Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:46 PM GMT

PDB ID	:	1CF5
Title	:	BETA-MOMORCHARIN STRUCTURE AT 2.55 A
Authors	:	Yuan, Y.-R.; He, Y.-N.; Xiong, J.-P.; Xia, Z.-X.
Deposited on	:	1999-03-24
Resolution	:	2.55 Å(reported)

The following versions of software and data (see references (i)) 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
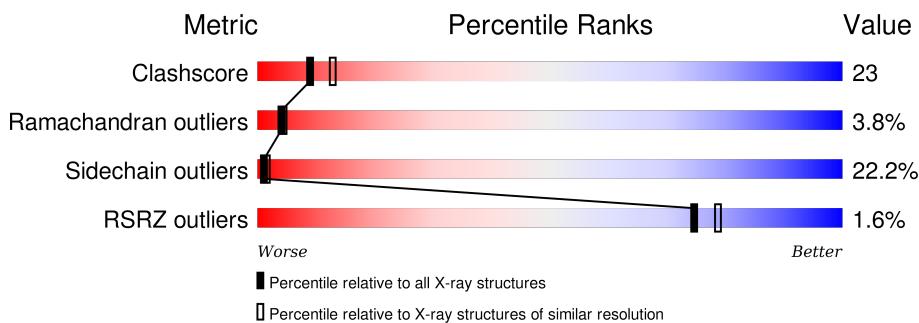
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
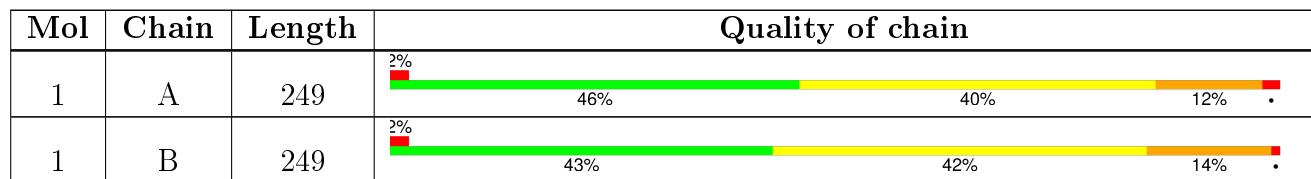
The reported resolution of this entry is 2.55 Å.

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	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		3.8%
Sidechain outliers		22.2%
RSRZ outliers		1.6%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 <=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	249	2% / 46% / 40% / 12% ·
1	B	249	2% / 43% / 42% / 14% ·

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	901	X	-	-	-
2	XYP	A	906	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	B	901	X	-	-	-
2	NAG	B	902	-	-	-	X
2	XYP	B	906	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4188 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 PROTEIN (BETA-MOMORCHARIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total 1991	C 1282	N 333	O 376	0	0	0
1	B	249	Total 1991	C 1282	N 333	O 376	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ASN	ASP	CONFLICT	UNP P29339
A	219	GLN	GLU	CONFLICT	UNP P29339

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total 69	C 39	N 2	O 28	0	0
2	B	6	Total 69	C 39	N 2	O 28	0	0
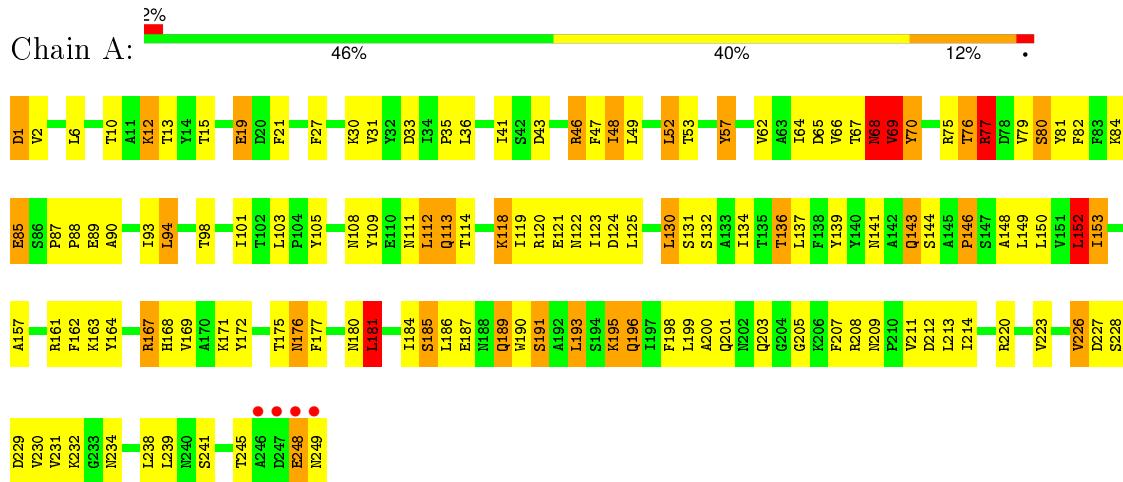
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total 31	O 31	0	0
3	B	37	Total 37	O 37	0	0
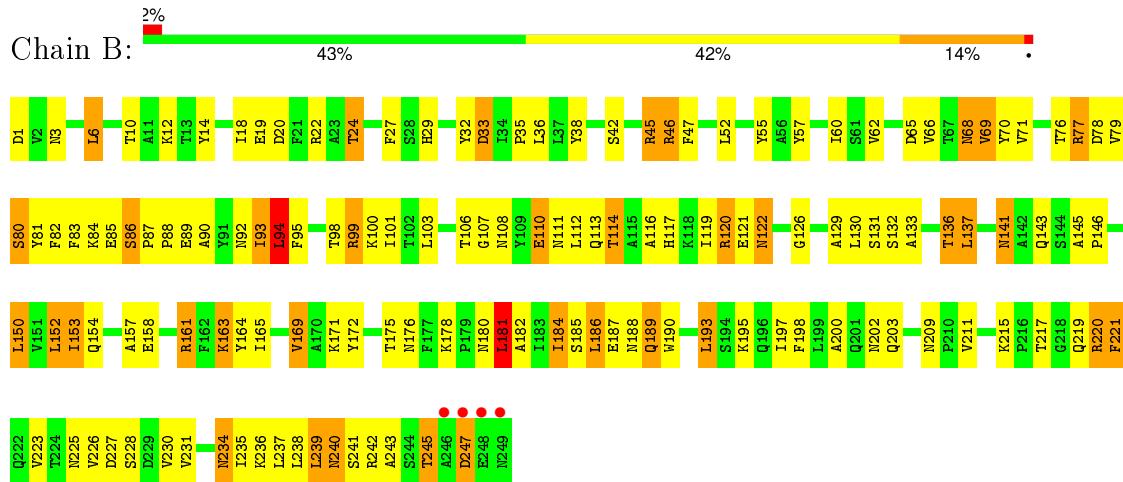
3 Residue-property plots ⓘ

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: PROTEIN (BETA-MOMORCHARIN)

- Molecule 1: PROTEIN (BETA-MOMORCHARIN)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.09Å 50.58Å 61.12Å 72.98° 78.39° 76.97°	Depositor
Resolution (Å)	10.00 – 2.55 32.81 – 2.43	Depositor EDS
% Data completeness (in resolution range)	79.3 (10.00-2.55) 75.0 (32.81-2.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.82 (at 2.42Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.172 , 0.278 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 94.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Outliers	0 of 16241 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4188	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: XYP, MAN, BMA, NAG, 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	0.61	0/2034	0.77	2/2767 (0.1%)
1	B	0.61	0/2034	0.78	2/2767 (0.1%)
All	All	0.61	0/4068	0.77	4/5534 (0.1%)

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
1	A	0	7
1	B	0	10
2	A	4	0
2	B	4	0
All	All	8	17

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	152	LEU	CA-CB-CG	6.64	130.58	115.30
1	A	152	LEU	CA-CB-CG	6.40	130.01	115.30
1	A	181	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	181	LEU	CA-CB-CG	5.93	128.93	115.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	FUC	C2,C3,C1,C4
2	B	901	FUC	C2,C3,C1,C4

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	139	TYR	Sidechain
1	A	168	HIS	Sidechain
1	A	176	ASN	Mainchain
1	A	198	PHE	Sidechain
1	A	70	TYR	Sidechain
1	A	77	ARG	Sidechain
1	B	120	ARG	Sidechain
1	B	14	TYR	Sidechain
1	B	161	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	38	TYR	Sidechain
1	B	55	TYR	Sidechain
1	B	70	TYR	Sidechain
1	B	77	ARG	Sidechain
1	B	80	SER	Mainchain
1	B	94	LEU	Mainchain

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	1991	0	2003	96	0
1	B	1991	0	2003	95	0
2	A	69	0	59	1	0
2	B	69	0	59	1	0
3	A	31	0	0	0	0
3	B	37	0	0	1	0
All	All	4188	0	4124	191	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 23.

All (191) 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:226:VAL:HG23	1:B:231:VAL:HG11	1.25	1.17
1:B:189:GLN:HE21	1:B:189:GLN:HA	1.32	0.94
1:A:47:PHE:HD2	1:A:93:ILE:HD11	1.33	0.92
1:A:241:SER:O	1:A:245:THR:HG22	1.73	0.88
1:B:180:ASN:O	1:B:181:LEU:HB2	1.74	0.88
1:B:190:TRP:CZ3	1:B:239:LEU:HG	2.11	0.85
1:A:230:VAL:O	1:A:234:ASN:HB3	1.76	0.85
1:A:196:GLN:HE21	1:A:209:ASN:H	1.28	0.81
1:B:172:TYR:HD2	1:B:175:THR:HG23	1.46	0.79
1:A:48:ILE:HG23	1:A:66:VAL:HG12	1.66	0.75
1:A:47:PHE:CD2	1:A:93:ILE:HD11	2.21	0.75
1:A:172:TYR:HB3	1:A:175:THR:O	1.85	0.75
1:B:132:SER:O	1:B:136:THR:HG23	1.85	0.74
1:A:6:LEU:HG	1:A:131:SER:HB2	1.71	0.73
1:B:231:VAL:HA	1:B:235:ILE:HD12	1.69	0.73
1:B:6:LEU:HD12	1:B:131:SER:HB2	1.70	0.72
1:A:109:TYR:CE1	1:A:153:ILE:HD11	2.26	0.71
1:B:113:GLN:HE22	1:B:120:ARG:HG2	1.55	0.71
1:A:118:LYS:HG2	1:A:123:ILE:HD11	1.73	0.71
1:B:163:LYS:HB2	1:B:236:LYS:HE2	1.72	0.70
1:A:205:GLY:O	1:A:226:VAL:HG12	1.92	0.69
1:A:196:GLN:NE2	1:A:209:ASN:H	1.89	0.69
1:B:80:SER:HB3	1:B:98:THR:HG21	1.74	0.68
1:B:215:LYS:HD2	1:B:219:GLN:HB2	1.74	0.68
1:A:2:VAL:HG11	1:A:21:PHE:HB2	1.76	0.66
1:B:80:SER:HG	1:B:82:PHE:HE1	1.43	0.66
1:A:193:LEU:HD13	1:A:211:VAL:HG11	1.77	0.66
1:A:149:LEU:O	1:A:153:ILE:HG23	1.96	0.66
1:A:48:ILE:HG12	1:A:64:ILE:HB	1.77	0.66
1:B:126:GLY:HA3	1:B:176:ASN:HD22	1.61	0.66
1:A:190:TRP:O	1:A:191:SER:HB2	1.96	0.66
1:A:109:TYR:O	1:A:113:GLN:HB2	1.95	0.65
1:B:242:ARG:O	1:B:245:THR:HG22	1.96	0.65
1:B:20:ASP:O	1:B:24:THR:HG23	1.96	0.65
1:B:165:ILE:O	1:B:169:VAL:HG12	1.97	0.64
1:A:48:ILE:HG23	1:A:66:VAL:CG1	2.26	0.64
1:A:75:ARG:HD2	1:A:98:THR:HG21	1.79	0.64
1:B:3:ASN:HD21	2:B:902:NAG:H2	1.63	0.63
1:A:113:GLN:HG3	1:A:119:ILE:HA	1.79	0.63
1:B:164:TYR:H	1:B:234:ASN:ND2	1.96	0.63
1:A:113:GLN:HG2	1:A:119:ILE:HG22	1.81	0.63
1:B:113:GLN:NE2	1:B:120:ARG:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:NE2	1:A:120:ARG:H	1.97	0.63
1:B:80:SER:OG	1:B:82:PHE:HE1	1.81	0.63
1:B:89:GLU:O	1:B:93:ILE:HG23	1.97	0.62
1:B:193:LEU:HD13	1:B:211:VAL:HG11	1.81	0.62
1:B:230:VAL:HG23	1:B:231:VAL:H	1.63	0.62
1:A:132:SER:O	1:A:136:THR:HG23	2.00	0.62
1:A:164:TYR:H	1:A:234:ASN:ND2	1.97	0.61
1:A:185:SER:O	1:A:189:GLN:HB2	2.00	0.61
1:A:87:PRO:HG2	1:A:90:ALA:HB2	1.82	0.61
1:A:214:ILE:HG13	1:A:220:ARG:HG3	1.83	0.61
1:B:189:GLN:HA	1:B:189:GLN:NE2	2.11	0.61
1:A:65:ASP:HB3	1:A:68:ASN:HD21	1.66	0.60
1:A:162:PHE:CE2	1:A:190:TRP:HB2	2.36	0.60
1:A:6:LEU:HD21	1:A:130:LEU:HD13	1.84	0.60
1:B:87:PRO:HG2	1:B:90:ALA:HB2	1.84	0.60
1:A:181:LEU:HD13	1:A:214:ILE:HG21	1.82	0.60
1:A:90:ALA:O	1:A:94:LEU:HB2	2.03	0.59
1:B:225:ASN:HB3	1:B:227:ASP:H	1.67	0.59
1:A:161:ARG:HG2	1:A:190:TRP:CE2	2.39	0.58
1:B:141:ASN:ND2	1:B:143:GLN:H	2.02	0.57
1:A:119:ILE:HD12	1:A:121:GLU:HB2	1.86	0.57
1:B:164:TYR:H	1:B:234:ASN:HD21	1.50	0.57
1:B:217:THR:OG1	1:B:219:GLN:HG3	2.05	0.57
1:A:46:ARG:HG3	1:A:46:ARG:HH11	1.70	0.57
1:A:113:GLN:HE22	1:A:120:ARG:HD3	1.69	0.57
1:B:95:PHE:O	1:B:98:THR:HG22	2.05	0.57
1:A:27:PHE:HB2	1:A:36:LEU:O	2.04	0.56
1:A:141:ASN:HB3	1:A:144:SER:OG	2.05	0.56
1:A:113:GLN:CG	1:A:119:ILE:HA	2.35	0.56
1:B:113:GLN:HE22	1:B:120:ARG:HH11	1.54	0.56
1:B:157:ALA:O	1:B:161:ARG:HD3	2.05	0.55
1:B:226:VAL:HA	1:B:231:VAL:HG21	1.89	0.55
1:B:10:THR:OG1	1:B:12:LYS:HB3	2.07	0.54
1:B:120:ARG:NH2	1:B:188:ASN:OD1	2.40	0.54
1:A:109:TYR:CZ	1:A:153:ILE:HD11	2.42	0.54
1:B:6:LEU:CD1	1:B:131:SER:HB2	2.39	0.53
1:B:80:SER:CB	1:B:98:THR:HG21	2.38	0.53
1:A:69:VAL:HB	1:A:161:ARG:HH11	1.74	0.53
1:B:18:ILE:O	1:B:22:ARG:HG3	2.09	0.53
1:B:161:ARG:HG2	1:B:190:TRP:NE1	2.23	0.53
1:B:180:ASN:O	1:B:181:LEU:CB	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:HA	1:A:177:PHE:O	2.10	0.52
1:B:36:LEU:HD12	1:B:238:LEU:HB3	1.92	0.52
1:A:84:LYS:O	1:A:85:GLU:HB2	2.10	0.51
1:B:153:ILE:HG13	1:B:153:ILE:O	2.07	0.51
1:B:113:GLN:NE2	1:B:120:ARG:H	2.08	0.51
1:B:90:ALA:HA	1:B:94:LEU:HD22	1.93	0.51
1:A:137:LEU:HD13	1:A:148:ALA:HB1	1.92	0.51
1:A:196:GLN:HE21	1:A:209:ASN:N	2.04	0.51
1:B:146:PRO:HD2	3:B:939:HOH:O	2.11	0.51
1:B:65:ASP:HB3	1:B:68:ASN:ND2	2.26	0.51
1:A:76:THR:CG2	1:A:81:TYR:HE1	2.24	0.51
1:B:240:ASN:ND2	1:B:243:ALA:H	2.08	0.51
1:A:27:PHE:CE2	1:A:30:LYS:HG2	2.46	0.51
1:A:57:TYR:HB3	2:A:903:NAG:H81	1.93	0.51
1:B:230:VAL:HG23	1:B:231:VAL:N	2.27	0.50
1:B:197:ILE:HD13	1:B:231:VAL:HG13	1.94	0.50
1:B:32:TYR:O	1:B:33:ASP:HB2	2.11	0.50
1:A:195:LYS:NZ	1:A:248:GLU:HA	2.26	0.50
1:A:68:ASN:ND2	1:A:70:TYR:H	2.10	0.50
1:A:195:LYS:HE3	1:A:208:ARG:NH2	2.27	0.50
1:A:6:LEU:HD21	1:A:130:LEU:CD1	2.42	0.49
1:B:195:LYS:O	1:B:198:PHE:HB3	2.12	0.49
1:A:10:THR:OG1	1:A:12:LYS:HD3	2.13	0.49
1:A:12:LYS:HG2	1:A:13:THR:N	2.28	0.49
1:B:197:ILE:O	1:B:200:ALA:HB3	2.12	0.48
1:B:221:PHE:CD1	1:B:221:PHE:N	2.79	0.48
1:A:65:ASP:OD1	1:A:67:THR:HB	2.12	0.48
1:A:125:LEU:O	1:A:176:ASN:HB3	2.13	0.48
1:B:171:LYS:HB3	1:B:171:LYS:HE2	1.59	0.48
1:A:52:LEU:HD23	1:A:152:LEU:HD21	1.95	0.48
1:B:193:LEU:CD1	1:B:211:VAL:HG11	2.44	0.48
1:A:130:LEU:O	1:A:134:ILE:HD12	2.13	0.48
1:A:157:ALA:O	1:A:161:ARG:HD3	2.13	0.48
1:B:110:GLU:O	1:B:114:THR:HG23	2.14	0.48
1:B:35:PRO:HG2	1:B:237:LEU:HD23	1.95	0.47
1:B:184:ILE:O	1:B:187:GLU:N	2.48	0.47
1:A:1:ASP:HB3	1:A:49:LEU:O	2.15	0.47
1:B:46:ARG:O	1:B:66:VAL:HG22	2.14	0.47
1:B:141:ASN:HD22	1:B:143:GLN:H	1.63	0.47
1:B:172:TYR:HD2	1:B:175:THR:CG2	2.22	0.46
1:B:83:PHE:O	1:B:86:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:H	1:B:176:ASN:HD21	1.63	0.46
1:B:133:ALA:O	1:B:137:LEU:HB2	2.15	0.46
1:B:137:LEU:HA	1:B:137:LEU:HD12	1.61	0.46
1:A:41:ILE:HG23	1:A:46:ARG:HG2	1.98	0.46
1:B:83:PHE:CE1	1:B:107:GLY:HA2	2.51	0.46
1:B:182:ALA:O	1:B:186:LEU:HB2	2.16	0.46
1:A:15:THR:O	1:A:19:GLU:HB2	2.16	0.45
1:B:172:TYR:CD2	1:B:175:THR:HG23	2.38	0.45
1:B:46:ARG:HB3	1:B:47:PHE:CD2	2.51	0.45
1:A:163:LYS:O	1:A:167:ARG:HG2	2.16	0.45
1:B:172:TYR:HB3	1:B:175:THR:O	2.16	0.45
1:B:65:ASP:HB3	1:B:68:ASN:HD21	1.81	0.45
1:A:196:GLN:OE1	1:A:249:ASN:ND2	2.50	0.45
1:A:31:VAL:HB	1:A:238:LEU:CD2	2.47	0.45
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.32	0.45
1:B:236:LYS:O	1:B:237:LEU:HD23	2.16	0.45
1:B:120:ARG:HG2	1:B:120:ARG:HH11	1.82	0.45
1:A:27:PHE:HE2	1:A:30:LYS:HG2	1.80	0.45
1:A:79:VAL:HG11	1:A:101:ILE:HD12	1.99	0.45
1:A:6:LEU:HG	1:A:131:SER:CB	2.45	0.44
1:A:195:LYS:HZ1	1:A:248:GLU:HA	1.81	0.44
1:A:6:LEU:CG	1:A:131:SER:HB2	2.45	0.44
1:B:161:ARG:HG2	1:B:190:TRP:CE2	2.53	0.44
1:A:195:LYS:O	1:A:199:LEU:HD13	2.18	0.44
1:B:113:GLN:NE2	1:B:120:ARG:CG	2.81	0.44
1:B:113:GLN:HG3	1:B:150:LEU:HD21	2.00	0.44
1:A:161:ARG:HG2	1:A:190:TRP:NE1	2.33	0.44
1:A:199:LEU:O	1:A:201:GLN:N	2.51	0.44
1:B:154:GLN:HA	1:B:158:GLU:HB2	1.99	0.44
1:A:46:ARG:O	1:A:66:VAL:HG13	2.17	0.43
1:A:226:VAL:HA	1:A:231:VAL:HG11	2.00	0.43
1:B:84:LYS:O	1:B:106:THR:HG22	2.19	0.43
1:A:43:ASP:OD2	1:A:89:GLU:HG2	2.18	0.43
1:A:76:THR:O	1:A:77:ARG:HB2	2.17	0.43
1:B:126:GLY:HA3	1:B:176:ASN:ND2	2.30	0.43
1:A:30:LYS:HD3	1:A:35:PRO:HG3	2.00	0.43
1:A:137:LEU:HD13	1:A:148:ALA:CB	2.48	0.43
1:B:197:ILE:CD1	1:B:231:VAL:HG13	2.49	0.43
1:B:90:ALA:O	1:B:94:LEU:HB2	2.19	0.43
1:B:108:ASN:C	1:B:108:ASN:OD1	2.57	0.43
1:A:53:THR:CG2	1:A:57:TYR:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:HA	1:A:88:PRO:HD2	1.69	0.42
1:B:230:VAL:HG23	1:B:231:VAL:HG23	2.01	0.42
1:B:80:SER:HB3	1:B:98:THR:CG2	2.46	0.42
1:B:87:PRO:HA	1:B:88:PRO:HD3	1.93	0.42
1:A:31:VAL:HB	1:A:238:LEU:HD22	2.00	0.42
1:B:116:ALA:O	1:B:117:HIS:HB2	2.20	0.42
1:B:122:ASN:HD22	1:B:178:LYS:NZ	2.18	0.42
1:A:171:LYS:HB3	1:A:171:LYS:HE2	1.83	0.42
1:A:180:ASN:O	1:A:181:LEU:HG	2.20	0.41
1:A:163:LYS:NZ	1:A:167:ARG:NH1	2.68	0.41
1:A:79:VAL:HG12	1:A:80:SER:N	2.34	0.41
1:B:27:PHE:HD2	1:B:29:HIS:O	2.03	0.41
1:B:42:SER:HB3	1:B:45:ARG:NH1	2.35	0.41
1:B:76:THR:O	1:B:78:ASP:N	2.54	0.41
1:B:79:VAL:HG12	1:B:80:SER:N	2.36	0.41
1:A:213:LEU:C	1:A:214:ILE:HD12	2.41	0.41
1:A:164:TYR:H	1:A:234:ASN:HD21	1.67	0.41
1:A:80:SER:HG	1:A:82:PHE:HE1	1.67	0.41
1:B:81:TYR:HA	1:B:101:ILE:O	2.21	0.41
1:A:189:GLN:HG2	1:A:211:VAL:CG1	2.51	0.41
1:B:60:ILE:O	1:B:60:ILE:HG13	2.21	0.41
1:A:48:ILE:CG2	1:A:66:VAL:HG12	2.44	0.40
1:A:184:ILE:O	1:A:187:GLU:HB2	2.21	0.40
1:A:196:GLN:HG2	1:A:207:PHE:HB3	2.03	0.40
1:B:145:ALA:O	1:B:146:PRO:C	2.59	0.40
1:A:143:GLN:O	1:A:146:PRO:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	247/249 (99%)	213 (86%)	24 (10%)	10 (4%)	4	4
1	B	247/249 (99%)	219 (89%)	19 (8%)	9 (4%)	4	5
All	All	494/498 (99%)	432 (87%)	43 (9%)	19 (4%)	4	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	191	SER
1	B	77	ARG
1	B	228	SER
1	A	68	ASN
1	A	112	LEU
1	A	181	LEU
1	B	181	LEU
1	B	185	SER
1	B	99	ARG
1	B	184	ILE
1	A	57	TYR
1	A	228	SER
1	B	247	ASP
1	A	200	ALA
1	B	57	TYR
1	A	77	ARG
1	A	69	VAL
1	B	69	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/218 (100%)	172 (79%)	46 (21%)	1	2
1	B	218/218 (100%)	167 (77%)	51 (23%)	1	1
All	All	436/436 (100%)	339 (78%)	97 (22%)	1	1

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	12	LYS
1	A	19	GLU
1	A	33	ASP
1	A	46	ARG
1	A	48	ILE
1	A	52	LEU
1	A	62	VAL
1	A	68	ASN
1	A	69	VAL
1	A	76	THR
1	A	77	ARG
1	A	80	SER
1	A	94	LEU
1	A	103	LEU
1	A	108	ASN
1	A	111	ASN
1	A	112	LEU
1	A	113	GLN
1	A	114	THR
1	A	118	LYS
1	A	122	ASN
1	A	130	LEU
1	A	136	THR
1	A	143	GLN
1	A	146	PRO
1	A	150	LEU
1	A	152	LEU
1	A	153	ILE
1	A	167	ARG
1	A	169	VAL
1	A	185	SER
1	A	186	LEU
1	A	189	GLN
1	A	193	LEU
1	A	195	LYS
1	A	196	GLN
1	A	203	GLN
1	A	212	ASP
1	A	223	VAL
1	A	226	VAL
1	A	227	ASP

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Mol	Chain	Res	Type
1	A	229	ASP
1	A	232	LYS
1	A	239	LEU
1	A	248	GLU
1	B	1	ASP
1	B	6	LEU
1	B	19	GLU
1	B	24	THR
1	B	33	ASP
1	B	45	ARG
1	B	46	ARG
1	B	52	LEU
1	B	62	VAL
1	B	68	ASN
1	B	69	VAL
1	B	71	VAL
1	B	85	GLU
1	B	86	SER
1	B	92	ASN
1	B	93	ILE
1	B	94	LEU
1	B	99	ARG
1	B	100	LYS
1	B	103	LEU
1	B	110	GLU
1	B	111	ASN
1	B	112	LEU
1	B	114	THR
1	B	119	ILE
1	B	121	GLU
1	B	122	ASN
1	B	130	LEU
1	B	136	THR
1	B	137	LEU
1	B	141	ASN
1	B	150	LEU
1	B	152	LEU
1	B	153	ILE
1	B	163	LYS
1	B	169	VAL
1	B	186	LEU
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	193	LEU
1	B	202	ASN
1	B	203	GLN
1	B	209	ASN
1	B	220	ARG
1	B	221	PHE
1	B	223	VAL
1	B	234	ASN
1	B	239	LEU
1	B	240	ASN
1	B	241	SER
1	B	245	THR
1	B	247	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	113	GLN
1	A	122	ASN
1	A	143	GLN
1	A	154	GLN
1	A	196	GLN
1	A	234	ASN
1	A	249	ASN
1	B	3	ASN
1	B	29	HIS
1	B	68	ASN
1	B	113	GLN
1	B	117	HIS
1	B	122	ASN
1	B	141	ASN
1	B	176	ASN
1	B	189	GLN
1	B	202	ASN
1	B	209	ASN
1	B	222	GLN
1	B	234	ASN
1	B	240	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 ⓘ

12 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	FUC	A	901	2	10,10,11	1.60	1 (10%)	14,14,16	1.25	1 (7%)
2	NAG	A	902	1,2	14,14,15	1.23	2 (14%)	15,19,21	1.79	4 (26%)
2	NAG	A	903	2	14,14,15	1.72	3 (21%)	15,19,21	2.74	8 (53%)
2	BMA	A	904	2	11,11,12	2.87	5 (45%)	14,15,17	1.79	4 (28%)
2	MAN	A	905	2	11,11,12	3.02	6 (54%)	14,15,17	1.58	2 (14%)
2	XYP	A	906	2	9,9,10	3.25	6 (66%)	12,12,14	1.88	2 (16%)
2	FUC	B	901	2	10,10,11	1.49	1 (10%)	14,14,16	1.25	2 (14%)
2	NAG	B	902	1,2	14,14,15	1.92	5 (35%)	15,19,21	3.44	8 (53%)
2	NAG	B	903	2	14,14,15	2.76	4 (28%)	15,19,21	1.84	5 (33%)
2	BMA	B	904	2	11,11,12	2.91	6 (54%)	14,15,17	3.19	6 (42%)
2	MAN	B	905	2	11,11,12	3.34	3 (27%)	14,15,17	2.32	5 (35%)
2	XYP	B	906	2	9,9,10	3.27	2 (22%)	12,12,14	1.51	2 (16%)

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	FUC	A	901	2	4/4/4/5	0/0/17/20	0/1/1/1
2	NAG	A	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	903	2	-	0/6/23/26	0/1/1/1
2	BMA	A	904	2	-	0/2/19/22	0/1/1/1
2	MAN	A	905	2	-	0/2/19/22	1/1/1/1
2	XYP	A	906	2	-	0/0/14/17	0/1/1/1
2	FUC	B	901	2	4/4/4/5	0/0/17/20	0/1/1/1
2	NAG	B	902	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	903	2	-	0/6/23/26	0/1/1/1
2	BMA	B	904	2	-	0/2/19/22	0/1/1/1
2	MAN	B	905	2	-	0/2/19/22	0/1/1/1
2	XYP	B	906	2	-	0/0/14/17	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903	NAG	O5-C1	-4.10	1.36	1.43
2	A	906	XYP	O5B-C1B	2.08	1.47	1.42
2	B	902	NAG	C4-C3	2.09	1.57	1.52
2	A	905	MAN	C4-C5	2.10	1.57	1.53
2	A	906	XYP	O5B-C5B	2.11	1.47	1.42
2	A	905	MAN	C4-C3	2.21	1.58	1.52
2	B	904	BMA	C4-C3	2.23	1.58	1.52
2	B	902	NAG	O5-C5	2.23	1.48	1.43
2	A	902	NAG	C4-C3	2.24	1.58	1.52
2	A	904	BMA	C6-C5	2.40	1.60	1.51
2	B	904	BMA	C6-C5	2.51	1.60	1.51
2	A	903	NAG	C3-C2	2.52	1.58	1.52
2	B	901	FUC	C1-C2	2.53	1.58	1.52
2	B	904	BMA	C4-C5	2.53	1.58	1.53
2	A	902	NAG	C3-C2	2.59	1.58	1.52
2	A	905	MAN	C1-C2	2.62	1.58	1.52
2	A	906	XYP	C5B-C4B	2.62	1.58	1.52
2	A	904	BMA	C2-C3	2.71	1.56	1.52
2	A	906	XYP	C1B-C2B	2.75	1.58	1.52
2	B	902	NAG	O3-C3	2.85	1.49	1.43
2	A	905	MAN	O5-C5	2.89	1.49	1.43
2	A	905	MAN	O5-C1	2.92	1.48	1.43
2	B	902	NAG	C1-C2	3.19	1.56	1.52
2	A	904	BMA	O2-C2	3.20	1.50	1.43
2	A	903	NAG	C2-N2	3.49	1.52	1.46
2	B	903	NAG	C4-C3	3.61	1.61	1.52
2	B	904	BMA	O2-C2	3.65	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	BMA	C1-C2	3.79	1.61	1.52
2	B	902	NAG	C4-C5	3.89	1.61	1.53
2	A	903	NAG	C4-C3	4.24	1.63	1.52
2	A	901	FUC	C4-C5	4.25	1.61	1.52
2	A	906	XYP	C4B-C3B	4.31	1.58	1.52
2	B	903	NAG	C3-C2	4.52	1.62	1.52
2	A	904	BMA	C4-C3	4.69	1.64	1.52
2	B	906	XYP	C2B-C3B	4.88	1.59	1.52
2	B	905	MAN	C4-C3	4.91	1.65	1.52
2	B	905	MAN	C1-C2	5.25	1.64	1.52
2	A	904	BMA	C4-C5	6.23	1.66	1.53
2	B	904	BMA	C2-C3	6.78	1.61	1.52
2	B	903	NAG	C1-C2	6.81	1.61	1.52
2	A	906	XYP	C2B-C3B	7.05	1.62	1.52
2	B	906	XYP	C4B-C3B	7.62	1.63	1.52
2	B	905	MAN	C2-C3	7.84	1.63	1.52
2	A	905	MAN	C2-C3	7.95	1.63	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	904	BMA	C1-C2-C3	-7.86	100.24	109.54
2	A	903	NAG	O7-C7-C8	-3.53	115.58	122.06
2	A	903	NAG	O4-C4-C5	-3.52	99.91	109.24
2	A	904	BMA	C1-C2-C3	-3.39	105.53	109.54
2	B	906	XYP	O3B-C3B-C2B	-3.00	104.57	110.00
2	B	903	NAG	O4-C4-C5	-3.00	101.30	109.24
2	B	903	NAG	C3-C2-N2	-2.85	103.73	110.56
2	B	905	MAN	C3-C4-C5	-2.82	105.27	110.20
2	B	902	NAG	C4-C3-C2	-2.80	106.88	111.23
2	A	902	NAG	O7-C7-C8	-2.65	117.20	122.06
2	B	902	NAG	C8-C7-N2	-2.50	111.32	116.11
2	B	902	NAG	O4-C4-C3	-2.33	105.10	110.34
2	B	905	MAN	O2-C2-C3	-2.27	105.55	110.12
2	A	903	NAG	C6-C5-C4	2.04	118.06	113.02
2	A	906	XYP	C5B-O5B-C1B	2.07	114.92	111.57
2	B	904	BMA	O3-C3-C2	2.17	113.92	110.00
2	B	902	NAG	O6-C6-C5	2.21	118.63	111.33
2	A	901	FUC	O5-C5-C4	2.22	113.37	109.53
2	A	904	BMA	C6-C5-C4	2.25	118.56	113.02
2	B	902	NAG	C3-C2-N2	2.31	116.08	110.56
2	A	903	NAG	C8-C7-N2	2.33	120.57	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	903	NAG	O4-C4-C3	2.39	115.72	110.34
2	B	901	FUC	C1-O5-C5	2.39	116.08	112.38
2	B	906	XYP	C5B-C4B-C3B	2.43	112.42	109.54
2	A	904	BMA	C3-C4-C5	2.44	114.45	110.20
2	B	901	FUC	O5-C1-C2	2.45	114.83	110.86
2	A	902	NAG	C3-C4-C5	2.46	114.48	110.20
2	B	902	NAG	C3-C4-C5	2.50	114.55	110.20
2	B	903	NAG	C2-N2-C7	2.56	126.33	123.04
2	A	905	MAN	O3-C3-C2	2.63	114.75	110.00
2	A	902	NAG	C1-O5-C5	2.67	115.64	112.25
2	B	905	MAN	O4-C4-C3	2.75	116.52	110.34
2	A	904	BMA	O2-C2-C1	2.85	114.92	109.21
2	B	904	BMA	O2-C2-C3	3.02	116.19	110.12
2	B	904	BMA	C3-C4-C5	3.06	115.53	110.20
2	A	903	NAG	O5-C5-C6	3.08	114.02	107.35
2	B	904	BMA	O2-C2-C1	3.11	115.43	109.21
2	A	903	NAG	C4-C3-C2	3.41	116.53	111.23
2	B	903	NAG	C3-C4-C5	3.54	116.36	110.20
2	A	902	NAG	C2-N2-C7	3.64	127.71	123.04
2	B	905	MAN	C1-C2-C3	4.20	114.51	109.54
2	A	905	MAN	C1-O5-C5	4.21	117.59	112.25
2	A	906	XYP	C1B-C2B-C3B	4.74	115.15	109.54
2	A	903	NAG	C3-C4-C5	4.76	118.49	110.20
2	A	903	NAG	C2-N2-C7	5.21	129.73	123.04
2	B	905	MAN	C6-C5-C4	5.47	126.50	113.02
2	B	904	BMA	C1-O5-C5	6.22	120.14	112.25
2	B	902	NAG	C2-N2-C7	7.36	132.49	123.04
2	B	902	NAG	C1-O5-C5	8.90	123.54	112.25

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	901	FUC	C2
2	B	901	FUC	C3
2	B	901	FUC	C1
2	B	901	FUC	C4
2	A	901	FUC	C2
2	A	901	FUC	C3
2	A	901	FUC	C1
2	A	901	FUC	C4

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	905	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	NAG	1	0
2	B	902	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	249/249 (100%)	-0.20	4 (1%)	74	79	3, 17, 49, 96	0
1	B	249/249 (100%)	-0.35	4 (1%)	74	79	2, 16, 51, 100	0
All	All	498/498 (100%)	-0.27	8 (1%)	74	79	2, 16, 50, 100	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASN	9.9
1	A	247	ASP	8.3
1	A	248	GLU	7.5
1	B	248	GLU	6.5
1	B	249	ASN	4.5
1	B	247	ASP	4.2
1	B	246	ALA	3.6
1	A	246	ALA	2.7

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(Å²)	Q<0.9
2	XYP	B	906	9/10	0.57	0.43	8.52	89,94,96,98	0
2	NAG	B	902	14/15	0.80	0.22	3.29	54,62,72,79	0
2	NAG	A	902	14/15	0.84	0.16	1.71	57,70,78,79	0
2	XYP	A	906	9/10	0.62	0.49	0.40	103,104,106,107	0
2	MAN	A	905	11/12	0.52	0.41	-	97,101,103,103	0
2	FUC	B	901	10/11	0.79	0.19	-	86,89,93,94	0
2	BMA	A	904	11/12	0.70	0.29	-	94,99,102,103	0
2	BMA	B	904	11/12	0.68	0.26	-	95,98,101,102	0
2	FUC	A	901	10/11	0.69	0.39	-	85,92,96,98	0
2	MAN	B	905	11/12	0.76	0.33	-	93,98,100,101	0
2	NAG	A	903	14/15	0.74	0.27	-	86,93,95,96	0
2	NAG	B	903	14/15	0.76	0.24	-	75,79,87,90	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.