4117 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ASP	N-CA	-10.05	1.26	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	GLY	N-CA-C	-8.84	91.00	113.10
1	A	351	ASP	N-CA-C	-5.78	95.39	111.00
1	A	300	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	298	SER	N-CA-C	-5.12	97.17	111.00

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	A	2944	628	2825	141	0
2	A	12	0	12	18	0
3	A	214	428	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3170	1056	2837	141	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 25.

All (141) 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: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	0.79
1:A:360:TRP:CZ2	2:A:800:GCS:O3	2.33	0.79
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:164:LYS:O	1:A:168:GLU:HG2	1.87	0.72
1:A:242:ASN:ND2	1:A:245:SER:H	1.87	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
1:A:297:GLU:CD	1:A:300:LEU:HB3	2.14	0.68
1:A:374:GLN:C	1:A:375:ARG:HG3	2.15	0.67
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: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: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:360:TRP:CE3	2:A:800:GCS:O3	2.49	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:57:ALA:O	1:A:58:PHE:CD2	2.58	0.57
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:22:TYR:HA	1:A:355:GLY:O	2.07	0.55
1:A:352:ASN:C	1:A:354:LEU:H	2.11	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: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:138:ASP:CG	2:A:800:GCS:N2	2.61	0.52
1:A:99:TRP:CD1	1:A:140:GLN:HG2	2.42	0.52
1:A:297:GLU:HG2	1:A:298:SER:N	2.24	0.52
1:A:137:LEU:HD11	1:A:162:MET:HE1	1.91	0.52
1:A:274:SER:HA	1:A:286:ILE:HD11	1.92	0.51
1:A:285:THR:HG23	1:A:286:ILE:N	2.25	0.51
1:A:231:SER:HB2	1:A:322:GLN:CD	2.31	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:291:PRO:CB	1:A:297:GLU:O	2.59	0.50
1:A:325:PRO:HG3	1:A:338:ASN:CG	2.32	0.50
1:A:78:GLU:HA	3:A:2048:HOH:O	2.11	0.50
1:A:352:ASN:C	1:A:354:LEU:HD12	2.32	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: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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:C	1:A:354:LEU:O	2.50	0.48
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:56:TYR:O	1:A:57:ALA:C	2.51	0.48
1:A:291:PRO:HG3	1:A:297:GLU:O	2.14	0.48
1:A:148:PRO:HD2	1:A:151:ASP:OD2	2.15	0.47
1:A:38:GLU:HG2	1:A:294:TYR:CE1	2.50	0.47
1:A:26:CYS:HB3	1:A:362:LEU:HG	1.97	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:175:ILE:O	1:A:176:PRO:C	2.52	0.46
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:231:SER:C	1:A:233:TYR:H	2.20	0.45
1:A:95:ALA:HA	1:A:136:ASN:O	2.16	0.45
1:A:56:TYR:HB3	1:A:94:LEU:HD12	1.98	0.45
1:A:53:HIS:HA	1:A:91:LYS:O	2.17	0.45
1:A:351:ASP:C	1:A:353:ASN:N	2.69	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:H4	2.53	0.43
1:A:291:PRO:HB3	1:A:297:GLU:O	2.18	0.43
1:A:352:ASN:C	1:A:354:LEU:N	2.72	0.43
1:A:139:TRP:C	1:A:139:TRP:CD1	2.92	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: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:212:TYR:HE1	2:A:800:GCS:C6	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CA	1:A:355:GLY:O	2.66	0.42
1:A:297:GLU:CG	1:A:298:SER:N	2.82	0.42
1:A:191:ILE:HD13	1:A:250:TRP:NE1	2.34	0.42
1:A:83:LEU:C	1:A:85:ASP:H	2.21	0.42
1:A:135:LEU:HG	1:A:136:ASN:N	2.34	0.42
1:A:210:MET:CE	2:A:800:GCS:H62	2.50	0.42
1:A:376:HIS:ND1	1:A:376:HIS:N	2.67	0.42
1:A:93:LEU:HD23	1:A:134:GLY:HA3	2.02	0.42
1:A:217:PRO:HB2	1:A:288:THR:HG22	2.02	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:291:PRO:HA	1:A:297:GLU:O	2.21	0.41
1:A:163:ARG:NH1	1:A:203:SER:O	2.45	0.41
1:A:258:GLU:HA	1:A:354:LEU:HB2	2.03	0.41
1:A:360:TRP:HA	1:A:361:PRO:HA	1.91	0.41
1:A:210:MET:CG	2:A:800:GCS:C6	2.87	0.41
1:A:217:PRO:CG	1:A:288:THR:HG22	2.48	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:81:ASN:HB2	3:A:2048:HOH:O	2.20	0.40
1:A:109:MET:HE3	1:A:109:MET:HB3	1.99	0.40
1:A:24:LEU:HD12	1:A:389:ILE:HG13	2.03	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%)	10	16

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%)	254 (80%)	64 (20%)	1	3

All (64) 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	89	GLU
1	A	96	ILE
1	A	99	TRP
1	A	100	LYS
1	A	117	GLN
1	A	125	ARG
1	A	127	LEU
1	A	128	ARG
1	A	129	GLN
1	A	131	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	137	LEU
1	A	138	ASP
1	A	140	GLN
1	A	144	SER
1	A	154	LEU
1	A	167	GLU
1	A	168	GLU
1	A	175	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
1	A	235	ILE
1	A	238	SER
1	A	242	ASN
1	A	251	LYS
1	A	273	LEU
1	A	274	SER
1	A	277	SER
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	326	TYR
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	351	ASP
1	A	352	ASN
1	A	362	LEU
1	A	374	GLN
1	A	375	ARG
1	A	384	LYS
1	A	387	LEU
1	A	393	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	70	HIS
1	A	115	ASN
1	A	117	GLN
1	A	242	ASN
1	A	338	ASN
1	A	352	ASN
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 carbohydrates 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	1	12,12,12	1.87	5 (41%)	15,17,17	2.32	6 (40%)

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	1	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	GCS	O5-C5	-2.00	1.39	1.44
2	A	800	GCS	C1-C2	2.07	1.55	1.53
2	A	800	GCS	C3-C2	2.53	1.56	1.53
2	A	800	GCS	O4-C4	2.84	1.49	1.43
2	A	800	GCS	O3-C3	2.98	1.50	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	GCS	O4-C4-C3	-3.46	102.56	110.34
2	A	800	GCS	O6-C6-C5	-3.11	101.07	111.33
2	A	800	GCS	C1-C2-N2	-2.99	105.22	111.10
2	A	800	GCS	O5-C5-C4	-2.03	105.87	109.68
2	A	800	GCS	O1-C1-O5	3.74	120.48	110.25
2	A	800	GCS	O5-C1-C2	4.68	115.13	109.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	GCS	18	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.