



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:09 AM BST

PDB ID : 2B7Y
Title : Fava Bean Lectin-Glucose Complex
Authors : Reeke Jr., G.N.; Becker, J.W.
Deposited on : 2005-10-05
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

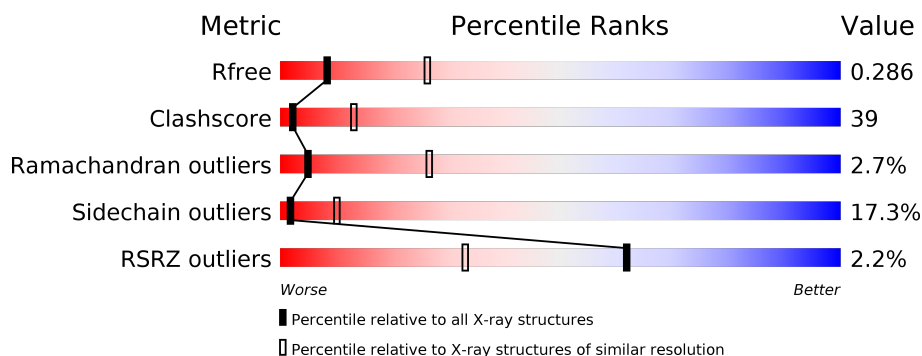
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	182	 2% 35% 49% 15% .
1	C	182	 4% 38% 47% 13% ..
2	B	51	 41% 43% 8% 8%
2	D	51	 35% 47% 10% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	A	801	-	-	-	X
4	NAG	A	803	X	-	-	-
4	NAG	C	804	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3620 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.

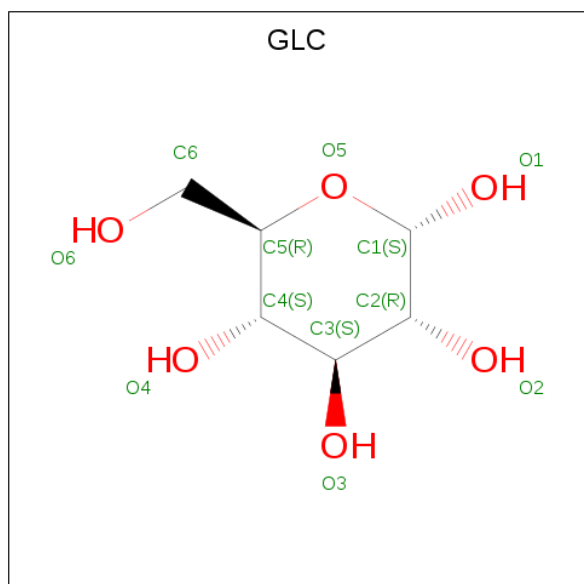
- Molecule 1 is a protein called Favin beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	0	0	0
			1409	905	229	275			
1	C	181	Total	C	N	O	0	0	0
			1409	905	229	275			

- Molecule 2 is a protein called Favin alpha chain.

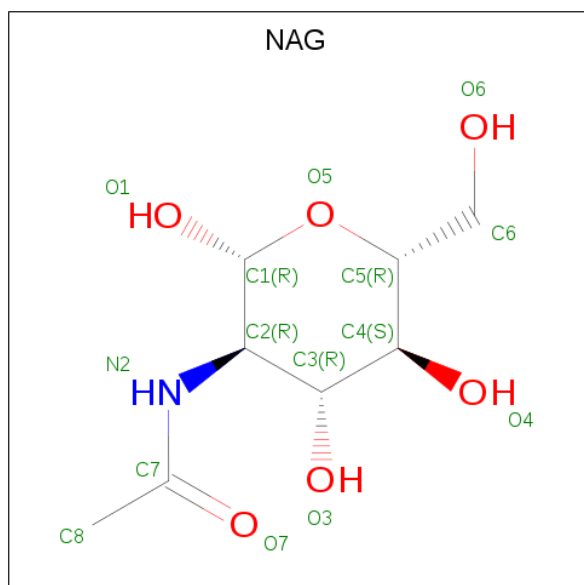
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			369	242	55	72			
2	D	47	Total	C	N	O	0	0	0
			369	242	55	72			

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

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

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

Continued on next page...

Continued from previous page...

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

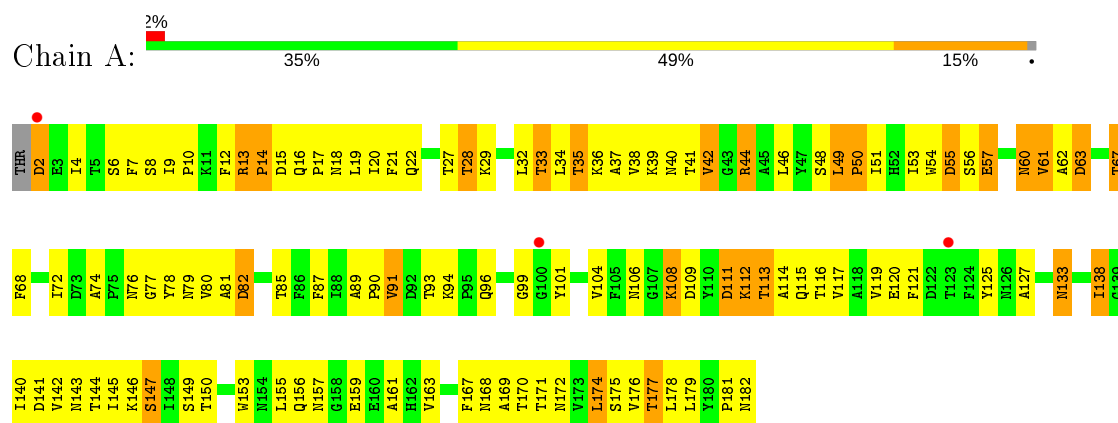
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	O	0	0
			4	4		
7	C	4	Total	O	0	0
			4	4		

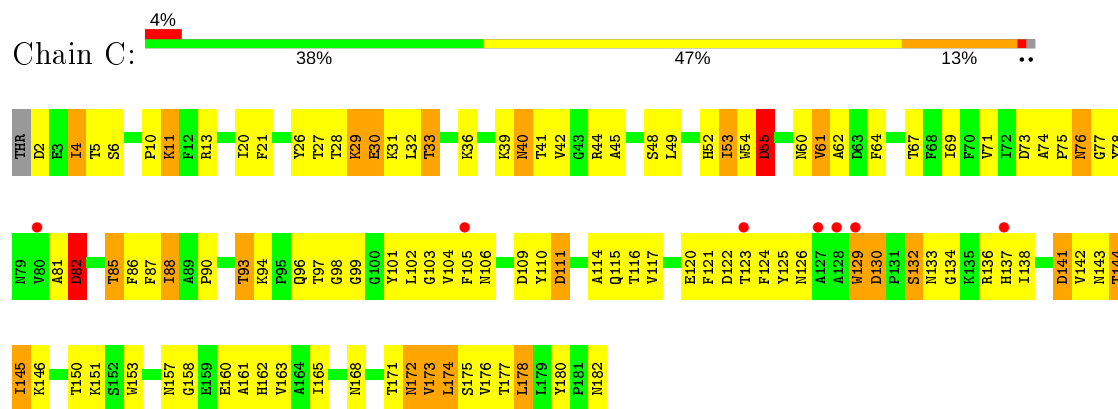
3 Residue-property plots

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 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.

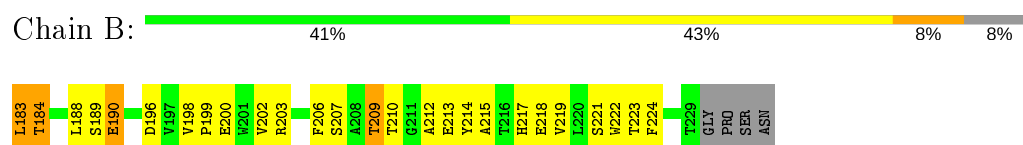
• Molecule 1: Favin beta chain



• Molecule 1: Favin beta chain



• Molecule 2: Favin alpha chain



• Molecule 2: Favin alpha chain



L183	T184	T187	L188	S189	E190	V191	V192	P193	L194	K195	D196	V197	P198	P199	E200	W201	V202	R203	I204	G205	F206	S207	K208	T209	T216	H217	E218	V219	L220	T223	F224	L225	S226	E227	L228	T229	GLY	PRO	SER	ASN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.00 Å 89.30 Å 67.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 3.00 46.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (46.18-3.00) 93.0 (46.18-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.01 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.300 0.197 , 0.286	Depositor DCC
R_{free} test set	545 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3620	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC, NAG, MN

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	0.97	1/1446 (0.1%)	1.14	8/1973 (0.4%)
1	C	0.86	0/1446	1.06	10/1973 (0.5%)
2	B	0.98	0/379	1.08	2/521 (0.4%)
2	D	0.94	0/379	1.04	1/521 (0.2%)
All	All	0.93	1/3650 (0.0%)	1.09	21/4988 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	PHE	CB-CG	-5.10	1.42	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	196	ASP	CB-CG-OD2	7.15	124.73	118.30
1	C	111	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	15	ASP	CB-CG-OD2	6.91	124.52	118.30
1	C	73	ASP	CB-CG-OD2	6.72	124.34	118.30
2	B	196	ASP	CB-CG-OD2	6.45	124.11	118.30
1	C	109	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	133	ASN	N-CA-C	-6.34	93.89	111.00
1	A	2	ASP	CB-CG-OD2	6.32	123.99	118.30
2	B	183	LEU	N-CA-C	-6.28	94.04	111.00
1	C	178	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	C	2	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	82	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	111	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	130	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	141	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	88	ILE	N-CA-C	-5.53	96.08	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	55	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	141	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	55	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	63	ASP	CB-CG-OD2	5.08	122.87	118.30

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	1409	0	1359	126	0
1	C	1409	0	1359	140	0
2	B	369	0	360	50	0
2	D	369	0	360	48	0
3	A	12	0	12	0	0
3	C	12	0	12	1	0
4	A	14	0	13	2	0
4	C	14	0	13	4	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
All	All	3620	0	3488	277	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 39.

All (277) 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:182:ASN:CB	2:B:183:LEU:N	2.02	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:HB2	2:B:183:LEU:N	1.60	1.12
1:A:44:ARG:HH22	1:A:93:THR:HB	1.14	1.11
1:C:174:LEU:HD12	1:C:175:SER:N	1.67	1.10
1:C:171:THR:OG1	1:C:173:VAL:HG12	1.54	1.06
1:C:174:LEU:HD12	1:C:175:SER:H	0.88	1.04
1:A:182:ASN:OXT	2:B:183:LEU:HB2	1.62	0.97
1:A:181:PRO:O	1:A:182:ASN:ND2	2.01	0.94
1:C:172:ASN:O	1:C:172:ASN:ND2	2.01	0.93
1:C:182:ASN:O	2:D:184:THR:HG23	1.69	0.92
1:C:90:PRO:HG3	1:C:115:GLN:HB2	1.55	0.89
1:C:172:ASN:HD22	1:C:172:ASN:C	1.74	0.88
1:C:153:TRP:HZ3	1:C:180:TYR:HH	0.93	0.87
1:A:174:LEU:HD12	1:A:175:SER:N	1.89	0.86
1:C:86:PHE:CE1	2:D:204:ILE:CG2	2.59	0.86
1:C:90:PRO:O	1:C:93:THR:HG22	1.75	0.86
1:A:49:LEU:CD1	1:C:49:LEU:HB2	2.06	0.85
1:A:89:ALA:HB1	1:A:93:THR:HG21	1.60	0.84
1:C:102:LEU:HA	2:D:209:THR:OG1	1.78	0.83
1:A:182:ASN:HB3	2:B:183:LEU:N	1.93	0.83
1:A:111:ASP:OD1	1:A:113:THR:HG22	1.79	0.83
1:C:86:PHE:CE1	2:D:204:ILE:HG21	2.14	0.83
1:C:53:ILE:HD13	2:D:202:VAL:CG2	2.10	0.82
1:C:171:THR:OG1	1:C:173:VAL:CG1	2.27	0.81
1:A:74:ALA:HB3	1:A:157:ASN:HD21	1.46	0.80
1:A:44:ARG:NH2	1:A:93:THR:HB	1.96	0.80
1:C:52:HIS:CE1	1:C:55:ASP:HB2	2.17	0.80
1:A:161:ALA:HB1	1:A:178:LEU:CD1	2.13	0.79
1:A:113:THR:CG2	1:A:114:ALA:H	1.95	0.79
1:A:44:ARG:HH22	1:A:93:THR:CB	1.96	0.78
1:A:113:THR:HG23	1:A:114:ALA:N	1.97	0.78
1:C:53:ILE:HD13	2:D:202:VAL:HG21	1.64	0.78
1:C:6:SER:HB3	2:D:225:LEU:HD12	1.65	0.78
1:A:49:LEU:HD13	1:C:49:LEU:HB2	1.66	0.76
1:C:174:LEU:CD1	1:C:175:SER:H	1.84	0.76
1:C:76:ASN:HD22	1:C:77:GLY:N	1.84	0.76
1:A:61:VAL:CG1	1:A:169:ALA:HB1	2.16	0.76
1:C:88:ILE:HG22	2:D:202:VAL:HG11	1.66	0.76
1:A:57:GLU:HA	1:A:57:GLU:OE1	1.85	0.75
1:A:182:ASN:CA	2:B:183:LEU:N	2.50	0.75
1:C:86:PHE:HE1	2:D:204:ILE:HG21	1.51	0.74
1:A:61:VAL:HG12	1:A:169:ALA:HB1	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:THR:HG22	2:D:207:SER:HB3	1.71	0.73
1:A:182:ASN:C	2:B:183:LEU:N	2.42	0.73
1:C:52:HIS:HE1	1:C:55:ASP:HB2	1.52	0.72
1:A:99:GLY:O	2:B:209:THR:HG21	1.89	0.72
1:C:81:ALA:HB1	1:C:82:ASP:HA	1.71	0.72
1:A:113:THR:CG2	1:A:114:ALA:N	2.53	0.72
1:A:33:THR:HG23	2:B:218:GLU:CG	2.19	0.72
1:A:181:PRO:O	1:A:182:ASN:CG	2.28	0.72
1:A:56:SER:CB	2:B:200:GLU:OE2	2.38	0.71
1:A:33:THR:HG23	2:B:218:GLU:HG3	1.73	0.70
1:C:96:GLN:HB3	1:C:106:ASN:OD1	1.91	0.70
1:A:67:THR:HB	2:B:223:THR:OG1	1.91	0.70
1:A:20:ILE:HD12	1:A:48:SER:HA	1.73	0.69
1:A:113:THR:HG23	1:A:114:ALA:H	1.54	0.69
1:C:110:TYR:HA	1:C:144:THR:HG22	1.76	0.67
1:A:56:SER:OG	2:B:200:GLU:OE2	2.09	0.67
1:A:161:ALA:HB1	1:A:178:LEU:HD11	1.77	0.67
1:A:115:GLN:HA	1:A:143:ASN:HD21	1.60	0.66
1:A:74:ALA:HB3	1:A:157:ASN:ND2	2.11	0.66
1:C:168:ASN:O	1:C:172:ASN:HA	1.96	0.66
1:A:49:LEU:HD12	1:C:49:LEU:HB2	1.75	0.66
1:C:161:ALA:HB1	1:C:178:LEU:CD1	2.26	0.65
1:C:71:VAL:HG22	1:C:160:GLU:HA	1.78	0.64
1:C:55:ASP:HA	2:D:200:GLU:OE2	1.97	0.64
1:A:76:ASN:O	1:A:78:TYR:N	2.31	0.64
1:C:32:LEU:HD23	2:D:219:VAL:CG1	2.28	0.64
1:A:168:ASN:OD1	1:A:171:THR:HG23	1.98	0.64
1:C:21:PHE:CE2	1:C:27:THR:HG23	2.32	0.63
1:A:20:ILE:CD1	1:A:48:SER:HA	2.29	0.63
1:A:96:GLN:HE21	1:A:106:ASN:HD21	1.45	0.62
1:A:8:SER:HB2	2:B:223:THR:HG22	1.82	0.62
1:C:76:ASN:ND2	1:C:78:TYR:H	1.97	0.62
2:D:194:LEU:HA	2:D:197:VAL:HG23	1.81	0.62
1:C:53:ILE:CD1	2:D:202:VAL:HG22	2.29	0.62
1:C:85:THR:CG2	2:D:207:SER:HB3	2.30	0.62
1:C:45:ALA:O	2:D:205:GLY:HA3	1.99	0.61
1:A:125:TYR:CZ	1:A:127:ALA:HA	2.36	0.61
1:A:38:VAL:HG12	1:A:38:VAL:O	2.00	0.61
1:A:79:ASN:HB3	2:B:213:GLU:CD	2.21	0.61
1:A:175:SER:HB3	2:B:189:SER:HB2	1.83	0.60
1:A:56:SER:HB3	2:B:200:GLU:OE2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ILE:HG12	1:C:176:VAL:HG22	1.82	0.60
1:C:97:THR:HG23	1:C:106:ASN:OD1	2.01	0.60
1:A:174:LEU:HD12	1:A:174:LEU:C	2.19	0.60
1:C:42:VAL:HA	2:D:209:THR:HG22	1.84	0.60
1:C:117:VAL:HG22	1:C:142:VAL:HG13	1.84	0.60
1:C:124:PHE:CE1	1:C:126:ASN:ND2	2.70	0.59
1:A:163:VAL:HA	1:A:177:THR:O	2.01	0.59
1:C:32:LEU:HG	1:C:32:LEU:O	2.02	0.59
1:A:85:THR:HG22	2:B:207:SER:O	2.03	0.59
1:C:110:TYR:HA	1:C:144:THR:CG2	2.33	0.59
1:A:55:ASP:OD2	1:A:57:GLU:HB2	2.02	0.59
1:A:32:LEU:HD23	2:B:219:VAL:HB	1.85	0.59
1:C:54:TRP:HB3	1:C:61:VAL:HG23	1.85	0.59
1:A:22:GLN:OE1	1:A:44:ARG:HD3	2.03	0.58
1:C:6:SER:HB3	2:D:225:LEU:CD1	2.32	0.58
1:C:53:ILE:CD1	2:D:202:VAL:CG2	2.80	0.58
1:C:101:TYR:HA	1:C:145:ILE:HD13	1.85	0.58
1:C:20:ILE:HD12	1:C:48:SER:HA	1.86	0.58
1:C:26:TYR:OH	1:C:36:LYS:HE3	2.04	0.57
1:C:171:THR:HG23	4:C:804:NAG:H2	1.85	0.57
1:C:171:THR:HG21	4:C:804:NAG:O7	2.05	0.57
1:A:63:ASP:HB2	1:A:167:PHE:O	2.05	0.57
1:C:124:PHE:CD1	1:C:126:ASN:ND2	2.72	0.57
1:C:85:THR:HG22	2:D:207:SER:O	2.04	0.57
1:C:87:PHE:CE1	2:D:207:SER:HB2	2.40	0.57
1:A:2:ASP:CG	1:C:13:ARG:HH12	2.08	0.56
1:C:29:LYS:O	1:C:30:GLU:HG2	2.05	0.56
1:C:182:ASN:HA	2:D:183:LEU:N	2.20	0.56
2:B:198:VAL:CG1	2:B:202:VAL:HG11	2.36	0.56
1:A:140:ILE:HD11	2:B:188:LEU:HG	1.86	0.56
1:C:97:THR:OG1	1:C:106:ASN:HA	2.06	0.56
1:C:121:PHE:CD2	1:C:121:PHE:N	2.73	0.55
1:C:153:TRP:HZ3	1:C:180:TYR:OH	1.75	0.55
1:A:7:PHE:CE2	2:B:224:PHE:HB3	2.41	0.55
1:C:54:TRP:O	2:D:200:GLU:HG3	2.07	0.55
1:C:11:LYS:NZ	1:C:13:ARG:HH21	2.04	0.55
1:C:172:ASN:OD1	2:D:193:PRO:HA	2.07	0.54
1:C:21:PHE:HE2	1:C:27:THR:HG23	1.72	0.54
1:A:147:SER:C	1:A:149:SER:H	2.11	0.54
1:C:125:TYR:CD1	1:C:134:GLY:HA2	2.43	0.54
1:C:182:ASN:O	2:D:184:THR:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:O	2:B:222:TRP:HA	2.08	0.54
1:C:53:ILE:HD13	2:D:202:VAL:HG22	1.84	0.54
1:C:125:TYR:OH	1:C:132:SER:HA	2.07	0.53
1:C:168:ASN:O	1:C:172:ASN:CA	2.56	0.53
1:A:28:THR:OG1	1:A:29:LYS:N	2.42	0.53
1:A:111:ASP:O	1:A:112:LYS:C	2.46	0.53
1:C:29:LYS:O	1:C:30:GLU:CG	2.57	0.53
1:C:62:ALA:HB2	2:D:228:LEU:HD13	1.91	0.52
1:C:11:LYS:HZ2	1:C:13:ARG:HH21	1.57	0.52
1:C:129:TRP:HB2	1:C:146:LYS:CG	2.40	0.52
1:C:153:TRP:CZ3	1:C:178:LEU:HD21	2.44	0.52
1:A:182:ASN:OXT	2:B:183:LEU:CB	2.47	0.52
1:A:89:ALA:HB1	1:A:93:THR:CG2	2.36	0.52
1:A:108:LYS:HZ2	1:A:108:LYS:HB2	1.74	0.52
1:A:35:THR:HG21	2:B:217:HIS:HD2	1.73	0.52
1:A:12:PHE:HA	1:A:16:GLN:NE2	2.24	0.52
1:A:13:ARG:HG2	1:A:14:PRO:HD2	1.91	0.51
1:A:13:ARG:H	1:A:16:GLN:NE2	2.08	0.51
1:A:168:ASN:HD22	4:A:803:NAG:C7	2.23	0.51
1:A:63:ASP:N	1:A:63:ASP:OD1	2.39	0.51
1:C:129:TRP:CE2	1:C:145:ILE:HG12	2.45	0.51
1:C:129:TRP:C	1:C:129:TRP:CD1	2.83	0.51
1:C:124:PHE:HD1	1:C:126:ASN:HD21	1.59	0.51
1:A:54:TRP:NE1	2:B:198:VAL:O	2.34	0.51
1:C:174:LEU:CD1	1:C:175:SER:N	2.57	0.50
2:D:224:PHE:C	2:D:224:PHE:CD2	2.85	0.50
1:C:39:LYS:HB3	1:C:40:ASN:ND2	2.26	0.50
1:C:123:THR:O	1:C:136:ARG:NH1	2.45	0.50
1:A:13:ARG:O	1:A:16:GLN:HG2	2.12	0.50
2:D:193:PRO:O	2:D:196:ASP:HB2	2.12	0.50
1:A:85:THR:CG2	2:B:207:SER:OG	2.60	0.49
1:C:165:ILE:HG23	1:C:174:LEU:HD11	1.94	0.49
1:C:114:ALA:O	1:C:143:ASN:OD1	2.30	0.49
1:C:53:ILE:HD11	2:D:202:VAL:HG13	1.94	0.49
4:A:803:NAG:H5	4:A:803:NAG:N2	2.27	0.49
1:A:2:ASP:OD2	1:C:10:PRO:HD2	2.12	0.49
1:A:79:ASN:HB3	2:B:213:GLU:OE1	2.13	0.49
1:A:33:THR:HG23	2:B:218:GLU:HG2	1.95	0.49
1:A:44:ARG:HA	2:B:206:PHE:O	2.13	0.49
1:A:155:LEU:HD12	1:A:156:GLN:H	1.78	0.48
1:A:144:THR:HG22	1:A:146:LYS:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:HA	1:A:143:ASN:ND2	2.28	0.48
1:A:182:ASN:HB2	2:B:183:LEU:CA	2.41	0.48
1:C:122:ASP:CG	1:C:137:HIS:CE1	2.87	0.48
1:A:108:LYS:NZ	1:A:108:LYS:HB2	2.29	0.48
1:C:82:ASP:OD1	3:C:802:GLC:H4	2.14	0.48
1:C:88:ILE:HG22	2:D:202:VAL:CG1	2.42	0.47
1:A:174:LEU:HD12	1:A:175:SER:H	1.76	0.47
1:A:61:VAL:HG13	1:A:62:ALA:O	2.14	0.47
1:C:145:ILE:HG13	1:C:145:ILE:O	2.15	0.47
1:C:171:THR:CG2	4:C:804:NAG:H2	2.44	0.47
1:A:155:LEU:HD12	1:A:156:GLN:N	2.30	0.47
1:C:168:ASN:O	1:C:172:ASN:N	2.48	0.47
1:C:129:TRP:HB2	1:C:146:LYS:HG2	1.97	0.47
1:C:129:TRP:CZ2	1:C:145:ILE:HG12	2.49	0.47
1:A:42:VAL:HG23	2:B:209:THR:OG1	2.15	0.47
2:B:214:TYR:CD2	2:B:214:TYR:N	2.83	0.47
1:C:85:THR:O	2:D:206:PHE:HA	2.15	0.47
1:A:101:TYR:HA	1:A:145:ILE:HG12	1.96	0.46
1:A:120:GLU:O	1:A:138:ILE:HA	2.15	0.46
1:C:52:HIS:HB2	2:D:201:TRP:CZ3	2.50	0.46
2:B:198:VAL:HG13	2:B:199:PRO:HD2	1.97	0.46
1:C:87:PHE:CE1	2:D:207:SER:CB	2.98	0.46
1:A:53:ILE:HG22	1:A:53:ILE:O	2.15	0.46
1:C:31:LYS:HG2	2:D:218:GLU:OE2	2.14	0.46
1:A:34:LEU:HD11	2:B:206:PHE:HB2	1.97	0.46
1:A:85:THR:O	1:A:85:THR:HG23	2.15	0.46
1:C:69:ILE:HG13	1:C:162:HIS:HB2	1.97	0.46
2:D:220:LEU:HA	2:D:220:LEU:HD23	1.66	0.46
1:C:173:VAL:CG2	1:C:174:LEU:O	2.64	0.46
1:A:53:ILE:O	1:A:53:ILE:CG2	2.64	0.46
1:C:161:ALA:HB1	1:C:178:LEU:HD11	1.98	0.46
1:C:31:LYS:HG3	2:D:220:LEU:HD21	1.97	0.46
1:C:85:THR:HG23	1:C:87:PHE:HD1	1.81	0.46
1:C:67:THR:HB	2:D:223:THR:OG1	2.15	0.46
1:A:91:VAL:O	2:B:203:ARG:HD2	2.16	0.46
2:B:190:GLU:OE1	2:B:190:GLU:HA	2.16	0.46
1:A:48:SER:O	1:A:50:PRO:HD3	2.16	0.45
1:C:81:ALA:HB2	1:C:124:PHE:HB2	1.98	0.45
1:A:76:ASN:C	1:A:78:TYR:H	2.20	0.45
1:C:81:ALA:CB	1:C:82:ASP:HA	2.40	0.45
1:A:60:ASN:N	1:A:60:ASN:OD1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TYR:CD1	1:C:130:ASP:HB3	2.52	0.45
1:C:172:ASN:C	1:C:172:ASN:ND2	2.48	0.45
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.75	0.45
1:A:153:TRP:NE1	1:A:178:LEU:HD21	2.32	0.45
1:A:63:ASP:HB3	1:A:169:ALA:N	2.32	0.45
1:A:68:PHE:HA	2:B:221:SER:O	2.16	0.45
1:C:64:PHE:C	1:C:64:PHE:CD1	2.90	0.45
1:C:87:PHE:HE1	2:D:206:PHE:C	2.20	0.45
1:A:61:VAL:CG1	1:A:169:ALA:CB	2.94	0.45
1:C:161:ALA:HB2	1:C:180:TYR:CE2	2.52	0.45
1:C:98:GLY:HA2	1:C:103:GLY:H	1.81	0.44
1:A:85:THR:HG21	2:B:207:SER:OG	2.17	0.44
1:C:142:VAL:O	1:C:143:ASN:HB2	2.17	0.44
1:C:153:TRP:CZ3	1:C:180:TYR:OH	2.49	0.44
1:A:46:LEU:HD21	1:A:87:PHE:HZ	1.82	0.44
1:C:176:VAL:HG12	1:C:177:THR:N	2.32	0.44
1:C:76:ASN:ND2	1:C:78:TYR:N	2.64	0.44
2:D:216:THR:HG23	2:D:218:GLU:HG2	1.99	0.44
1:C:4:ILE:HD11	2:D:225:LEU:HD11	1.99	0.43
1:C:39:LYS:O	1:C:41:THR:HG23	2.18	0.43
1:C:120:GLU:OE2	1:C:141:ASP:OD2	2.35	0.43
1:A:175:SER:HB3	2:B:189:SER:CB	2.47	0.43
1:C:69:ILE:HG22	2:D:220:LEU:HB2	2.00	0.43
1:C:173:VAL:HG22	1:C:174:LEU:O	2.19	0.43
1:C:168:ASN:HD22	4:C:804:NAG:H82	1.84	0.43
1:A:85:THR:CG2	1:A:85:THR:O	2.66	0.43
1:A:40:ASN:HA	2:B:210:THR:O	2.18	0.43
1:A:113:THR:HG22	1:A:114:ALA:H	1.79	0.43
1:A:8:SER:CB	2:B:223:THR:HG22	2.49	0.42
1:C:176:VAL:CG1	1:C:177:THR:N	2.82	0.42
2:B:183:LEU:HD12	2:B:183:LEU:HA	1.62	0.42
1:A:72:ILE:HG21	1:A:72:ILE:HD13	1.79	0.42
1:C:173:VAL:HA	2:D:191:VAL:HA	2.02	0.42
1:A:156:GLN:HE22	2:B:184:THR:HG21	1.85	0.42
1:C:4:ILE:CG1	1:C:5:THR:N	2.82	0.42
1:A:18:ASN:OD1	1:A:19:LEU:HG	2.20	0.42
1:A:39:LYS:HD3	2:B:212:ALA:O	2.20	0.42
1:C:111:ASP:O	1:C:143:ASN:HB3	2.20	0.42
1:A:145:ILE:HA	1:A:145:ILE:HD12	1.88	0.41
1:C:133:ASN:OD1	1:C:134:GLY:N	2.53	0.41
1:C:32:LEU:HD23	2:D:219:VAL:HG13	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ASN:OD1	1:C:158:GLY:N	2.52	0.41
1:A:111:ASP:O	1:A:113:THR:N	2.54	0.41
1:A:57:GLU:OE1	1:A:57:GLU:CA	2.64	0.41
1:C:120:GLU:OE1	1:C:122:ASP:HB2	2.21	0.41
1:C:124:PHE:HE1	1:C:126:ASN:ND2	2.14	0.41
1:A:36:LYS:O	1:A:38:VAL:N	2.54	0.41
1:A:6:SER:HA	2:B:224:PHE:O	2.20	0.41
2:B:198:VAL:HG11	2:B:202:VAL:HG11	2.02	0.41
1:C:104:VAL:HG13	1:C:105:PHE:CD2	2.55	0.41
1:C:88:ILE:CG2	2:D:202:VAL:HG11	2.43	0.41
1:A:90:PRO:HG3	1:A:115:GLN:HG3	2.03	0.41
2:D:204:ILE:HG22	2:D:205:GLY:N	2.35	0.41
1:C:28:THR:HG23	1:C:33:THR:CG2	2.51	0.41
1:C:74:ALA:HA	1:C:75:PRO:HD3	1.82	0.41
1:A:178:LEU:HD12	1:A:179:LEU:H	1.86	0.41
1:A:61:VAL:CG1	1:A:61:VAL:O	2.65	0.41
2:B:214:TYR:O	2:B:215:ALA:HB2	2.21	0.41
2:B:224:PHE:CD2	2:B:224:PHE:C	2.94	0.41
1:C:138:ILE:O	1:C:151:LYS:N	2.54	0.41
1:A:119:VAL:HG12	1:A:121:PHE:CE1	2.56	0.40
1:A:17:PRO:HG2	2:D:201:TRP:CD2	2.55	0.40
1:A:81:ALA:HB1	1:A:82:ASP:HA	2.02	0.40
1:C:124:PHE:HE1	1:C:126:ASN:HD22	1.69	0.40
2:D:193:PRO:O	2:D:197:VAL:HG22	2.20	0.40
1:A:35:THR:HG21	2:B:217:HIS:CD2	2.56	0.40
1:C:126:ASN:OD1	1:C:129:TRP:CZ2	2.75	0.40
1:A:142:VAL:O	1:A:142:VAL:HG23	2.21	0.40
1:A:32:LEU:O	2:B:218:GLU:HA	2.22	0.40
1:A:9:ILE:HA	1:A:10:PRO:HD3	1.86	0.40
1:C:153:TRP:HZ3	1:C:180:TYR:CZ	2.39	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	179/182 (98%)	150 (84%)	20 (11%)	9 (5%)	2	12
1	C	179/182 (98%)	161 (90%)	15 (8%)	3 (2%)	9	39
2	B	45/51 (88%)	40 (89%)	5 (11%)	0	100	100
2	D	45/51 (88%)	39 (87%)	6 (13%)	0	100	100
All	All	448/466 (96%)	390 (87%)	46 (10%)	12 (3%)	5	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLY
1	A	133	ASN
1	C	129	TRP
1	A	113	THR
1	A	37	ALA
1	A	172	ASN
1	A	4	ILE
1	A	112	LYS
1	C	30	GLU
1	A	50	PRO
1	C	99	GLY
1	A	14	PRO

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	153/154 (99%)	123 (80%)	30 (20%)	1	7
1	C	153/154 (99%)	129 (84%)	24 (16%)	2	13
2	B	41/44 (93%)	38 (93%)	3 (7%)	14	44
2	D	41/44 (93%)	31 (76%)	10 (24%)	0	3
All	All	388/396 (98%)	321 (83%)	67 (17%)	2	10

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	27	THR
1	A	28	THR
1	A	33	THR
1	A	35	THR
1	A	41	THR
1	A	42	VAL
1	A	44	ARG
1	A	49	LEU
1	A	51	ILE
1	A	57	GLU
1	A	60	ASN
1	A	61	VAL
1	A	67	THR
1	A	80	VAL
1	A	82	ASP
1	A	91	VAL
1	A	94	LYS
1	A	104	VAL
1	A	108	LYS
1	A	116	THR
1	A	117	VAL
1	A	138	ILE
1	A	147	SER
1	A	150	THR
1	A	159	GLU
1	A	170	THR
1	A	174	LEU
1	A	176	VAL
1	A	177	THR
2	B	184	THR
2	B	190	GLU
2	B	209	THR
1	C	4	ILE
1	C	11	LYS
1	C	29	LYS
1	C	33	THR
1	C	40	ASN
1	C	44	ARG
1	C	53	ILE
1	C	55	ASP
1	C	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	VAL
1	C	76	ASN
1	C	82	ASP
1	C	85	THR
1	C	93	THR
1	C	94	LYS
1	C	116	THR
1	C	132	SER
1	C	144	THR
1	C	145	ILE
1	C	150	THR
1	C	163	VAL
1	C	172	ASN
1	C	173	VAL
1	C	174	LEU
2	D	187	THR
2	D	189	SER
2	D	191	VAL
2	D	192	VAL
2	D	197	VAL
2	D	198	VAL
2	D	202	VAL
2	D	216	THR
2	D	226	SER
2	D	229	THR

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

Mol	Chain	Res	Type
1	A	16	GLN
1	A	76	ASN
1	A	96	GLN
1	A	143	ASN
2	B	217	HIS
1	C	40	ASN
1	C	52	HIS
1	C	76	ASN
1	C	79	ASN
1	C	126	ASN
1	C	172	ASN
1	C	182	ASN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	GLC	A	801	-	12,12,12	0.75	0	17,17,17	0.88	0
3	GLC	C	802	-	12,12,12	0.68	0	17,17,17	1.01	1 (5%)
4	NAG	C	804	1	14,14,15	1.00	0	17,19,21	2.25	6 (35%)
4	NAG	A	803	1	14,14,15	0.82	0	17,19,21	2.55	7 (41%)

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
4	NAG	A	803	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	C	804	1	1/1/5/7	4/6/23/26	0/1/1/1
3	GLC	C	802	-	-	2/2/22/22	0/1/1/1
3	GLC	A	801	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	NAG	O5-C5-C6	7.38	118.78	107.20
4	C	804	NAG	C1-O5-C5	6.06	120.40	112.19
4	C	804	NAG	C4-C3-C2	3.48	116.12	111.02
4	A	803	NAG	C8-C7-N2	3.34	121.75	116.10
4	C	804	NAG	C2-N2-C7	3.05	127.24	122.90
4	A	803	NAG	O7-C7-C8	-2.90	116.68	122.06
4	A	803	NAG	C1-O5-C5	2.83	116.03	112.19
4	A	803	NAG	C2-N2-C7	2.51	126.48	122.90
4	A	803	NAG	O4-C4-C3	2.47	116.07	110.35
4	A	803	NAG	C3-C4-C5	-2.44	105.89	110.24
4	C	804	NAG	O5-C5-C4	2.43	116.73	110.83
3	C	802	GLC	O2-C2-C1	-2.10	104.28	109.16
4	C	804	NAG	O7-C7-C8	-2.00	118.34	122.06
4	C	804	NAG	O5-C1-C2	2.00	114.45	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	803	NAG	C1
4	C	804	NAG	C1

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	NAG	C8-C7-N2-C2
4	A	803	NAG	O7-C7-N2-C2
4	C	804	NAG	C8-C7-N2-C2
4	C	804	NAG	O7-C7-N2-C2
4	A	803	NAG	C4-C5-C6-O6
4	C	804	NAG	O5-C5-C6-O6
4	A	803	NAG	O5-C5-C6-O6
4	C	804	NAG	C4-C5-C6-O6
4	A	803	NAG	C1-C2-N2-C7
3	C	802	GLC	O5-C5-C6-O6
3	C	802	GLC	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	GLC	1	0
4	C	804	NAG	4	0
4	A	803	NAG	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 [i](#)

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

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	181/182 (99%)	-0.28	3 (1%) 70 41	4, 19, 40, 52	0
1	C	181/182 (99%)	-0.02	7 (3%) 39 15	8, 32, 51, 57	0
2	B	47/51 (92%)	-0.36	0 100 100	6, 15, 23, 29	0
2	D	47/51 (92%)	-0.33	0 100 100	8, 29, 39, 46	0
All	All	456/466 (97%)	-0.19	10 (2%) 62 33	4, 24, 47, 57	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASP	3.7
1	C	123	THR	3.0
1	C	105	PHE	2.5
1	C	137	HIS	2.3
1	C	80	VAL	2.3
1	C	128	ALA	2.2
1	C	127	ALA	2.2
1	A	100	GLY	2.1
1	C	129	TRP	2.0
1	A	123	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
4	NAG	C	804	14/15	0.71	0.27	51,56,63,64	0
3	GLC	A	801	12/12	0.73	0.60	2,2,2,2	12
3	GLC	C	802	12/12	0.83	0.32	2,2,2,2	12
4	NAG	A	803	14/15	0.84	0.20	42,47,51,52	0
5	MN	C	601	1/1	0.94	0.10	41,41,41,41	0
6	CA	C	602	1/1	0.98	0.06	33,33,33,33	0
6	CA	A	502	1/1	0.99	0.06	13,13,13,13	0
5	MN	A	501	1/1	0.99	0.05	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.