



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:03 PM GMT

PDB ID : 1WBL
Title : WINGED BEAN LECTIN COMPLEXED WITH METHYL-ALPHA-D-GA
LACTOSE
Authors : Prabu, M.M.; Sankaranarayanan, R.; Puri, K.D.; Sharma, V.; Surolia, A.;
Vijayan, M.; Suguna, K.
Deposited on : 1997-04-04
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

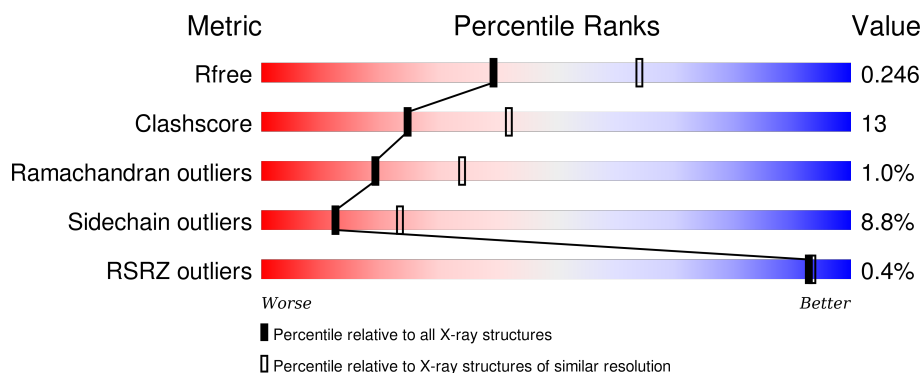
1 Overall quality at a glance

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))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	A	241	 70% 25% . .
1	B	241	 66% 29% . .
1	C	241	 65% 30% . .
1	D	241	 67% 27% . .

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	FUC	A	502	X	-	-	-
2	NAG	A	503	X	-	-	-
2	FUC	B	602	X	-	-	-
2	NAG	B	603	X	-	-	-
2	FUC	C	502	X	-	-	-
2	FUC	D	502	X	-	-	-
2	NAG	D	503	X	-	-	-
3	NAG	B	501	X	-	-	-
3	NAG	B	503	X	-	-	-
6	CA	B	303	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8139 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 WINGED BEAN LECTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	0	0	0
			1831	1179	307	345			
1	B	237	Total	C	N	O	0	0	0
			1818	1171	301	346			
1	C	237	Total	C	N	O	0	0	0
			1823	1173	304	346			
1	D	237	Total	C	N	O	0	0	0
			1815	1170	300	345			

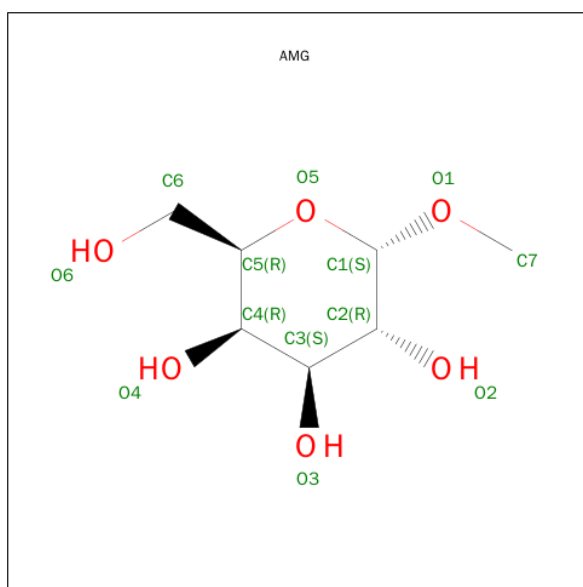
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			38	22	2	14		
2	B	3	Total	C	N	O	0	0
			38	22	2	14		
2	C	3	Total	C	N	O	0	0
			38	22	2	14		
2	D	3	Total	C	N	O	0	0
			38	22	2	14		
2	D	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is ALPHA-METHYL-D-GALACTOSIDE (three-letter code: AMG) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	7	6		
4	B	1	Total	C	O	0	0
			13	7	6		
4	C	1	Total	C	O	0	0
			13	7	6		
4	D	1	Total	C	O	0	0
			13	7	6		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	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	B	1	Total	Ca	0	0
			1	1		

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

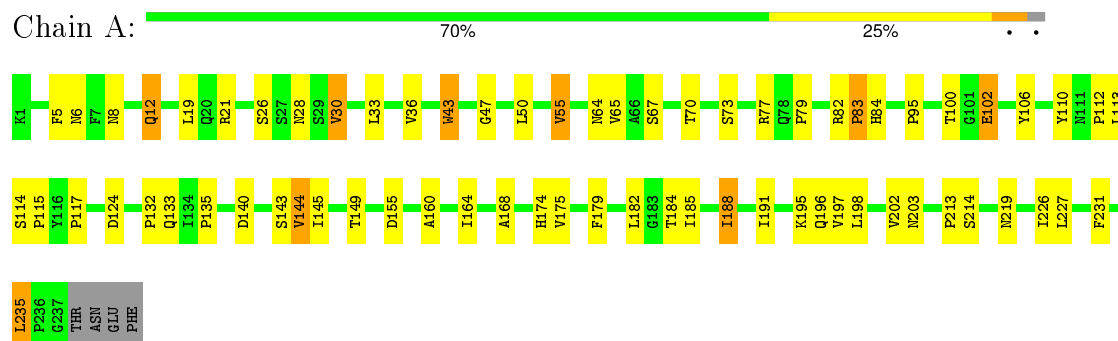
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	153	Total 153	O 153	0	0
7	B	130	Total 130	O 130	0	0
7	C	132	Total 132	O 132	0	0
7	D	131	Total 131	O 131	0	0

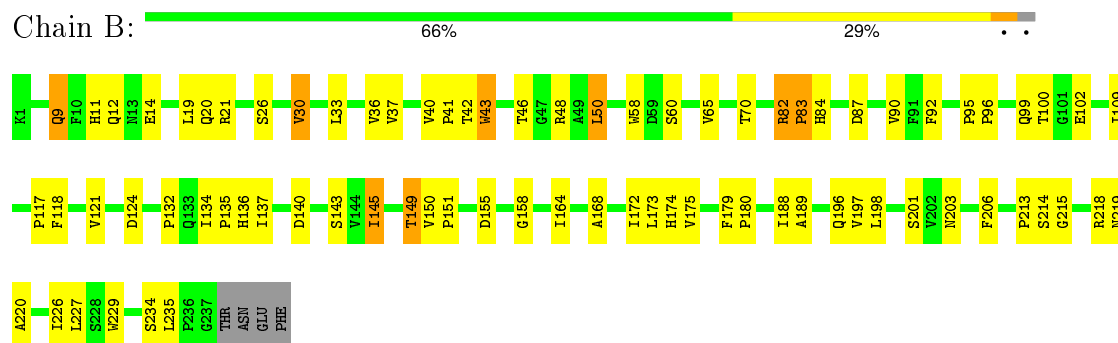
3 Residue-property plots

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.

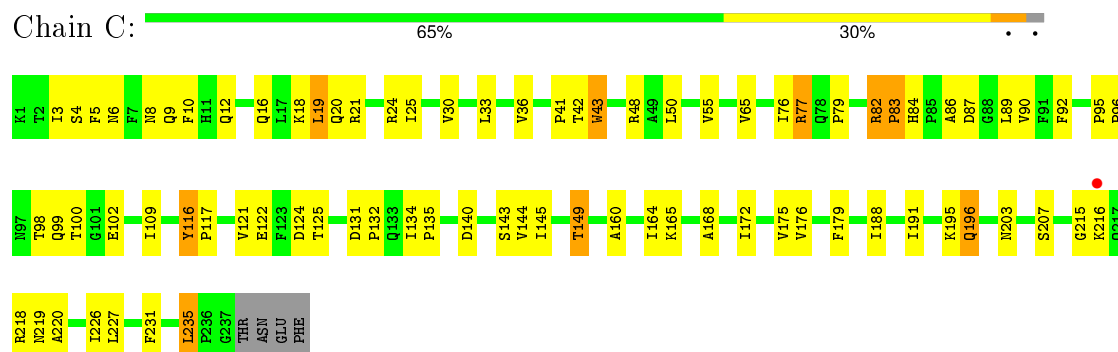
• Molecule 1: WINGED BEAN LECTIN



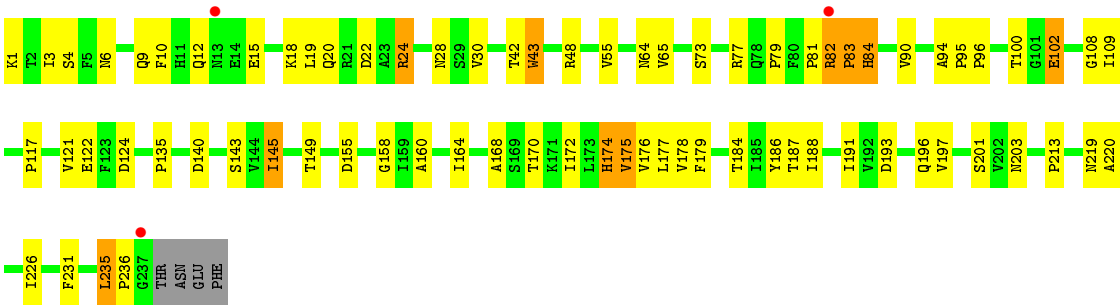
• Molecule 1: WINGED BEAN LECTIN



• Molecule 1: WINGED BEAN LECTIN



• Molecule 1: WINGED BEAN LECTIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.59 Å 91.91 Å 73.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50 9.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	77.3 (100.00-2.50) 76.6 (9.89-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.50 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , 0.259 0.184 , 0.246	Depositor DCC
R_{free} test set	1373 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 64.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 28257 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8139	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MN, NAG, AMG, FUC

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	0.44	0/1884	0.74	0/2580
1	B	0.47	0/1871	0.76	0/2564
1	C	0.46	0/1876	0.76	1/2569 (0.0%)
1	D	0.44	0/1867	0.74	0/2558
All	All	0.45	0/7498	0.75	1/10271 (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	A	2	0
2	B	2	0
2	C	1	0
2	D	2	0
3	B	2	0
All	All	9	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	GLY	N-CA-C	-6.16	97.71	113.10

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	502	FUC	C1
2	A	503	NAG	C1

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Mol	Chain	Res	Type	Atom
3	B	501	NAG	C1
3	B	503	NAG	C1
2	B	602	FUC	C1
2	B	603	NAG	C1
2	C	502	FUC	C1
2	D	502	FUC	C1
2	D	503	NAG	C1

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	1831	0	1776	47	0
1	B	1818	0	1744	52	0
1	C	1823	0	1756	55	0
1	D	1815	0	1751	44	0
2	A	38	0	34	1	0
2	B	38	0	34	2	0
2	C	38	0	34	1	0
2	D	76	0	68	1	0
3	A	28	0	25	0	0
3	B	28	0	25	3	0
4	A	13	0	14	0	0
4	B	13	0	14	0	0
4	C	13	0	14	0	0
4	D	13	0	14	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	153	0	0	2	0
7	B	130	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	132	0	0	4	0
7	D	131	0	0	2	0
All	All	8139	0	7303	190	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 13.

All (190) 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:B:65:VAL:HG13	1:B:168:ALA:HB1	1.53	0.88
1:D:65:VAL:HG13	1:D:168:ALA:HB1	1.57	0.86
1:B:175:VAL:HG22	1:B:188:ILE:HG22	1.62	0.79
1:C:48:ARG:HD2	1:C:100:THR:HG23	1.65	0.79
1:A:195:LYS:HG2	1:D:145:ILE:HD11	1.65	0.79
1:D:175:VAL:HG22	1:D:188:ILE:HG22	1.66	0.76
1:B:82:ARG:HD3	3:B:501:NAG:H4	1.68	0.73
1:C:175:VAL:HG22	1:C:188:ILE:HG22	1.70	0.73
1:A:143:SER:OG	1:A:145:ILE:HG22	1.89	0.73
1:B:82:ARG:HB2	1:B:83:PRO:HD3	1.72	0.72
1:D:83:PRO:HG2	1:D:219:ASN:HB2	1.70	0.72
1:D:140:ASP:HB3	1:D:143:SER:O	1.90	0.72
1:B:83:PRO:HG2	1:B:219:ASN:HB2	1.71	0.71
1:A:77:ARG:O	1:A:79:PRO:HD3	1.91	0.69
1:B:82:ARG:HD2	3:B:501:NAG:O6	1.91	0.69
1:C:121:VAL:HG21	1:C:164:ILE:HD13	1.75	0.68
1:C:132:PRO:HG3	1:C:149:THR:HG21	1.76	0.68
1:D:90:VAL:HG21	1:D:109:ILE:HD13	1.78	0.66
1:A:43:TRP:CZ3	1:A:213:PRO:HA	2.32	0.64
1:A:140:ASP:HB3	1:A:143:SER:O	1.97	0.64
1:A:65:VAL:HG13	1:A:168:ALA:HB1	1.79	0.64
1:C:21:ARG:HD3	7:C:543:HOH:O	1.97	0.63
1:C:16:GLN:HA	1:C:16:GLN:HE21	1.64	0.63
1:B:70:THR:HG22	1:B:164:ILE:HB	1.80	0.63
1:D:82:ARG:HB2	2:D:503:NAG:O6	1.99	0.63
1:B:145:ILE:HG23	1:C:196:GLN:HE22	1.65	0.62
1:D:48:ARG:HD2	1:D:100:THR:HA	1.80	0.62
1:A:83:PRO:HG2	1:A:219:ASN:HB2	1.81	0.61
1:C:143:SER:OG	1:C:145:ILE:HG22	2.00	0.61
1:C:77:ARG:O	1:C:79:PRO:HD3	2.01	0.60
1:B:124:ASP:O	1:B:135:PRO:HA	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASP:HB3	1:B:143:SER:O	2.01	0.60
1:B:21:ARG:HB3	1:B:46:THR:O	2.02	0.60
1:D:3:ILE:HD13	1:D:55:VAL:HG12	1.86	0.57
1:C:165:LYS:HD2	1:D:187:THR:HG23	1.85	0.57
1:A:6:ASN:HD21	1:A:8:ASN:ND2	2.02	0.57
1:D:64:ASN:HB3	1:D:236:PRO:HG2	1.86	0.57
1:B:43:TRP:CZ3	1:B:213:PRO:HA	2.39	0.57
1:B:82:ARG:HG3	3:B:501:NAG:O5	2.05	0.56
1:C:124:ASP:O	1:C:135:PRO:HA	2.05	0.56
1:C:43:TRP:CE3	1:C:218:ARG:HA	2.40	0.56
1:A:83:PRO:HG3	2:A:501:NAG:C7	2.35	0.56
1:B:33:LEU:HD11	1:B:226:ILE:HD12	1.87	0.56
1:D:10:PHE:HE2	1:D:226:ILE:O	1.88	0.56
1:D:95:PRO:HD3	1:D:117:PRO:O	2.05	0.56
1:B:36:VAL:HA	1:B:41:PRO:HA	1.86	0.56
1:D:203:ASN:HA	7:D:617:HOH:O	2.06	0.56
1:C:98:THR:HB	1:C:116:TYR:CE2	2.40	0.56
1:C:96:PRO:HA	1:C:203:ASN:OD1	2.06	0.55
1:C:82:ARG:CB	1:C:83:PRO:HD3	2.36	0.55
1:A:82:ARG:HB2	1:A:83:PRO:HD3	1.89	0.55
1:A:84:HIS:O	1:A:84:HIS:HD2	1.89	0.55
1:A:5:PHE:CZ	1:A:231:PHE:HB3	2.42	0.55
1:A:198:LEU:HD13	1:A:202:VAL:HG11	1.90	0.54
1:D:77:ARG:O	1:D:79:PRO:HD3	2.08	0.54
1:D:84:HIS:O	1:D:220:ALA:HA	2.08	0.53
1:B:84:HIS:O	1:B:220:ALA:HA	2.07	0.53
1:B:145:ILE:HD11	1:C:195:LYS:HG2	1.90	0.53
1:C:50:LEU:HD11	1:C:92:PHE:CZ	2.43	0.53
1:D:193:ASP:O	1:D:197:VAL:HG22	2.08	0.52
1:A:33:LEU:HD11	1:A:226:ILE:HD12	1.90	0.52
1:A:84:HIS:CD2	1:A:84:HIS:O	2.62	0.52
1:A:175:VAL:HG22	1:A:188:ILE:HG22	1.92	0.52
1:B:145:ILE:HG23	1:C:196:GLN:NE2	2.25	0.52
1:B:82:ARG:CB	1:B:83:PRO:HD3	2.40	0.52
1:C:203:ASN:HA	7:C:518:HOH:O	2.09	0.51
1:D:90:VAL:HG12	1:D:122:GLU:HA	1.91	0.51
1:A:113:LEU:HD23	1:A:113:LEU:H	1.75	0.51
1:D:121:VAL:HG21	1:D:164:ILE:HD13	1.92	0.51
1:B:90:VAL:HG21	1:B:109:ILE:HD13	1.93	0.51
1:A:203:ASN:HA	7:A:617:HOH:O	2.09	0.51
1:A:124:ASP:O	1:A:135:PRO:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PHE:HA	1:B:198:LEU:HD21	1.92	0.50
1:B:82:ARG:HB2	1:B:83:PRO:CD	2.41	0.50
1:D:73:SER:HA	1:D:160:ALA:O	2.11	0.50
1:B:121:VAL:HG21	1:B:164:ILE:HD13	1.94	0.50
1:A:185:ILE:HD12	7:B:696:HOH:O	2.10	0.50
1:C:145:ILE:HG23	1:C:145:ILE:O	2.11	0.50
1:C:4:SER:HA	1:C:231:PHE:O	2.12	0.50
1:C:76:ILE:HD11	1:C:89:LEU:HD23	1.93	0.50
1:C:83:PRO:HG2	1:C:219:ASN:HB2	1.94	0.49
1:B:11:HIS:O	1:B:14:GLU:HG2	2.12	0.49
1:C:19:LEU:HD21	1:C:25:ILE:HG13	1.95	0.49
1:C:33:LEU:HD11	1:C:226:ILE:HD11	1.95	0.49
1:C:90:VAL:HG21	1:C:109:ILE:HD13	1.94	0.49
1:D:83:PRO:HG2	1:D:219:ASN:CB	2.42	0.48
1:C:50:LEU:HD11	1:C:92:PHE:HZ	1.77	0.48
1:A:175:VAL:HG22	1:A:188:ILE:CG2	2.43	0.48
1:B:50:LEU:N	1:B:50:LEU:HD22	2.28	0.48
1:C:95:PRO:HD3	1:C:117:PRO:O	2.14	0.48
1:C:165:LYS:HE2	7:C:565:HOH:O	2.14	0.48
1:B:197:VAL:HG23	1:B:198:LEU:N	2.28	0.48
1:D:155:ASP:OD2	1:D:158:GLY:HA3	2.13	0.48
1:B:50:LEU:HD11	1:B:92:PHE:CZ	2.48	0.48
1:B:50:LEU:HD11	1:B:92:PHE:HZ	1.79	0.48
1:B:9:GLN:HG3	7:B:733:HOH:O	2.13	0.48
1:A:132:PRO:HG3	1:A:149:THR:HG21	1.96	0.47
1:D:4:SER:HA	1:D:231:PHE:O	2.14	0.47
1:D:43:TRP:CZ3	1:D:213:PRO:HA	2.48	0.47
1:C:84:HIS:CD2	1:C:84:HIS:O	2.68	0.47
1:D:160:ALA:HB2	1:D:179:PHE:CE1	2.49	0.47
1:B:213:PRO:HB3	2:B:601:NAG:H82	1.97	0.47
1:D:79:PRO:O	1:D:81:PRO:HD3	2.14	0.47
1:C:6:ASN:HD21	1:C:8:ASN:HD21	1.63	0.47
1:A:83:PRO:HG2	1:A:219:ASN:CB	2.45	0.47
1:C:6:ASN:HD21	1:C:8:ASN:ND2	2.12	0.47
1:B:203:ASN:HA	7:B:621:HOH:O	2.14	0.47
1:A:26:SER:OG	1:A:30:VAL:HG13	2.15	0.47
1:C:36:VAL:HA	1:C:41:PRO:HA	1.95	0.47
1:A:179:PHE:HB2	1:A:184:THR:OG1	2.14	0.47
1:D:102:GLU:O	1:D:108:GLY:N	2.49	0.46
1:C:90:VAL:HG12	1:C:122:GLU:CB	2.46	0.46
1:B:149:THR:HB	7:B:705:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:O	1:A:145:ILE:HG23	2.15	0.46
1:B:95:PRO:HD3	1:B:117:PRO:O	2.15	0.46
1:A:110:TYR:CE2	1:A:112:PRO:HG3	2.51	0.46
1:D:1:LYS:N	1:D:235:LEU:O	2.45	0.46
1:C:134:ILE:HB	1:C:135:PRO:HA	1.97	0.45
1:A:149:THR:HB	7:A:659:HOH:O	2.16	0.45
1:A:70:THR:HG22	1:A:164:ILE:HB	1.97	0.45
1:D:177:LEU:HB3	1:D:186:TYR:HB2	1.98	0.45
1:B:206:PHE:HE1	1:B:229:TRP:CE3	2.34	0.45
1:D:94:ALA:HB1	1:D:95:PRO:CD	2.46	0.45
1:C:48:ARG:HG2	1:C:207:SER:OG	2.17	0.45
2:B:602:FUC:H5	2:B:603:NAG:C1	2.46	0.45
1:A:5:PHE:CE1	1:A:231:PHE:HB3	2.52	0.45
1:A:95:PRO:HD3	1:A:117:PRO:O	2.16	0.44
1:A:160:ALA:HB2	1:A:179:PHE:CE1	2.52	0.44
1:D:172:ILE:HD12	7:D:611:HOH:O	2.17	0.44
1:B:136:HIS:HA	1:B:151:PRO:HA	1.99	0.44
1:B:173:LEU:O	1:B:189:ALA:HA	2.17	0.44
1:A:21:ARG:HG3	1:A:100:THR:HG21	1.99	0.44
1:A:36:VAL:HG13	1:A:36:VAL:O	2.17	0.44
1:C:3:ILE:HD13	1:C:55:VAL:HG12	1.99	0.44
1:C:144:VAL:HG13	7:C:504:HOH:O	2.17	0.44
1:B:96:PRO:HD3	1:B:201:SER:O	2.17	0.44
1:D:175:VAL:HG22	1:D:188:ILE:CG2	2.42	0.44
1:C:125:THR:O	1:C:134:ILE:HD13	2.18	0.44
1:D:96:PRO:HD3	1:D:201:SER:O	2.18	0.44
1:C:5:PHE:CZ	1:C:231:PHE:HB3	2.53	0.44
2:C:501:NAG:H61	2:C:503:NAG:C1	2.47	0.44
1:D:102:GLU:O	1:D:108:GLY:HA2	2.17	0.43
1:B:132:PRO:HG3	1:B:149:THR:HG21	1.99	0.43
1:B:134:ILE:HB	1:B:135:PRO:HA	1.99	0.43
1:C:160:ALA:HB2	1:C:179:PHE:CE1	2.52	0.43
1:A:191:ILE:HG13	1:B:172:ILE:HD11	2.00	0.43
1:A:33:LEU:O	1:A:47:GLY:HA3	2.18	0.43
1:B:58:TRP:HZ3	1:B:60:SER:HA	1.82	0.43
1:C:140:ASP:HB3	1:C:143:SER:O	2.19	0.43
1:C:176:VAL:HG11	1:D:176:VAL:HG11	2.01	0.43
1:A:64:ASN:O	1:A:235:LEU:HD21	2.19	0.43
1:B:134:ILE:HG22	1:B:136:HIS:CE1	2.54	0.43
1:D:124:ASP:O	1:D:135:PRO:HA	2.19	0.43
1:D:20:GLN:HB2	1:D:48:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:HIS:O	1:C:220:ALA:HA	2.19	0.42
1:B:172:ILE:HD12	7:B:614:HOH:O	2.19	0.42
1:A:197:VAL:HG23	1:A:198:LEU:HG	2.01	0.42
1:D:84:HIS:CD2	1:D:84:HIS:O	2.72	0.42
1:D:174:HIS:CD2	1:D:174:HIS:N	2.88	0.42
1:C:43:TRP:C	1:C:43:TRP:CD1	2.91	0.42
1:B:20:GLN:OE1	1:B:48:ARG:HD3	2.18	0.42
1:A:102:GLU:O	1:A:106:TYR:HB2	2.19	0.42
1:D:178:VAL:HA	1:D:184:THR:O	2.19	0.42
1:B:48:ARG:HD2	1:B:100:THR:HA	2.01	0.42
1:C:227:LEU:HD22	1:C:227:LEU:N	2.35	0.42
1:B:155:ASP:OD2	1:B:158:GLY:HA3	2.20	0.42
1:A:155:ASP:HB2	1:A:182:LEU:HD12	2.02	0.42
1:C:235:LEU:HA	1:C:235:LEU:HD23	1.86	0.42
1:B:137:ILE:HB	1:B:150:VAL:HG12	2.02	0.42
1:C:20:GLN:OE1	1:C:48:ARG:NH1	2.51	0.42
1:A:113:LEU:CD2	1:A:113:LEU:H	2.32	0.42
1:D:22:ASP:O	1:D:24:ARG:HD2	2.20	0.42
1:B:145:ILE:CD1	1:C:195:LYS:HG2	2.50	0.42
1:B:26:SER:OG	1:B:30:VAL:HG13	2.19	0.42
1:C:10:PHE:CD1	1:C:10:PHE:N	2.88	0.41
1:C:83:PRO:CG	1:C:219:ASN:HB2	2.50	0.41
1:A:73:SER:HA	1:A:160:ALA:O	2.21	0.41
1:A:106:TYR:HA	1:A:144:VAL:HG21	2.03	0.41
1:A:55:VAL:HG22	1:A:202:VAL:HG23	2.03	0.41
1:A:114:SER:N	1:A:115:PRO:HD3	2.36	0.41
1:D:10:PHE:CE2	1:D:226:ILE:O	2.72	0.41
1:A:12:GLN:HE21	1:A:12:GLN:HB2	1.70	0.41
1:B:179:PHE:HA	1:B:180:PRO:HD2	1.91	0.41
1:C:191:ILE:HD12	1:D:170:THR:HB	2.03	0.40
1:B:213:PRO:C	1:B:215:GLY:H	2.25	0.40
1:C:65:VAL:HG13	1:C:168:ALA:HB1	2.02	0.40
1:C:172:ILE:HD11	1:D:191:ILE:HG13	2.02	0.40
1:C:86:ALA:HA	1:C:87:ASP:HA	1.82	0.40
1:A:33:LEU:HD11	1:A:226:ILE:CD1	2.50	0.40
1:B:37:VAL:N	1:B:40:VAL:O	2.55	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	235/241 (98%)	214 (91%)	19 (8%)	2 (1%)	21	37
1	B	235/241 (98%)	216 (92%)	17 (7%)	2 (1%)	21	37
1	C	235/241 (98%)	216 (92%)	16 (7%)	3 (1%)	15	26
1	D	235/241 (98%)	217 (92%)	16 (7%)	2 (1%)	21	37
All	All	940/964 (98%)	863 (92%)	68 (7%)	9 (1%)	19	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	PRO
1	C	82	ARG
1	A	83	PRO
1	C	83	PRO
1	C	216	LYS
1	A	214	SER
1	D	83	PRO
1	B	214	SER
1	D	84	HIS

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	202/210 (96%)	186 (92%)	16 (8%)	15	28
1	B	199/210 (95%)	180 (90%)	19 (10%)	11	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	200/210 (95%)	184 (92%)	16 (8%)	15	28
1	D	199/210 (95%)	180 (90%)	19 (10%)	11	20
All	All	800/840 (95%)	730 (91%)	70 (9%)	12	23

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	19	LEU
1	A	28	ASN
1	A	30	VAL
1	A	43	TRP
1	A	50	LEU
1	A	55	VAL
1	A	67	SER
1	A	102	GLU
1	A	133	GLN
1	A	144	VAL
1	A	174	HIS
1	A	188	ILE
1	A	196	GLN
1	A	227	LEU
1	A	235	LEU
1	B	9	GLN
1	B	12	GLN
1	B	19	LEU
1	B	30	VAL
1	B	42	THR
1	B	43	TRP
1	B	50	LEU
1	B	82	ARG
1	B	87	ASP
1	B	99	GLN
1	B	102	GLU
1	B	145	ILE
1	B	149	THR
1	B	174	HIS
1	B	196	GLN
1	B	218	ARG
1	B	227	LEU
1	B	234	SER

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Mol	Chain	Res	Type
1	B	235	LEU
1	C	9	GLN
1	C	12	GLN
1	C	18	LYS
1	C	19	LEU
1	C	24	ARG
1	C	30	VAL
1	C	42	THR
1	C	43	TRP
1	C	77	ARG
1	C	99	GLN
1	C	102	GLU
1	C	116	TYR
1	C	131	ASP
1	C	149	THR
1	C	196	GLN
1	C	235	LEU
1	D	6	ASN
1	D	9	GLN
1	D	12	GLN
1	D	15	GLU
1	D	18	LYS
1	D	19	LEU
1	D	24	ARG
1	D	28	ASN
1	D	30	VAL
1	D	42	THR
1	D	43	TRP
1	D	82	ARG
1	D	102	GLU
1	D	145	ILE
1	D	149	THR
1	D	174	HIS
1	D	175	VAL
1	D	196	GLN
1	D	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	GLN

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Mol	Chain	Res	Type
1	A	38	ASN
1	A	64	ASN
1	A	97	ASN
1	A	196	GLN
1	A	203	ASN
1	A	217	GLN
1	B	9	GLN
1	B	12	GLN
1	B	38	ASN
1	B	64	ASN
1	B	78	GLN
1	B	97	ASN
1	B	99	GLN
1	B	217	GLN
1	C	8	ASN
1	C	16	GLN
1	C	38	ASN
1	C	78	GLN
1	C	97	ASN
1	C	196	GLN
1	D	8	ASN
1	D	12	GLN
1	D	16	GLN
1	D	38	ASN
1	D	64	ASN
1	D	196	GLN
1	D	217	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 ⓘ

19 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
2	NAG	A	501	1,2	14,14,15	1.18	2 (14%)	15,19,21	1.39	2 (13%)
2	FUC	A	502	2	10,10,11	1.31	2 (20%)	14,14,16	1.09	1 (7%)
2	NAG	A	503	2	14,14,15	1.12	1 (7%)	15,19,21	2.15	1 (6%)
3	NAG	A	601	1,3	14,14,15	1.10	1 (7%)	15,19,21	2.15	3 (20%)
3	NAG	A	603	3	14,14,15	1.71	4 (28%)	15,19,21	1.72	3 (20%)
3	NAG	B	501	1,3	14,14,15	1.01	1 (7%)	15,19,21	1.59	4 (26%)
3	NAG	B	503	3	14,14,15	0.77	0	15,19,21	1.64	4 (26%)
2	NAG	B	601	1,2	14,14,15	1.11	1 (7%)	15,19,21	2.31	3 (20%)
2	FUC	B	602	2	10,10,11	1.42	1 (10%)	14,14,16	1.80	4 (28%)
2	NAG	B	603	2	14,14,15	1.19	2 (14%)	15,19,21	1.99	2 (13%)
2	NAG	C	501	1,2	14,14,15	1.12	2 (14%)	15,19,21	1.74	5 (33%)
2	FUC	C	502	2	10,10,11	1.64	2 (20%)	14,14,16	1.72	5 (35%)
2	NAG	C	503	2	14,14,15	0.79	0	15,19,21	1.59	4 (26%)
2	NAG	D	501	1,2	14,14,15	0.59	0	15,19,21	1.40	3 (20%)
2	FUC	D	502	2	10,10,11	0.81	0	14,14,16	2.22	5 (35%)
2	NAG	D	503	2	14,14,15	0.73	0	15,19,21	1.21	2 (13%)
2	NAG	D	601	1,2	14,14,15	1.57	2 (14%)	15,19,21	2.33	5 (33%)
2	FUC	D	602	2	10,10,11	1.50	2 (20%)	14,14,16	1.72	4 (28%)
2	NAG	D	603	2	14,14,15	0.89	0	15,19,21	1.22	2 (13%)

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	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	502	2	1/1/4/5	0/0/17/20	0/1/1/1
2	NAG	A	503	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	603	3	-	0/6/23/26	0/1/1/1
3	NAG	B	501	1,3	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	503	3	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	601	1,2	-	0/6/23/26	0/1/1/1
2	FUC	B	602	2	1/1/4/5	0/0/17/20	0/1/1/1
2	NAG	B	603	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	501	1,2	-	0/6/23/26	0/1/1/1
2	FUC	C	502	2	1/1/4/5	0/0/17/20	0/1/1/1
2	NAG	C	503	2	-	0/6/23/26	0/1/1/1
2	NAG	D	501	1,2	-	0/6/23/26	0/1/1/1
2	FUC	D	502	2	1/1/4/5	0/0/17/20	0/1/1/1
2	NAG	D	503	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	601	1,2	-	0/6/23/26	0/1/1/1
2	FUC	D	602	2	-	0/0/17/20	0/1/1/1
2	NAG	D	603	2	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAG	C1-C2	-2.71	1.48	1.52
2	A	501	NAG	O5-C1	-2.70	1.39	1.43
2	C	501	NAG	C1-C2	-2.51	1.49	1.52
2	B	601	NAG	O3-C3	-2.20	1.37	1.43
2	B	602	FUC	C1-C2	-2.14	1.47	1.52
2	C	501	NAG	C2-N2	-2.11	1.42	1.46
2	A	503	NAG	C4-C5	2.13	1.57	1.53
3	A	603	NAG	O5-C1	2.14	1.47	1.43
3	B	501	NAG	C1-C2	2.16	1.55	1.52
2	B	603	NAG	C6-C5	2.22	1.59	1.51
2	B	603	NAG	C4-C5	2.33	1.58	1.53
2	D	602	FUC	C6-C5	2.43	1.57	1.51
2	A	502	FUC	C4-C3	2.54	1.59	1.52
3	A	603	NAG	O5-C5	2.66	1.49	1.43
2	D	601	NAG	C1-C2	2.67	1.56	1.52
2	A	502	FUC	C2-C3	2.80	1.56	1.52
2	D	601	NAG	C4-C5	2.82	1.59	1.53
2	C	502	FUC	C4-C5	2.98	1.59	1.52
2	D	602	FUC	C4-C5	3.00	1.59	1.52
3	A	603	NAG	C1-C2	3.11	1.56	1.52
2	C	502	FUC	C2-C3	3.17	1.56	1.52
3	A	601	NAG	C1-C2	3.34	1.57	1.52
3	A	603	NAG	C4-C5	3.34	1.60	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	FUC	O5-C1-C2	-4.36	103.79	110.86
2	B	601	NAG	C3-C4-C5	-4.06	103.13	110.20
2	B	602	FUC	C1-C2-C3	-3.92	104.91	109.54
2	D	601	NAG	C4-C3-C2	-3.80	105.33	111.23
3	A	601	NAG	C4-C3-C2	-3.78	105.35	111.23
2	C	503	NAG	C3-C4-C5	-3.61	103.91	110.20
2	D	601	NAG	C3-C4-C5	-3.14	104.72	110.20
2	B	603	NAG	C3-C2-N2	-3.14	103.05	110.56
2	D	602	FUC	C1-C2-C3	-3.12	105.85	109.54
2	D	602	FUC	O5-C1-C2	-2.73	106.43	110.86
3	B	501	NAG	C4-C3-C2	-2.71	107.02	111.23
3	A	603	NAG	C4-C3-C2	-2.63	107.14	111.23
2	C	502	FUC	O5-C1-C2	-2.62	106.61	110.86
2	C	502	FUC	C2-C3-C4	-2.62	106.60	111.04
2	C	501	NAG	C3-C2-N2	-2.53	104.50	110.56
2	D	502	FUC	O3-C3-C2	-2.50	105.48	110.00
2	C	501	NAG	O4-C4-C3	-2.35	105.04	110.34
2	C	501	NAG	C2-N2-C7	-2.30	120.08	123.04
3	B	503	NAG	C3-C4-C5	-2.24	106.29	110.20
2	B	602	FUC	O3-C3-C2	-2.19	106.03	110.00
2	D	603	NAG	C3-C2-N2	-2.18	105.34	110.56
3	B	503	NAG	C2-N2-C7	-2.15	120.28	123.04
3	B	503	NAG	O7-C7-C8	-2.08	118.25	122.06
2	C	503	NAG	O7-C7-C8	-2.04	118.31	122.06
2	C	501	NAG	C4-C3-C2	-2.03	108.07	111.23
2	D	501	NAG	O3-C3-C2	2.05	113.18	109.11
2	C	503	NAG	O4-C4-C5	2.06	114.69	109.24
3	A	603	NAG	O3-C3-C2	2.08	113.22	109.11
2	D	503	NAG	O5-C5-C6	2.12	111.93	107.35
2	D	503	NAG	C6-C5-C4	2.13	118.28	113.02
2	B	601	NAG	O4-C4-C5	2.15	114.93	109.24
2	D	501	NAG	C3-C4-C5	2.15	113.94	110.20
2	A	502	FUC	O4-C4-C3	2.17	115.21	110.34
3	B	501	NAG	O3-C3-C2	2.19	113.46	109.11
3	A	601	NAG	O3-C3-C2	2.21	113.48	109.11
2	D	603	NAG	C2-N2-C7	2.29	125.98	123.04
2	C	502	FUC	O2-C2-C1	2.33	113.89	109.21
2	C	502	FUC	C1-C2-C3	2.34	112.31	109.54
3	B	501	NAG	C3-C4-C5	2.35	114.29	110.20
2	A	501	NAG	O3-C3-C2	2.35	113.77	109.11
2	C	502	FUC	O5-C5-C4	2.50	113.87	109.53
2	D	601	NAG	O4-C4-C5	2.56	116.02	109.24
2	B	602	FUC	C1-O5-C5	2.59	116.37	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	FUC	O2-C2-C1	2.63	114.47	109.21
2	C	503	NAG	C6-C5-C4	2.74	119.78	113.02
2	D	502	FUC	C1-O5-C5	2.80	116.71	112.38
2	B	602	FUC	C6-C5-C4	2.87	118.73	113.08
3	B	501	NAG	C6-C5-C4	2.91	120.19	113.02
2	D	602	FUC	C1-O5-C5	2.97	116.96	112.38
2	D	501	NAG	C1-O5-C5	3.12	116.21	112.25
2	D	502	FUC	C6-C5-C4	3.28	119.54	113.08
2	C	501	NAG	C1-O5-C5	3.48	116.67	112.25
3	B	503	NAG	C1-O5-C5	3.59	116.81	112.25
2	D	601	NAG	O3-C3-C2	3.62	116.28	109.11
2	D	502	FUC	O2-C2-C1	3.93	117.08	109.21
2	A	501	NAG	C1-O5-C5	3.96	117.27	112.25
2	D	601	NAG	C6-C5-C4	4.64	124.47	113.02
3	A	603	NAG	C1-O5-C5	4.86	118.42	112.25
2	B	603	NAG	C1-O5-C5	6.28	120.22	112.25
3	A	601	NAG	C1-O5-C5	6.55	120.56	112.25
2	B	601	NAG	C1-O5-C5	6.59	120.62	112.25
2	A	503	NAG	C1-O5-C5	7.66	121.97	112.25

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	602	FUC	C1
2	D	502	FUC	C1
2	C	502	FUC	C1
3	B	501	NAG	C1
2	B	603	NAG	C1
3	B	503	NAG	C1
2	D	503	NAG	C1
2	A	503	NAG	C1
2	A	502	FUC	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAG	1	0
3	B	501	NAG	3	0
2	B	601	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	FUC	1	0
2	B	603	NAG	1	0
2	C	501	NAG	1	0
2	C	503	NAG	1	0
2	D	503	NAG	1	0

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 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
4	AMG	A	400	-	13,13,13	0.66	0	18,18,18	1.03	0
4	AMG	B	400	-	13,13,13	1.32	1 (7%)	18,18,18	1.56	4 (22%)
4	AMG	C	400	-	13,13,13	1.37	3 (23%)	18,18,18	1.99	7 (38%)
4	AMG	D	400	-	13,13,13	0.67	0	18,18,18	1.32	2 (11%)

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	AMG	A	400	-	-	0/4/24/24	0/1/1/1
4	AMG	B	400	-	-	0/4/24/24	0/1/1/1
4	AMG	C	400	-	-	0/4/24/24	0/1/1/1
4	AMG	D	400	-	-	0/4/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	400	AMG	O4-C4	-2.17	1.37	1.43
4	C	400	AMG	O5-C1	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	400	AMG	O1-C1	2.54	1.44	1.40
4	B	400	AMG	O1-C1	3.68	1.46	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	400	AMG	O4-C4-C3	-2.91	103.79	110.34
4	C	400	AMG	O3-C3-C2	-2.43	104.86	110.34
4	B	400	AMG	O1-C1-C2	-2.40	105.39	108.21
4	C	400	AMG	O2-C2-C3	-2.30	105.16	110.34
4	C	400	AMG	O4-C4-C5	-2.29	103.17	109.24
4	C	400	AMG	O3-C3-C4	2.22	115.33	110.34
4	B	400	AMG	C6-C5-C4	2.27	118.62	113.02
4	B	400	AMG	O5-C1-O1	2.34	116.52	110.88
4	C	400	AMG	O1-C1-C2	2.54	111.20	108.21
4	C	400	AMG	C3-C4-C5	2.95	115.35	110.20
4	D	400	AMG	C1-O5-C5	3.06	119.68	113.75
4	D	400	AMG	C7-O1-C1	3.17	118.48	113.29
4	C	400	AMG	C7-O1-C1	4.28	120.30	113.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	237/241 (98%)	-0.86	0	100 100	3, 14, 43, 62	0
1	B	237/241 (98%)	-0.87	0	100 100	2, 13, 42, 60	0
1	C	237/241 (98%)	-0.78	1 (0%)	93 93	3, 17, 51, 61	0
1	D	237/241 (98%)	-0.72	3 (1%)	79 82	3, 20, 52, 76	0
All	All	948/964 (98%)	-0.81	4 (0%)	93 93	2, 16, 47, 76	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	3.4
1	C	216	LYS	2.7
1	D	13	ASN	2.7
1	D	82	ARG	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	D	501	14/15	0.86	0.20	0.33	48,56,61,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	501	14/15	0.87	0.16	0.25	40,49,59,61	0
2	NAG	C	501	14/15	0.89	0.18	0.23	32,37,44,47	0
2	NAG	A	501	14/15	0.92	0.15	0.12	38,43,48,51	0
2	FUC	C	502	10/11	0.55	0.55	-	58,63,70,70	0
2	FUC	D	502	10/11	0.76	0.23	-	58,62,66,67	0
2	NAG	D	601	14/15	0.89	0.20	-	36,47,50,50	0
2	FUC	B	602	10/11	0.92	0.19	-	49,53,55,56	0
2	NAG	B	601	14/15	0.86	0.21	-	43,52,60,60	0
2	NAG	B	603	14/15	0.82	0.22	-	57,62,69,70	0
3	NAG	A	601	14/15	0.91	0.14	-	35,46,56,59	0
3	NAG	B	503	14/15	0.85	0.24	-	61,64,68,72	0
2	FUC	D	602	10/11	0.69	0.46	-	55,60,62,66	0
2	NAG	C	503	14/15	0.88	0.18	-	47,50,56,59	0
2	NAG	D	503	14/15	0.84	0.24	-	51,56,59,63	0
2	NAG	A	503	14/15	0.85	0.21	-	49,53,59,63	0
3	NAG	A	603	14/15	0.73	0.43	-	76,81,89,89	0
2	NAG	D	603	14/15	0.74	0.43	-	76,80,90,90	0
2	FUC	A	502	10/11	0.87	0.18	-	45,53,57,63	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	CA	B	303	1/1	0.98	0.20	5.45	28,28,28,28	0
4	AMG	A	400	13/13	0.96	0.12	0.43	27,32,39,40	0
5	MN	D	300	1/1	0.95	0.09	-0.34	34,34,34,34	0
4	AMG	C	400	13/13	0.95	0.10	-0.42	23,25,29,29	0
4	AMG	D	400	13/13	0.97	0.09	-0.55	8,20,28,30	0
4	AMG	B	400	13/13	0.97	0.07	-0.80	10,18,25,25	0
5	MN	A	300	1/1	0.92	0.07	-1.29	32,32,32,32	0
6	CA	D	303	1/1	0.99	0.08	-1.41	28,28,28,28	0
6	CA	C	303	1/1	0.98	0.04	-2.11	22,22,22,22	0
5	MN	C	300	1/1	0.96	0.04	-2.23	29,29,29,29	0
6	CA	A	303	1/1	0.99	0.03	-2.86	13,13,13,13	0
5	MN	B	300	1/1	0.99	0.03	-3.02	13,13,13,13	0

6.5 Other polymers

There are no such residues in this entry.