Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 08:59 am GMT

PDB ID	:	4C1Y
Title	:	Crystal Structure of Fucose binding lectin from Aspergillus Fumigatus (AFL) in complex with b-methylfucoside
Authors	:	Houser, J.; Komarek, J.; Kostlanova, N.; Lahmann, M.; Cioci, G.; Varrot, A.; Imberty, A.; Wimmerova, M.
Deposited on	:	2013-08-14
Resolution	:	2.23 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:

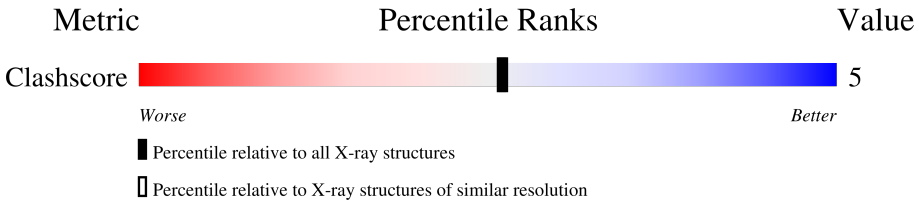
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.23 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	141614	2539 (2.26-2.22)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	314	85% 15%
2	B	314	87% 13%
2	C	314	85% 15%
2	D	314	89% 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10093 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 FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2439	1554	421	460	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	LEU	variant	UNP Q4WW81
A	111	CYS	ARG	variant	UNP Q4WW81

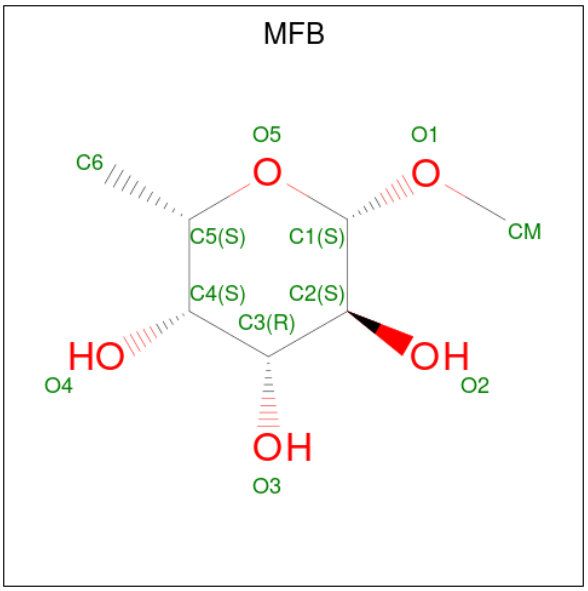
- Molecule 2 is a protein called FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2443	1557	422	460	4			
2	C	314	Total	C	N	O	S	0	0	0
			2434	1553	418	459	4			
2	D	314	Total	C	N	O	S	0	0	0
			2438	1556	419	459	4			

There are 6 discrepancies between the modelled and reference sequences:

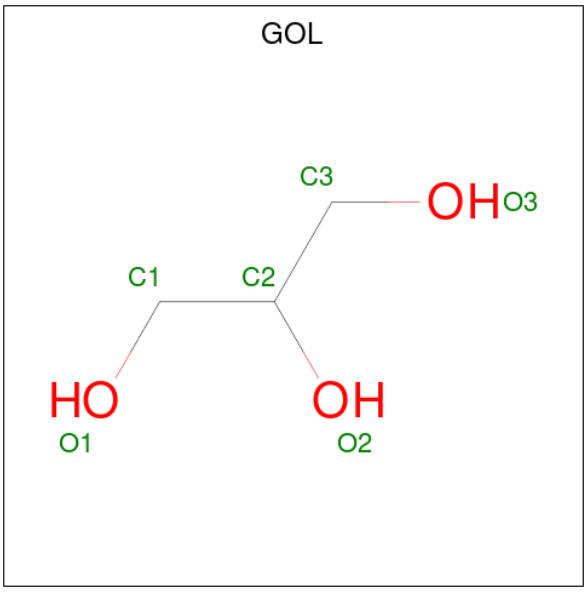
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	LEU	variant	UNP Q4WW81
B	111	CYS	ARG	variant	UNP Q4WW81
C	20	SER	LEU	variant	UNP Q4WW81
C	111	CYS	ARG	variant	UNP Q4WW81
D	20	SER	LEU	variant	UNP Q4WW81
D	111	CYS	ARG	variant	UNP Q4WW81

- Molecule 3 is methyl beta-L-fucopyranoside (three-letter code: MFB) (formula: $C_7H_{14}O_5$).



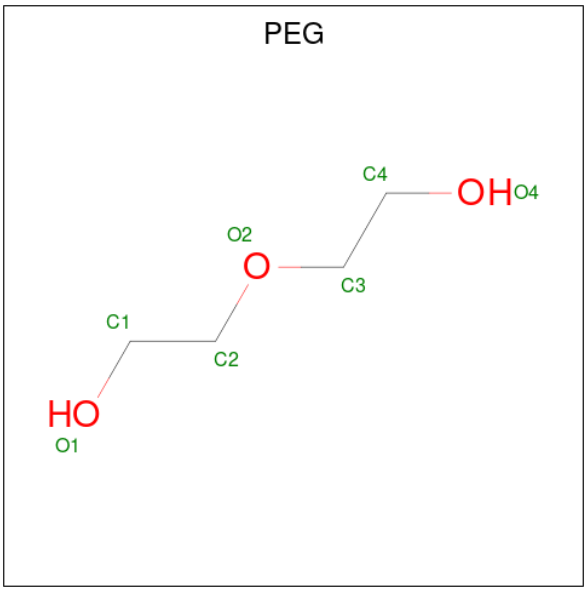
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 7 5	0	0
3	A	1	Total C O 12 7 5	0	0
3	A	1	Total C O 12 7 5	0	0
3	B	1	Total C O 12 7 5	0	0
3	B	1	Total C O 12 7 5	0	0
3	B	1	Total C O 12 7 5	0	0
3	C	1	Total C O 12 7 5	0	0
3	C	1	Total C O 12 7 5	0	0
3	C	1	Total C O 12 7 5	0	0
3	C	1	Total C O 12 7 5	0	0
3	D	1	Total C O 12 7 5	0	0
3	D	1	Total C O 12 7 5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	53	Total O 53 53	0	0
7	B	46	Total O 46 46	0	0
7	C	19	Total O 19 19	0	0
7	D	18	Total O 18 18	0	0

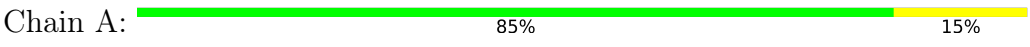
3 Residue-property plots (i)

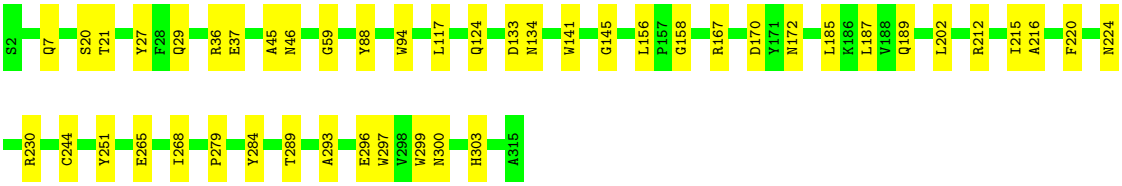
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 failed to run properly.

• Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

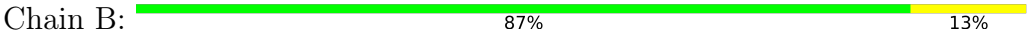
Chain A:

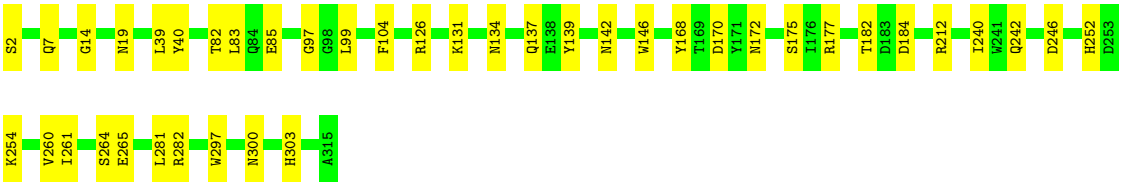




• Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA

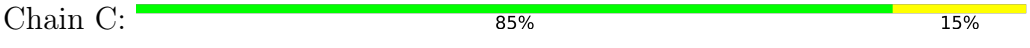
Chain B:

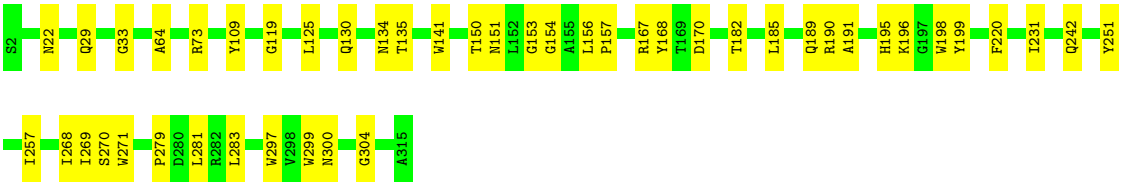




• Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA

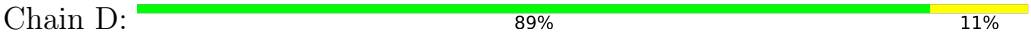
Chain C:





• Molecule 2: FUCOSE-SPECIFIC LECTIN FLEA

Chain D:




I269
R282
Q286
S292
A315

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 90.33Å 189.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.23	Depositor
% Data completeness (in resolution range)	99.0 (48.14-2.23)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.243 , 0.313	Depositor
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.139	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10093	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, MFB, GOL, PEG, CSX

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	0.70	0/2502	0.82	1/3412 (0.0%)
2	B	0.68	0/2514	0.80	1/3427 (0.0%)
2	C	0.57	0/2505	0.73	0/3418
2	D	0.55	0/2509	0.71	0/3422
All	All	0.63	0/10030	0.77	2/13679 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	ARG	NE-CZ-NH2	-7.15	116.73	120.30
2	B	39	LEU	CA-CB-CG	5.89	128.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	19	ASN	Peptide

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	2439	0	2317	27	0
2	B	2443	0	2329	26	0
2	C	2434	0	2311	33	0
2	D	2438	0	2322	23	0
3	A	36	0	42	0	0
3	B	36	0	42	1	0
3	C	48	0	56	0	0
3	D	24	0	28	0	0
4	A	30	0	40	3	0
4	B	18	0	24	2	0
4	D	6	0	8	2	0
5	A	4	0	5	0	0
6	A	1	0	0	0	0
7	A	53	0	0	0	0
7	B	46	0	0	0	0
7	C	19	0	0	0	0
7	D	18	0	0	0	0
All	All	10093	0	9524	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (107) 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:212:ARG:O	4:A:991:GOL:H2	1.75	0.84
2:B:212:ARG:O	4:B:990:GOL:O2	1.97	0.81
2:D:246:ASP:OD2	2:D:252:HIS:HE1	1.67	0.77
2:C:109:TYR:OH	2:C:134:ASN:OD1	2.06	0.71
2:B:300:ASN:ND2	2:B:303:HIS:H	1.93	0.66
2:D:146:TRP:HE1	4:D:920:GOL:HO3	1.44	0.66
2:D:195:HIS:CD2	2:D:196:LYS:HG3	2.35	0.62
2:B:246:ASP:OD2	2:B:252:HIS:HE1	1.83	0.61
2:B:182:THR:OG1	2:B:184:ASP:OD1	2.14	0.60
2:B:300:ASN:HD22	2:B:300:ASN:C	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH2	1:A:172:ASN:HA	2.18	0.59
2:C:242:GLN:CB	2:C:257:ILE:HD11	2.34	0.57
2:B:40:TYR:CE2	3:B:960:MFB:H62	2.40	0.56
1:A:189:GLN:NE2	1:A:251:TYR:OH	2.38	0.56
2:C:125:LEU:HB2	2:C:141:TRP:HB3	1.88	0.56
2:B:175:SER:HB3	2:B:177:ARG:HH12	1.71	0.56
2:B:212:ARG:O	4:B:990:GOL:C2	2.54	0.56
1:A:300:ASN:ND2	1:A:303:HIS:H	2.05	0.55
1:A:284:TYR:CE1	1:A:296:GLU:HG3	2.42	0.55
2:D:182:THR:OG1	2:D:184:ASP:OD1	2.17	0.55
2:B:300:ASN:HD21	2:B:303:HIS:H	1.54	0.54
2:C:300:ASN:HD22	2:C:300:ASN:C	2.11	0.54
1:A:170:ASP:OD1	1:A:224:ASN:HA	2.08	0.54
2:B:172:ASN:H	2:B:172:ASN:HD22	1.56	0.53
2:C:119:GLY:HA3	2:C:167:ARG:HD3	1.91	0.53
2:D:246:ASP:OD2	2:D:252:HIS:CE1	2.54	0.53
2:D:13:THR:HG22	2:D:286:GLN:NE2	2.23	0.52
2:C:135:THR:HA	2:C:154:GLY:HA2	1.91	0.52
2:C:242:GLN:HB3	2:C:257:ILE:HD11	1.91	0.52
2:D:61:PRO:O	2:D:76:THR:HG22	2.10	0.52
2:D:269:ILE:HG13	2:D:282:ARG:HB2	1.91	0.51
2:C:150:THR:HG21	2:C:198:TRP:CD1	2.46	0.51
2:B:14:GLY:HA2	2:B:265:GLU:HG3	1.92	0.51
2:B:126:ARG:HH12	2:B:142:ASN:HD21	1.58	0.50
1:A:230:ARG:NH2	4:A:950:GOL:O3	2.37	0.49
2:D:172:ASN:ND2	2:D:172:ASN:H	2.10	0.49
2:C:283:LEU:HB2	2:C:297:TRP:HB3	1.94	0.49
2:C:195:HIS:CG	2:C:196:LYS:H	2.31	0.49
1:A:117:LEU:HD12	1:A:124:GLN:HB3	1.95	0.48
1:A:289:THR:O	1:A:293:ALA:HB3	2.13	0.48
2:D:205:ILE:HB	2:D:243:VAL:HG11	1.94	0.48
2:C:190:ARG:NH2	2:C:199:TYR:O	2.42	0.48
2:C:182:THR:O	2:C:185:LEU:N	2.43	0.47
2:C:189:GLN:NE2	2:C:251:TYR:OH	2.47	0.47
1:A:300:ASN:C	1:A:300:ASN:HD22	2.16	0.47
2:C:29:GLN:OE1	2:C:33:GLY:O	2.32	0.47
1:A:29:GLN:HE22	1:A:59:GLY:H	1.62	0.47
2:C:242:GLN:HB2	2:C:257:ILE:HD11	1.96	0.47
2:B:131:LYS:HD2	2:B:137:GLN:HB2	1.95	0.47
2:C:191:ALA:O	2:C:198:TRP:CE3	2.67	0.47
2:D:167:ARG:NH2	2:D:172:ASN:HA	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:HIS:CG	2:C:196:LYS:N	2.83	0.46
2:C:299:TRP:HA	2:C:304:GLY:O	2.15	0.46
1:A:265:GLU:OE2	4:A:991:GOL:H12	2.15	0.46
1:A:27:TYR:CE1	1:A:37:GLU:HG3	2.50	0.46
2:C:191:ALA:O	2:C:198:TRP:HE3	1.98	0.46
2:D:75:TYR:CZ	2:D:127:ILE:HD11	2.51	0.46
1:A:220:PHE:CE2	1:A:279:PRO:HG3	2.51	0.46
2:D:151:ASN:ND2	2:D:153:GLY:H	2.14	0.46
2:B:168:TYR:HB3	2:B:170:ASP:OD1	2.16	0.45
1:A:133:ASP:O	1:A:134:ASN:HB2	2.15	0.45
1:A:216:ALA:HB1	1:A:268:ILE:HG22	1.99	0.45
2:B:2:SER:HB3	2:B:7:GLN:HE21	1.82	0.45
2:D:34:SER:OG	2:D:55:ASN:ND2	2.49	0.45
2:C:297:TRP:CH2	2:C:299:TRP:HB2	2.52	0.45
2:D:82:THR:HA	2:D:104:PHE:O	2.17	0.45
2:D:146:TRP:C	2:D:147:LYS:HG2	2.37	0.45
2:D:192:TYR:CE2	2:D:197:GLY:HA2	2.52	0.45
2:B:240:ILE:HG13	2:B:260:VAL:HG11	1.99	0.45
2:C:231:ILE:HD12	2:C:231:ILE:N	2.32	0.44
2:B:82:THR:HA	2:B:104:PHE:O	2.17	0.44
1:A:45:ALA:O	1:A:46:ASN:HB2	2.16	0.44
2:D:181:GLN:HA	2:D:186:LYS:O	2.17	0.44
2:D:6:ALA:O	2:D:292:SER:OG	2.32	0.44
2:C:64:ALA:HA	2:C:73:ARG:O	2.19	0.43
2:C:156:LEU:C	2:C:156:LEU:HD23	2.39	0.43
2:C:151:ASN:ND2	2:C:153:GLY:H	2.17	0.43
2:B:261:ILE:HG12	2:B:264:SER:HB2	2.01	0.43
2:C:168:TYR:C	2:C:170:ASP:H	2.22	0.43
1:A:202:LEU:HD12	1:A:202:LEU:N	2.34	0.43
2:B:99:LEU:HD13	2:B:146:TRP:CD2	2.53	0.42
2:C:130:GLN:HA	2:C:135:THR:O	2.19	0.42
1:A:141:TRP:CZ3	1:A:145:GLY:HA2	2.54	0.42
2:B:242:GLN:O	2:B:254:LYS:HA	2.19	0.42
2:D:146:TRP:NE1	4:D:920:GOL:O3	2.38	0.42
1:A:20:SER:O	1:A:21:THR:C	2.57	0.42
2:D:239:THR:OG1	2:D:241:TRP:CD1	2.72	0.42
2:C:268:ILE:HG13	2:C:269:ILE:N	2.34	0.42
2:D:189:GLN:NE2	2:D:251:TYR:OH	2.53	0.42
2:D:151:ASN:HD22	2:D:153:GLY:H	1.68	0.42
2:C:22:ASN:HB3	2:C:271:TRP:CZ2	2.55	0.42
2:C:283:LEU:HD12	2:C:297:TRP:CE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:LEU:O	2:B:282:ARG:HD3	2.21	0.41
2:C:270:SER:HB3	2:C:281:LEU:HD23	2.01	0.41
1:A:158:GLY:HA3	1:A:212:ARG:NE	2.35	0.41
2:C:220:PHE:CE2	2:C:279:PRO:HG3	2.55	0.41
1:A:7:GLN:NE2	2:B:134:ASN:HD21	2.19	0.41
1:A:187:LEU:HD22	1:A:215:ILE:HD11	2.02	0.41
2:B:282:ARG:HA	2:B:297:TRP:O	2.20	0.41
1:A:156:LEU:HD12	1:A:185:LEU:HD23	2.03	0.41
1:A:7:GLN:HE22	2:B:134:ASN:HD21	1.69	0.41
1:A:88:TYR:HB2	1:A:94:TRP:CD2	2.56	0.41
2:B:85:GLU:OE1	2:B:97:GLY:HA3	2.20	0.41
2:B:83:LEU:HD11	2:B:139:TYR:CE2	2.56	0.41
2:C:151:ASN:HD22	2:C:153:GLY:H	1.69	0.40
1:A:297:TRP:CH2	1:A:299:TRP:HB2	2.57	0.40
2:C:156:LEU:HA	2:C:157:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSX	A	244	1	3,6,7	0.72	0	1,6,8	2.32	1 (100%)

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
1	CSX	A	244	1	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	CSX	CA-CB-SG	-2.32	108.28	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MFB	D	960	-	12,12,12	0.80	1 (8%)	17,17,17	1.02	1 (5%)
4	GOL	B	990	-	5,5,5	0.79	0	5,5,5	1.12	0
4	GOL	D	920	-	5,5,5	0.53	0	5,5,5	0.51	0
3	MFB	B	910	-	12,12,12	0.87	1 (8%)	17,17,17	0.86	1 (5%)
3	MFB	B	930	-	12,12,12	0.81	0	17,17,17	1.25	2 (11%)
4	GOL	A	940	-	5,5,5	0.49	0	5,5,5	0.46	0
3	MFB	C	950	-	12,12,12	0.84	0	17,17,17	0.78	0
4	GOL	A	950	-	5,5,5	0.51	0	5,5,5	0.99	0
3	MFB	C	960	-	12,12,12	0.58	0	17,17,17	1.04	0
4	GOL	B	920	-	5,5,5	0.50	0	5,5,5	0.75	0
3	MFB	D	930	-	12,12,12	0.77	0	17,17,17	1.10	1 (5%)
3	MFB	A	960	-	12,12,12	0.68	0	17,17,17	0.98	1 (5%)
3	MFB	C	910	-	12,12,12	0.95	1 (8%)	17,17,17	0.93	0
3	MFB	A	910	-	12,12,12	0.87	1 (8%)	17,17,17	0.90	1 (5%)
3	MFB	B	960	-	12,12,12	0.94	1 (8%)	17,17,17	1.55	4 (23%)
4	GOL	A	990	-	5,5,5	0.85	0	5,5,5	0.83	0
3	MFB	C	930	-	12,12,12	0.85	1 (8%)	17,17,17	1.19	2 (11%)
3	MFB	A	930	-	12,12,12	0.83	0	17,17,17	1.15	2 (11%)
4	GOL	A	920	-	5,5,5	0.60	0	5,5,5	0.25	0
4	GOL	A	991	-	5,5,5	0.27	0	5,5,5	0.49	0
4	GOL	B	950	-	5,5,5	0.50	0	5,5,5	0.40	0
5	PEG	A	992	-	3,3,6	0.78	0	2,2,5	0.18	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	MFB	D	960	-	-	0/2/22/22	0/1/1/1
4	GOL	B	990	-	-	2/4/4/4	-
4	GOL	D	920	-	-	2/4/4/4	-
3	MFB	B	910	-	-	0/2/22/22	0/1/1/1
3	MFB	B	930	-	-	0/2/22/22	0/1/1/1
4	GOL	A	940	-	-	2/4/4/4	-
3	MFB	C	950	-	-	0/2/22/22	0/1/1/1
4	GOL	A	950	-	-	4/4/4/4	-
3	MFB	C	960	-	-	0/2/22/22	0/1/1/1
4	GOL	B	920	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MFB	D	930	-	-	0/2/22/22	0/1/1/1
3	MFB	A	960	-	-	0/2/22/22	0/1/1/1
3	MFB	C	910	-	-	0/2/22/22	0/1/1/1
3	MFB	A	910	-	-	0/2/22/22	0/1/1/1
3	MFB	B	960	-	-	0/2/22/22	0/1/1/1
4	GOL	A	990	-	-	2/4/4/4	-
3	MFB	C	930	-	-	2/2/22/22	0/1/1/1
3	MFB	A	930	-	-	0/2/22/22	0/1/1/1
4	GOL	A	920	-	-	0/4/4/4	-
4	GOL	A	991	-	-	2/4/4/4	-
4	GOL	B	950	-	-	4/4/4/4	-
5	PEG	A	992	-	-	1/1/1/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	960	MFB	O1-C1	2.59	1.44	1.40
3	A	910	MFB	O1-C1	2.48	1.44	1.40
3	C	930	MFB	O1-C1	2.46	1.44	1.40
3	C	910	MFB	O1-C1	2.37	1.44	1.40
3	B	910	MFB	O1-C1	2.22	1.44	1.40
3	D	960	MFB	O1-C1	2.01	1.43	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	930	MFB	O1-C1-C2	3.02	111.69	108.15
3	B	960	MFB	C1-C2-C3	2.93	116.09	110.00
3	B	960	MFB	O5-C5-C6	2.87	112.90	106.70
3	B	930	MFB	C1-O5-C5	-2.79	108.87	113.67
3	B	960	MFB	C3-C4-C5	-2.66	105.63	109.77
3	B	910	MFB	O1-C1-C2	2.59	111.18	108.15
3	C	930	MFB	O1-C1-C2	2.56	111.15	108.15
3	A	930	MFB	O3-C3-C2	-2.42	104.75	110.35
3	A	910	MFB	C1-C2-C3	2.23	114.63	110.00
3	A	930	MFB	C1-O5-C5	-2.16	109.95	113.67
3	B	930	MFB	O1-C1-C2	2.10	110.62	108.15
3	D	960	MFB	O3-C3-C4	2.05	115.10	110.35
3	A	960	MFB	C1-O5-C5	-2.04	110.16	113.67
3	B	960	MFB	C1-O5-C5	-2.03	110.17	113.67
3	C	930	MFB	O5-C5-C6	2.00	111.03	106.70

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	950	GOL	O1-C1-C2-C3
4	A	990	GOL	C1-C2-C3-O3
4	A	991	GOL	O1-C1-C2-C3
4	B	950	GOL	O1-C1-C2-C3
4	B	950	GOL	C1-C2-C3-O3
3	C	930	MFB	O5-C1-O1-CM
3	C	930	MFB	C2-C1-O1-CM
4	A	940	GOL	C1-C2-C3-O3
4	A	950	GOL	C1-C2-C3-O3
4	B	990	GOL	O1-C1-C2-C3
4	D	920	GOL	O1-C1-C2-C3
4	A	940	GOL	O2-C2-C3-O3
4	A	990	GOL	O2-C2-C3-O3
4	B	950	GOL	O2-C2-C3-O3
4	D	920	GOL	O1-C1-C2-O2
4	A	950	GOL	O2-C2-C3-O3
4	B	950	GOL	O1-C1-C2-O2
4	B	920	GOL	C1-C2-C3-O3
4	A	950	GOL	O1-C1-C2-O2
4	A	991	GOL	O1-C1-C2-O2
4	B	990	GOL	O1-C1-C2-O2
5	A	992	PEG	O1-C1-C2-O2
4	B	920	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	990	GOL	2	0
4	D	920	GOL	2	0
4	A	950	GOL	1	0
3	B	960	MFB	1	0
4	A	991	GOL	2	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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.