



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:52 AM GMT

PDB ID : 2OLH
Title : Crystal structure of a signalling protein (SPG-40) complex with cellobiose at 2.78 Å resolution
Authors : Sharma, P.; Singh, N.; Sharma, S.; Bhushan, A.; Kaur, P.; Singh, T.P.
Deposited on : 2007-01-19
Resolution : 2.78 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
<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

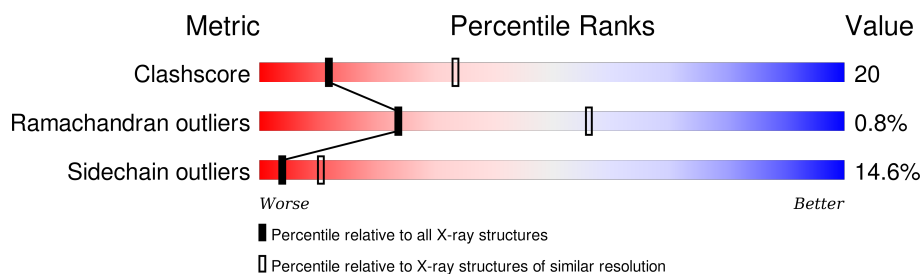
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)

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. 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	361	

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	CBI	A	840	X	-	-	-
3	NAG	A	842	X	-	-	-
3	MAN	A	843	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3067 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.

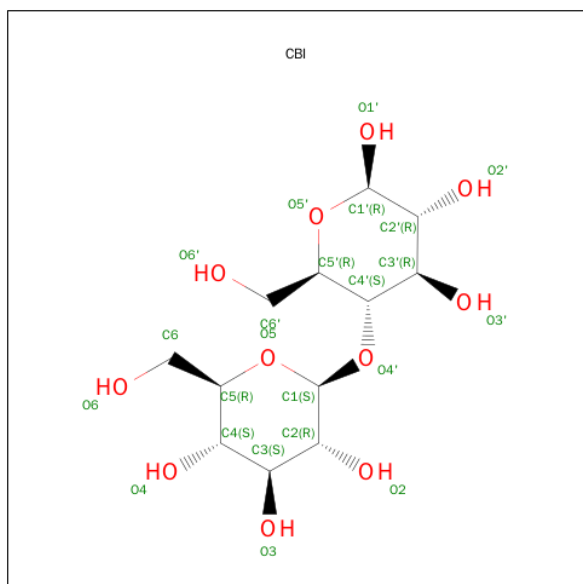
- Molecule 1 is a protein called Chitinase-3-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2876	1836	508	523	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	VAL	ILE	SEE REMARK 999	UNP Q8SPQ0
A	131	ALA	GLY	SEE REMARK 999	UNP Q8SPQ0
A	205	ASN	GLN	SEE REMARK 999	UNP Q8SPQ0
A	206	SER	GLU	SEE REMARK 999	UNP Q8SPQ0
A	?	-	ASP	SEE REMARK 999	UNP Q8SPQ0
A	361	ARG	GLU	SEE REMARK 999	UNP Q8SPQ0

- Molecule 2 is SUGAR (CELLOBIOSE) (three-letter code: CBI) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is water.

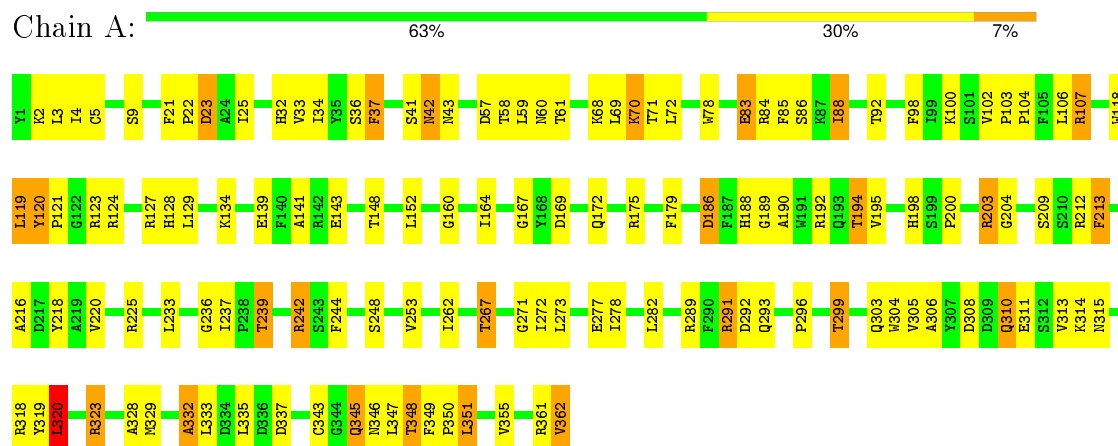
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		

3 Residue-property plots

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: Chitinase-3-like protein 1



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.69 Å 66.45 Å 107.53 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.78	Depositor
% Data completeness (in resolution range)	97.9 (19.94-2.78)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.191 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3067	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: CBI, NAG, MAN

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	0/2952	0.83	8/4001 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	2	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	119	LEU	CA-CB-CG	-6.35	100.70	115.30
1	A	320	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	212	ARG	N-CA-C	5.64	126.22	111.00
1	A	188	HIS	N-CA-C	-5.53	96.06	111.00
1	A	37	PHE	N-CA-C	5.46	125.73	111.00
1	A	36	SER	N-CA-C	5.28	125.25	111.00
1	A	167	GLY	N-CA-C	5.16	126.00	113.10
1	A	343	CYS	N-CA-C	5.12	124.82	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	842	NAG	C1
3	A	843	MAN	C1

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	2876	0	2817	114	0
2	A	23	0	21	5	0
3	A	39	0	34	3	0
4	A	129	0	0	27	0
All	All	3067	0	2872	117	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 20.

All (117) 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:78:TRP:HB2	2:A:840:CBI:H61	1.44	1.00
1:A:242:ARG:HH22	2:A:840:CBI:H2'	1.26	0.97
1:A:78:TRP:HB2	2:A:840:CBI:C6	1.97	0.94
1:A:141:ALA:HB2	4:A:946:HOH:O	1.70	0.90
1:A:203:ARG:HB2	4:A:885:HOH:O	1.79	0.82
3:A:841:NAG:H62	3:A:842:NAG:O7	1.78	0.82
1:A:25:ILE:HD12	1:A:333:LEU:HD13	1.61	0.81
1:A:134:LYS:HE2	4:A:961:HOH:O	1.84	0.77
1:A:192:ARG:HD3	1:A:194:THR:HG22	1.66	0.76
1:A:57:ASP:O	1:A:61:THR:HG23	1.87	0.73
1:A:242:ARG:NH2	2:A:840:CBI:H2'	2.02	0.71
1:A:200:PRO:HB3	1:A:293:GLN:HB3	1.71	0.71
1:A:213:PHE:HB3	1:A:218:TYR:CD2	2.26	0.70
1:A:348:THR:HG23	1:A:349:PHE:HD2	1.57	0.70
1:A:278:ILE:CD1	1:A:305:VAL:HG11	2.21	0.69
1:A:134:LYS:HE3	4:A:866:HOH:O	1.93	0.68
1:A:348:THR:HG23	1:A:349:PHE:CD2	2.29	0.67
1:A:103:PRO:HB2	1:A:104:PRO:HD3	1.76	0.66
1:A:239:THR:HG22	1:A:335:LEU:HB2	1.77	0.66
1:A:278:ILE:HD12	1:A:305:VAL:HG11	1.78	0.65
1:A:267:THR:HB	1:A:277:GLU:OE1	1.96	0.64
1:A:124:ARG:HG2	4:A:941:HOH:O	1.98	0.64
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:O	1:A:164:ILE:HG13	1.98	0.62
1:A:84:ARG:HD2	4:A:958:HOH:O	2.00	0.61
3:A:843:MAN:H62	4:A:863:HOH:O	2.00	0.61
1:A:332:ALA:HB3	1:A:335:LEU:HD12	1.83	0.60
1:A:169:ASP:OD2	1:A:172:GLN:HG3	2.02	0.60
1:A:291:ARG:CZ	1:A:291:ARG:HB2	2.31	0.60
1:A:345:GLN:HB3	4:A:953:HOH:O	2.04	0.58
1:A:323:ARG:NH1	1:A:323:ARG:HG2	2.18	0.58
1:A:332:ALA:CB	1:A:335:LEU:HD12	2.33	0.57
1:A:124:ARG:HD2	4:A:887:HOH:O	2.05	0.56
1:A:107:ARG:HD3	1:A:143:GLU:OE2	2.06	0.56
1:A:107:ARG:NH1	1:A:148:THR:HG21	2.21	0.56
1:A:278:ILE:HD11	1:A:305:VAL:HG11	1.89	0.55
1:A:107:ARG:NH1	1:A:148:THR:CG2	2.70	0.54
1:A:83:GLU:HB3	4:A:855:HOH:O	2.06	0.54
1:A:123:ARG:CD	4:A:922:HOH:O	2.56	0.54
1:A:34:ILE:HG12	1:A:72:LEU:HB2	1.91	0.53
1:A:271:GLY:C	1:A:272:ILE:HD12	2.29	0.53
1:A:361:ARG:HG3	1:A:361:ARG:O	2.09	0.53
1:A:127:ARG:HB3	4:A:960:HOH:O	2.07	0.53
1:A:361:ARG:O	1:A:362:VAL:HG12	2.11	0.51
1:A:216:ALA:O	1:A:220:VAL:HG23	2.11	0.51
1:A:332:ALA:HB1	1:A:335:LEU:HG	1.92	0.51
1:A:361:ARG:O	1:A:362:VAL:CB	2.59	0.51
1:A:70:LYS:HE3	4:A:950:HOH:O	2.11	0.50
1:A:37:PHE:HB2	4:A:857:HOH:O	2.12	0.50
1:A:239:THR:O	1:A:239:THR:CG2	2.60	0.50
1:A:78:TRP:CE3	1:A:119:LEU:HD13	2.46	0.50
1:A:318:ARG:HE	1:A:361:ARG:HH12	1.60	0.50
1:A:204:GLY:HA2	1:A:292:ASP:HB3	1.93	0.50
1:A:271:GLY:O	1:A:272:ILE:HD12	2.12	0.50
1:A:4:ILE:HD13	1:A:179:PHE:CE2	2.47	0.50
1:A:5:CYS:HB3	1:A:333:LEU:HG	1.94	0.49
1:A:32:HIS:HA	1:A:70:LYS:O	2.12	0.49
1:A:152:LEU:HD23	4:A:884:HOH:O	2.12	0.49
1:A:186:ASP:CG	1:A:186:ASP:O	2.50	0.49
1:A:273:LEU:HD12	1:A:278:ILE:CD1	2.42	0.49
1:A:78:TRP:HB2	2:A:840:CBI:H62	1.91	0.49
1:A:127:ARG:NH1	4:A:878:HOH:O	2.46	0.49
1:A:262:ILE:H	1:A:303:GLN:HE22	1.61	0.49
1:A:361:ARG:O	1:A:362:VAL:HB	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HG2	4:A:867:HOH:O	2.13	0.48
1:A:239:THR:HG22	1:A:335:LEU:CB	2.43	0.48
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.95	0.48
1:A:304:TRP:CZ3	1:A:306:ALA:HB2	2.49	0.48
1:A:289:ARG:HD3	4:A:964:HOH:O	2.14	0.48
1:A:319:TYR:CZ	1:A:323:ARG:HD2	2.49	0.47
1:A:192:ARG:HD3	1:A:194:THR:CG2	2.39	0.47
1:A:313:VAL:HG13	1:A:355:VAL:HG22	1.95	0.47
1:A:320:LEU:CD1	1:A:328:ALA:HB2	2.45	0.47
1:A:213:PHE:HB3	1:A:218:TYR:CE2	2.49	0.47
1:A:237:ILE:CG2	1:A:313:VAL:HG22	2.44	0.47
1:A:128:HIS:HE1	4:A:912:HOH:O	1.98	0.46
1:A:253:VAL:HG13	4:A:853:HOH:O	2.14	0.46
1:A:323:ARG:CG	1:A:323:ARG:HH11	2.28	0.46
1:A:123:ARG:HD2	4:A:913:HOH:O	2.14	0.46
1:A:320:LEU:HD11	1:A:328:ALA:HB2	1.98	0.46
1:A:123:ARG:HD3	4:A:922:HOH:O	2.15	0.45
1:A:41:SER:O	1:A:42:ASN:HB2	2.16	0.45
1:A:123:ARG:HD2	4:A:922:HOH:O	2.15	0.45
1:A:120:TYR:N	1:A:120:TYR:CD2	2.78	0.45
1:A:43:ASN:OD1	1:A:88:ILE:HD11	2.16	0.45
1:A:239:THR:O	1:A:239:THR:HG23	2.17	0.45
1:A:273:LEU:HD12	1:A:278:ILE:HD13	1.97	0.45
1:A:310:GLN:O	1:A:314:LYS:CG	2.64	0.45
1:A:60:ASN:ND2	1:A:71:THR:OG1	2.49	0.45
1:A:107:ARG:NH1	1:A:143:GLU:OE1	2.51	0.44
1:A:345:GLN:HB2	1:A:345:GLN:HE21	1.61	0.44
1:A:237:ILE:HG21	1:A:313:VAL:HG22	2.00	0.44
1:A:313:VAL:HG13	1:A:355:VAL:CG2	2.48	0.43
1:A:78:TRP:HZ2	4:A:959:HOH:O	2.01	0.43
1:A:244:PHE:HD2	1:A:304:TRP:CE3	2.37	0.43
1:A:22:PRO:HB2	1:A:58:THR:HG22	2.01	0.43
1:A:118:TRP:CE3	1:A:129:LEU:HD23	2.53	0.43
1:A:33:VAL:HG11	1:A:59:LEU:HD11	2.00	0.43
1:A:190:ALA:HA	4:A:858:HOH:O	2.17	0.42
1:A:198:HIS:CD2	1:A:198:HIS:H	2.37	0.42
1:A:299:THR:HA	1:A:303:GLN:O	2.19	0.42
1:A:310:GLN:O	1:A:314:LYS:HG3	2.19	0.42
1:A:21:PHE:C	1:A:23:ASP:N	2.73	0.42
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.47	0.42
1:A:139:GLU:OE1	1:A:139:GLU:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:TYR:HA	1:A:121:PRO:HD2	1.73	0.41
1:A:351:LEU:HA	1:A:351:LEU:HD12	1.81	0.41
1:A:128:HIS:CE1	4:A:912:HOH:O	2.73	0.41
1:A:43:ASN:O	1:A:98:PHE:HA	2.21	0.41
1:A:291:ARG:H	1:A:291:ARG:HG3	1.67	0.41
1:A:43:ASN:OD1	1:A:88:ILE:CD1	2.69	0.41
1:A:236:GLY:HA3	1:A:329:MET:CE	2.50	0.41
1:A:337:ASP:HB3	1:A:350:PRO:CD	2.51	0.40
3:A:841:NAG:C6	3:A:842:NAG:O7	2.61	0.40
1:A:107:ARG:NH1	1:A:148:THR:HG23	2.37	0.40
1:A:103:PRO:HB3	1:A:143:GLU:HG3	2.04	0.40
1:A:291:ARG:HB3	4:A:918:HOH:O	2.21	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	359/361 (99%)	326 (91%)	30 (8%)	3 (1%)	24	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLY
1	A	332	ALA
1	A	120	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	302/302 (100%)	258 (85%)	44 (15%)	4 10

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	SER
1	A	23	ASP
1	A	42	ASN
1	A	68	LYS
1	A	69	LEU
1	A	70	LYS
1	A	83	GLU
1	A	85	PHE
1	A	86	SER
1	A	88	ILE
1	A	92	THR
1	A	100	LYS
1	A	106	LEU
1	A	107	ARG
1	A	175	ARG
1	A	186	ASP
1	A	194	THR
1	A	195	VAL
1	A	203	ARG
1	A	209	SER
1	A	213	PHE
1	A	225	ARG
1	A	233	LEU
1	A	239	THR
1	A	242	ARG
1	A	248	SER
1	A	267	THR
1	A	282	LEU
1	A	291	ARG
1	A	296	PRO
1	A	299	THR
1	A	308	ASP
1	A	310	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	311	GLU
1	A	315	ASN
1	A	320	LEU
1	A	323	ARG
1	A	345	GLN
1	A	346	ASN
1	A	347	LEU
1	A	348	THR
1	A	351	LEU
1	A	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	303	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

3 carbohydrates are 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	NAG	A	841	1,3	14,14,15	0.83	0	15,19,21	1.35	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	842	3	14,14,15	1.41	2 (14%)	15,19,21	1.26	2 (13%)
3	MAN	A	843	3	11,11,12	1.00	0	14,15,17	1.68	2 (14%)

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	NAG	A	841	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	842	3	1/1/5/7	0/6/23/26	0/1/1/1
3	MAN	A	843	3	1/1/4/5	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	842	NAG	C8-C7	2.34	1.55	1.50
3	A	842	NAG	C1-C2	3.59	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	842	NAG	C4-C3-C2	2.58	115.24	111.23
3	A	843	MAN	C1-O5-C5	2.83	115.84	112.25
3	A	842	NAG	C2-N2-C7	2.91	126.78	123.04
3	A	841	NAG	C4-C3-C2	3.53	116.72	111.23
3	A	843	MAN	C1-C2-C3	5.33	115.84	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	843	MAN	C1
3	A	842	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	841	NAG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	842	NAG	2	0
3	A	843	MAN	1	0

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	$\# Z > 2$
2	CBI	A	840	-	24,24,24	2.40	10 (41%)	35,35,35	2.67	9 (25%)

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	CBI	A	840	-	1/1/10/10	0/8/48/48	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	840	CBI	C6-C5	2.05	1.59	1.51
2	A	840	CBI	C3'-C4'	2.10	1.58	1.52
2	A	840	CBI	C3'-C2'	2.18	1.58	1.52
2	A	840	CBI	O4'-C4'	2.38	1.49	1.43
2	A	840	CBI	O2-C2	2.68	1.49	1.43
2	A	840	CBI	C1'-C2'	3.18	1.59	1.52
2	A	840	CBI	O5'-C1'	3.20	1.49	1.43
2	A	840	CBI	C4'-C5'	3.68	1.63	1.52
2	A	840	CBI	O5-C5	4.72	1.56	1.44
2	A	840	CBI	O5-C1	5.65	1.56	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	840	CBI	O4'-C4'-C3'	-5.06	94.12	107.17
2	A	840	CBI	O5-C1-C2	-3.14	103.84	110.28
2	A	840	CBI	C1'-C2'-C3'	-2.68	106.44	110.43
2	A	840	CBI	C2'-C3'-C4'	2.11	114.23	109.60
2	A	840	CBI	O2'-C2'-C3'	2.13	115.13	110.34
2	A	840	CBI	C1-C2-C3	2.20	114.31	109.97
2	A	840	CBI	C6-C5-C4	2.26	118.58	113.02
2	A	840	CBI	C1-O5-C5	2.34	118.29	113.75
2	A	840	CBI	O4'-C1-C2	12.22	137.85	108.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	840	CBI	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	840	CBI	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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