Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2016 – 10:23 AM EDT

PDB ID	:	4JZJ
Title	:	Crystal Structure of Receptor-Fab Complex
Authors	:	Broughton, S.E.; Parker, M.W.
Deposited on	:	2013-04-03
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

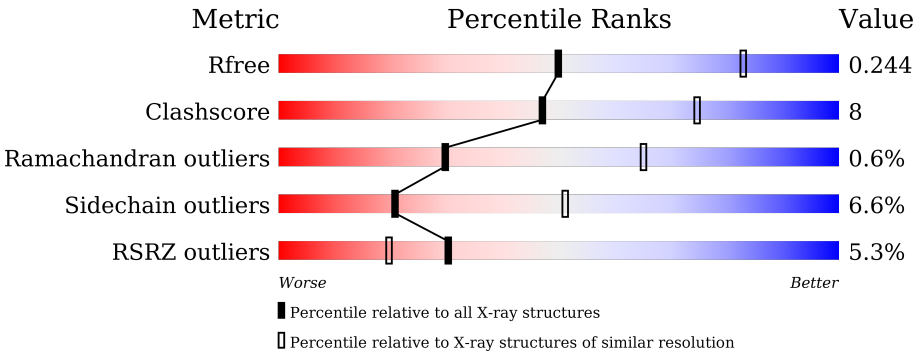
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	C	287	10% 70% 15% • 13%
1	D	287	10% 65% 21% • 13%
2	A	221	2% 78% 17% • •
2	H	221	84% 13% •
3	B	220	4% 90% 8% •
3	L	220	% 85% 12% •

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
4	FUL	C	402	-	-	-	X
6	NAG	D	401	-	-	X	-
6	NAG	D	402	-	-	X	-
6	FUL	D	405	-	-	X	-
7	NAG	D	407	-	-	X	-
8	GOL	H	301	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10972 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 Interleukin-3 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	250	Total	C	N	O	S	0	0	0
			2024	1283	359	369	13			
1	D	251	Total	C	N	O	S	0	0	0
			2035	1293	359	370	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	144	LYS	ASN	SEE REMARK 999	UNP P26951
C	?	-	ARG	DELETION	UNP P26951
C	298	VAL	ALA	ENGINEERED MUTATION	UNP P26951
D	144	LYS	ASN	SEE REMARK 999	UNP P26951
D	?	-	ARG	DELETION	UNP P26951
D	298	VAL	ALA	ENGINEERED MUTATION	UNP P26951

- Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	214	Total	C	N	O	S	0	0	0
			1628	1041	267	311	9			
2	H	215	Total	C	N	O	S	0	0	0
			1634	1044	268	313	9			

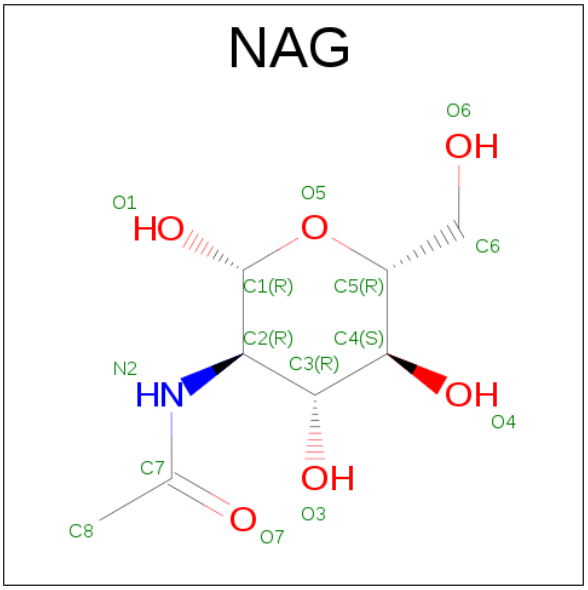
- Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	219	Total	C	N	O	S	0	0	0
			1699	1062	282	350	5			
3	L	219	Total	C	N	O	S	0	0	0
			1699	1062	282	350	5			

- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	7	Total	C	N	O	0	0
			81	46	2	33		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

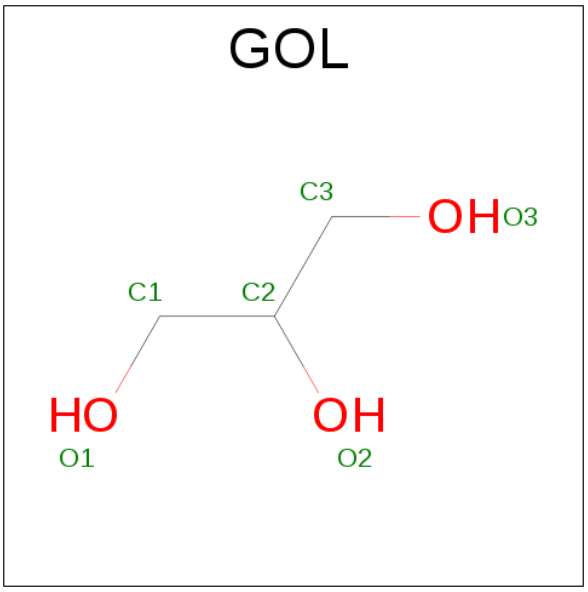
- Molecule 6 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	5	Total	C	N	O	0	0
			59	34	2	23		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	3	Total	C	N	O	0	0
			34	20	1	13		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C O 6 3 3	0	0
8	H	1	Total C O 6 3 3	0	0

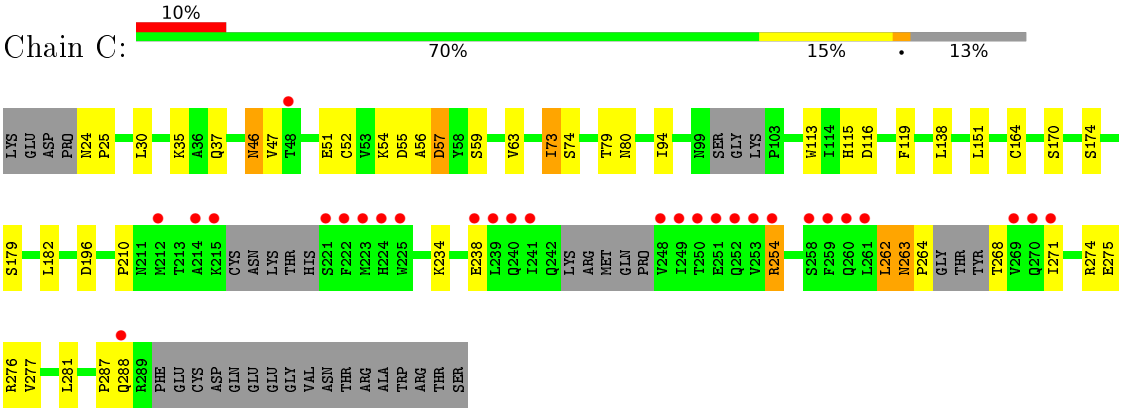
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	9	Total O 9 9	0	0
9	D	7	Total O 7 7	0	0
9	A	2	Total O 2 2	0	0
9	B	6	Total O 6 6	0	0
9	H	12	Total O 12 12	0	0
9	L	3	Total O 3 3	0	0

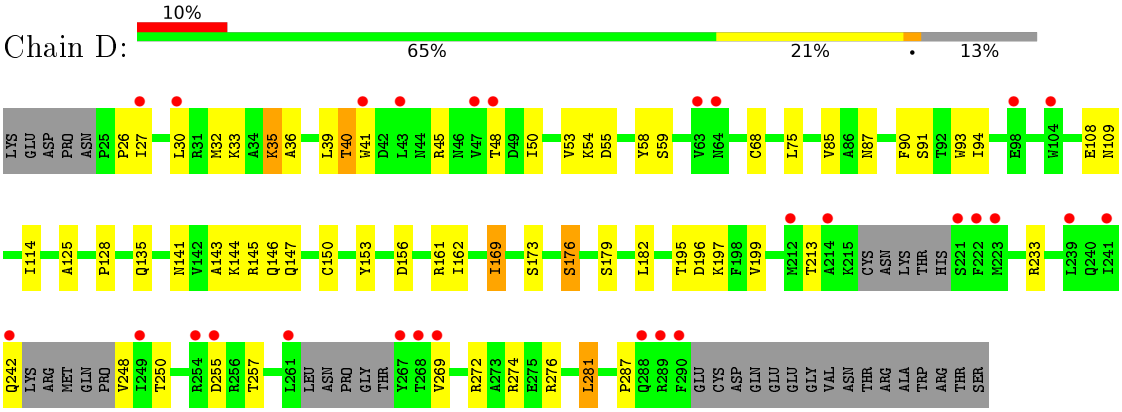
3 Residue-property plots (i)

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.

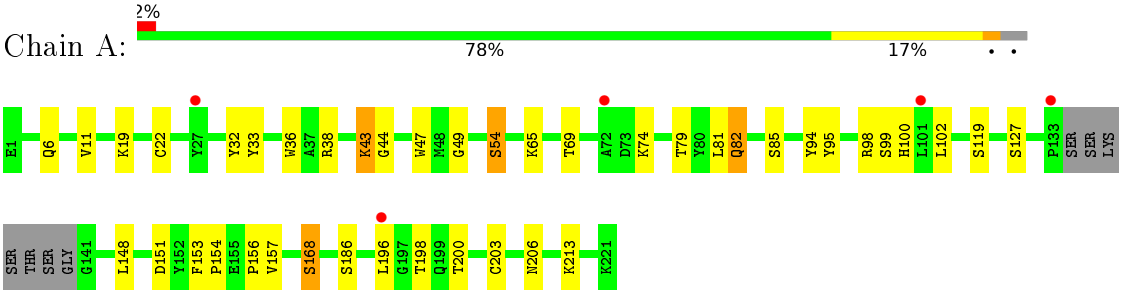
- Molecule 1: Interleukin-3 receptor subunit alpha



- Molecule 1: Interleukin-3 receptor subunit alpha

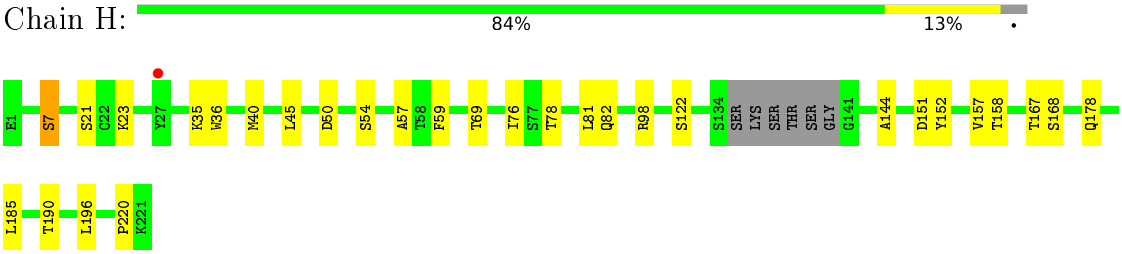


- Molecule 2: Fab Heavy Chain



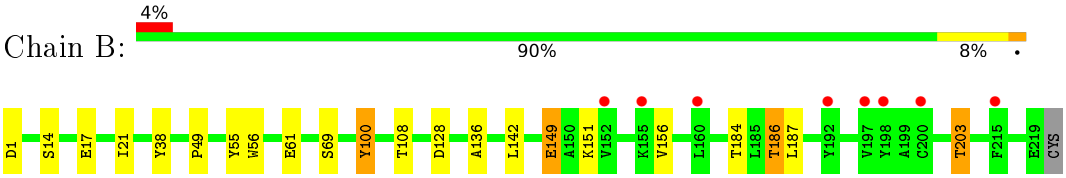
• Molecule 2: Fab Heavy Chain

Chain H:



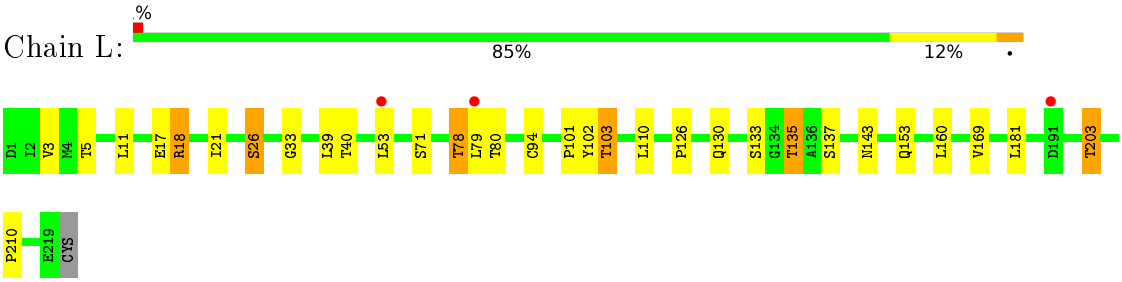
• Molecule 3: Fab Light Chain

Chain B:



• Molecule 3: Fab Light Chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.30Å 120.65Å 92.97Å 90.00° 97.45° 90.00°	Depositor
Resolution (Å)	49.67 – 2.80 49.67 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.67-2.80) 99.1 (49.67-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1218)	Depositor
R, R_{free}	0.185 , 0.244 0.188 , 0.244	Depositor DCC
R_{free} test set	2378 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 15.5	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 47191 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10972	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: GOL, BMA, NAG, FUC, FUL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.60	1/2074 (0.0%)	0.72	1/2814 (0.0%)
1	D	0.51	0/2087	0.70	1/2830 (0.0%)
2	A	0.48	0/1671	0.63	0/2270
2	H	0.56	0/1677	0.68	1/2278 (0.0%)
3	B	0.52	0/1737	0.65	0/2362
3	L	0.58	0/1737	0.65	0/2362
All	All	0.54	1/10983 (0.0%)	0.68	3/14916 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	THR	C-N	5.69	1.47	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	281	LEU	CA-CB-CG	7.03	131.47	115.30
1	C	151	LEU	CA-CB-CG	5.75	128.52	115.30
2	H	185	LEU	CA-CB-CG	5.04	126.90	115.30

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	C	2024	0	1958	28	0
1	D	2035	0	1968	39	0
2	A	1628	0	1608	19	0
2	H	1634	0	1613	12	0
3	B	1699	0	1630	10	0
3	L	1699	0	1630	18	0
4	C	81	0	70	9	0
5	C	14	0	13	2	0
5	D	14	0	13	2	0
6	D	59	0	51	33	0
7	D	34	0	31	10	0
8	D	6	0	8	1	0
8	H	6	0	8	1	0
9	A	2	0	0	1	0
9	B	6	0	0	0	0
9	C	9	0	0	0	0
9	D	7	0	0	0	0
9	H	12	0	0	3	0
9	L	3	0	0	0	0
All	All	10972	0	10601	159	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 8.

All (159) 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:C:46:ASN:HD22	5:C:408:NAG:C1	0.99	1.57
6:D:401:NAG:H62	6:D:402:NAG:C7	1.36	1.51
1:D:109:ASN:HD21	7:D:407:NAG:C1	1.22	1.48
6:D:401:NAG:C6	6:D:402:NAG:C7	2.27	1.11
1:C:80:ASN:CG	4:C:401:NAG:C1	2.23	1.06
6:D:401:NAG:H62	6:D:402:NAG:O7	1.57	1.01
6:D:401:NAG:C6	6:D:402:NAG:O7	2.09	1.01
6:D:401:NAG:C5	6:D:402:NAG:O7	2.09	1.01
6:D:401:NAG:H62	6:D:402:NAG:C8	1.99	0.91
1:C:80:ASN:OD1	4:C:401:NAG:C1	2.20	0.88
6:D:401:NAG:H5	6:D:402:NAG:O7	1.73	0.87
6:D:401:NAG:O7	6:D:405:FUL:C1	2.22	0.87
6:D:401:NAG:C7	6:D:405:FUL:C1	2.57	0.83
1:C:56:ALA:HB2	4:C:402:FUL:O3	1.79	0.82
6:D:401:NAG:C6	6:D:402:NAG:C1	2.59	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:401:NAG:O3	6:D:401:NAG:C7	2.28	0.80
3:B:151:LYS:HB3	3:B:203:THR:HG23	1.65	0.78
4:C:404:BMA:H62	4:C:405:MAN:O2	1.84	0.77
1:C:80:ASN:ND2	4:C:401:NAG:C2	2.48	0.77
1:C:37:GLN:HE21	1:C:73:ILE:HG12	1.51	0.76
1:C:238:GLU:OE2	1:C:274:ARG:NH1	2.20	0.73
1:C:262:LEU:HG	1:C:263:ASN:HB3	1.72	0.72
1:D:125:ALA:CB	7:D:407:NAG:H82	2.19	0.72
1:D:109:ASN:CG	7:D:407:NAG:C1	2.59	0.71
1:C:80:ASN:ND2	4:C:401:NAG:O5	2.25	0.70
1:D:109:ASN:HD21	7:D:407:NAG:C2	2.04	0.70
6:D:401:NAG:O4	6:D:405:FUL:C2	2.41	0.69
1:D:30:LEU:HD13	1:D:94:ILE:HG23	1.76	0.68
1:C:51:GLU:OE2	3:L:102:TYR:OH	2.05	0.67
1:D:153:TYR:CD1	1:D:161:ARG:HG2	2.30	0.66
3:L:17:GLU:HG3	3:L:18:ARG:H	1.63	0.64
6:D:402:NAG:O7	6:D:402:NAG:C1	2.41	0.64
1:C:46:ASN:HD21	5:C:408:NAG:C1	2.02	0.64
6:D:402:NAG:C1	6:D:404:FUL:H61	2.29	0.63
6:D:402:NAG:H5	6:D:404:FUL:H61	1.82	0.62
2:H:36:TRP:CE3	2:H:81:LEU:HD22	2.34	0.62
3:B:14:SER:HB2	3:B:17:GLU:HG3	1.82	0.62
6:D:401:NAG:O4	6:D:405:FUL:O2	2.16	0.62
2:H:151:ASP:OD1	2:H:178:GLN:NE2	2.33	0.61
6:D:401:NAG:H81	6:D:405:FUL:O5	2.00	0.61
6:D:401:NAG:C8	6:D:405:FUL:O5	2.48	0.61
1:C:24:ASN:HB3	1:C:25:PRO:HD3	1.85	0.59
6:D:401:NAG:O4	6:D:405:FUL:H2	2.02	0.58
1:D:125:ALA:HB1	7:D:407:NAG:H82	1.85	0.58
8:H:301:GOL:H2	9:H:409:HOH:O	2.04	0.57
1:D:93:TRP:CE2	6:D:401:NAG:H3	2.39	0.57
1:C:37:GLN:NE2	1:C:73:ILE:HG12	2.20	0.56
1:D:50:ILE:HG12	1:D:85:VAL:HG12	1.87	0.56
1:D:109:ASN:OD1	7:D:407:NAG:C1	2.54	0.56
1:D:53:VAL:HA	1:D:59:SER:HB2	1.88	0.55
6:D:401:NAG:C7	6:D:405:FUL:O5	2.54	0.55
6:D:401:NAG:H4	6:D:401:NAG:O7	2.07	0.55
6:D:401:NAG:O7	6:D:405:FUL:O5	2.23	0.55
6:D:401:NAG:C4	6:D:402:NAG:O7	2.54	0.55
1:C:30:LEU:HD23	1:C:94:ILE:HG23	1.88	0.54
3:L:102:TYR:N	3:L:102:TYR:CD1	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:407:NAG:O4	5:D:409:NAG:C1	2.55	0.54
1:D:144:LYS:N	1:D:145:ARG:HA	2.22	0.54
3:B:38:TYR:CE1	3:B:56:TRP:HZ3	2.26	0.53
6:D:401:NAG:O4	6:D:402:NAG:O7	2.25	0.53
2:A:36:TRP:CD2	2:A:81:LEU:HD13	2.43	0.53
1:D:26:PRO:HB3	1:D:45:ARG:HD3	1.91	0.53
3:L:11:LEU:HD23	3:L:110:LEU:HD13	1.91	0.53
3:B:55:TYR:HE2	3:B:61:GLU:OE1	1.92	0.52
6:D:401:NAG:O7	6:D:401:NAG:C4	2.58	0.51
4:C:404:BMA:C6	4:C:405:MAN:O2	2.57	0.51
6:D:402:NAG:H82	6:D:404:FUL:C1	2.40	0.51
3:L:169:VAL:HG22	3:L:181:LEU:HD12	1.92	0.51
1:C:63:VAL:HG13	3:L:33:GLY:HA3	1.93	0.51
1:C:182:LEU:HD12	1:C:196:ASP:HB3	1.94	0.50
2:A:32:TYR:CG	2:A:98:ARG:HD3	2.46	0.50
1:D:156:ASP:HB3	1:D:162:ILE:HD13	1.94	0.50
3:L:39:LEU:HG	3:L:40:THR:N	2.26	0.50
2:A:33:TYR:HB2	2:A:99:SER:HB3	1.93	0.49
1:C:263:ASN:HB2	1:C:264:PRO:HA	1.93	0.49
1:C:234:LYS:HD2	1:C:276:ARG:NH2	2.27	0.49
1:D:144:LYS:HB2	1:D:146:GLN:N	2.27	0.49
1:D:182:LEU:HD12	1:D:196:ASP:HB3	1.93	0.49
1:D:272:ARG:HH21	1:D:274:ARG:NH1	2.10	0.48
2:H:168:SER:HB2	9:H:411:HOH:O	2.12	0.48
3:B:184:THR:HG22	3:B:186:THR:HG23	1.95	0.48
2:H:152:TYR:CE1	2:H:157:VAL:HG13	2.49	0.48
3:L:21:ILE:HD12	3:L:79:LEU:HD23	1.95	0.48
1:C:138:LEU:HD22	1:C:164:CYS:HB3	1.96	0.48
1:D:32:MET:HE2	1:D:39:LEU:HD13	1.96	0.47
2:A:43:LYS:HD3	2:A:43:LYS:HA	1.52	0.47
6:D:402:NAG:H3	6:D:404:FUL:H61	1.95	0.47
1:C:56:ALA:HB2	4:C:402:FUL:HO3	1.77	0.47
2:H:76:ILE:O	2:H:78:THR:HG23	2.13	0.47
1:D:75:LEU:HB3	8:D:410:GOL:H32	1.97	0.47
2:A:196:LEU:HA	2:A:196:LEU:HD12	1.71	0.46
3:L:71:SER:OG	3:L:78:THR:HG22	2.16	0.46
2:A:38:ARG:HB3	2:A:94:TYR:CE1	2.51	0.46
1:D:35:LYS:HG3	1:D:36:ALA:H	1.79	0.46
1:D:85:VAL:HG22	1:D:90:PHE:O	2.16	0.46
2:A:95:TYR:CE1	3:B:49:PRO:HB3	2.51	0.46
2:H:7:SER:HB3	2:H:21:SER:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:O	1:C:57:ASP:HB2	2.16	0.46
1:D:143:ALA:HA	1:D:145:ARG:NE	2.31	0.45
1:D:173:SER:HB2	1:D:176:SER:HB2	1.99	0.45
1:D:150:CYS:HB3	1:D:153:TYR:CZ	2.52	0.45
2:A:69:THR:HG23	2:A:82:GLN:HB3	1.99	0.45
2:H:168:SER:CB	9:H:411:HOH:O	2.64	0.45
1:D:242:GLN:HB3	1:D:248:VAL:HA	1.99	0.45
2:A:47:TRP:CZ2	2:A:49:GLY:HA2	2.52	0.45
7:D:407:NAG:HO4	5:D:409:NAG:C1	2.28	0.45
3:L:3:VAL:H	3:L:26:SER:HB2	1.82	0.45
1:D:135:GLN:CD	1:D:161:ARG:HD3	2.37	0.45
1:D:114:ILE:HD12	1:D:169:ILE:HD13	1.99	0.44
1:D:141:ASN:OD1	1:D:147:GLN:HG2	2.17	0.44
1:D:54:LYS:HD2	1:D:58:TYR:CE2	2.52	0.44
3:L:153:GLN:HG2	3:L:160:LEU:HD22	2.00	0.44
2:A:11:VAL:HG21	2:A:154:PRO:HG3	2.00	0.44
1:D:125:ALA:HB1	7:D:407:NAG:C8	2.48	0.44
1:C:274:ARG:CZ	1:C:281:LEU:HD21	2.48	0.44
1:D:30:LEU:HD22	1:D:94:ILE:HD13	2.00	0.44
3:L:126:PRO:HB3	3:L:137:SER:H	1.83	0.44
3:L:17:GLU:CG	3:L:18:ARG:H	2.30	0.44
1:D:40:THR:HG22	1:D:41:TRP:H	1.82	0.44
1:C:268:THR:HA	1:C:288:GLN:O	2.18	0.43
1:D:93:TRP:NE1	6:D:401:NAG:H3	2.34	0.43
2:A:148:LEU:HA	2:A:148:LEU:HD12	1.88	0.43
2:A:148:LEU:HD12	2:A:186:SER:HB3	1.99	0.43
2:A:100:HIS:CE1	2:A:102:LEU:HD12	2.53	0.43
1:C:210:PRO:HG2	1:C:271:ILE:HG23	1.99	0.43
1:D:153:TYR:CG	1:D:161:ARG:HG2	2.54	0.43
1:D:125:ALA:HB3	7:D:407:NAG:H82	1.98	0.43
2:A:19:LYS:HG3	2:A:82:GLN:HG3	1.99	0.43
6:D:401:NAG:O3	6:D:401:NAG:O7	2.30	0.43
6:D:401:NAG:C3	6:D:401:NAG:O7	2.56	0.43
1:C:254:ARG:HA	1:C:254:ARG:HD2	1.97	0.42
2:H:35:LYS:HG2	2:H:50:ASP:OD1	2.19	0.42
3:B:136:ALA:N	3:B:187:LEU:O	2.41	0.42
2:H:144:ALA:HB2	2:H:190:THR:HG22	2.01	0.42
3:B:21:ILE:HG12	3:B:108:THR:HG21	2.02	0.42
3:B:149:GLU:O	3:B:149:GLU:HG3	2.19	0.42
1:D:108:GLU:OE2	1:D:128:PRO:HD2	2.19	0.42
6:D:402:NAG:O5	6:D:405:FUL:H2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:100:TYR:CD2	3:B:100:TYR:C	2.92	0.42
3:L:203:THR:HG22	3:L:210:PRO:HB3	2.02	0.42
4:C:405:MAN:H61	2:H:57:ALA:HB2	2.01	0.41
3:L:39:LEU:HD11	3:L:94:CYS:HB2	2.02	0.41
3:L:130:GLN:HG2	3:L:135:THR:O	2.20	0.41
1:D:169:ILE:HG13	1:D:169:ILE:H	1.59	0.41
3:L:3:VAL:H	3:L:26:SER:CB	2.34	0.41
2:H:23:LYS:CB	2:H:78:THR:HG22	2.50	0.41
1:D:54:LYS:HD3	1:D:54:LYS:O	2.20	0.41
2:H:196:LEU:HA	2:H:196:LEU:HD23	1.84	0.41
1:C:113:TRP:HD1	1:C:115:HIS:HB3	1.85	0.41
1:C:52:CYS:O	1:C:59:SER:HB2	2.21	0.41
2:A:153:PHE:HA	2:A:154:PRO:HA	1.71	0.41
2:A:168:SER:HB2	9:A:401:HOH:O	2.20	0.41
2:A:206:ASN:OD1	2:A:213:LYS:HE2	2.20	0.41
1:D:33:LYS:HE2	1:D:40:THR:OG1	2.21	0.41
3:L:101:PRO:O	3:L:103:THR:N	2.53	0.41
6:D:402:NAG:C5	6:D:404:FUL:H61	2.49	0.40
2:A:54:SER:O	2:A:74:LYS:HE3	2.21	0.40
2:A:6:GLN:HG2	2:A:22:CYS:HB2	2.02	0.40
1:C:116:ASP:HB2	1:C:119:PHE:HD2	1.86	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	C	240/287 (84%)	222 (92%)	15 (6%)	3 (1%)	15	44
1	D	243/287 (85%)	220 (90%)	20 (8%)	3 (1%)	16	47
2	A	210/221 (95%)	197 (94%)	12 (6%)	1 (0%)	34	69
2	H	211/221 (96%)	201 (95%)	9 (4%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	217/220 (99%)	205 (94%)	12 (6%)	0	100	100
3	L	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
All	All	1338/1456 (92%)	1257 (94%)	73 (6%)	8 (1%)	30	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	ARG
1	D	35	LYS
1	D	48	THR
1	D	287	PRO
2	H	220	PRO
1	C	73	ILE
1	C	287	PRO
2	A	44	GLY

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	C	223/256 (87%)	210 (94%)	13 (6%)	25	57
1	D	223/256 (87%)	203 (91%)	20 (9%)	12	34
2	A	181/187 (97%)	166 (92%)	15 (8%)	14	38
2	H	182/187 (97%)	171 (94%)	11 (6%)	24	56
3	B	194/195 (100%)	185 (95%)	9 (5%)	33	67
3	L	194/195 (100%)	183 (94%)	11 (6%)	25	58
All	All	1197/1276 (94%)	1118 (93%)	79 (7%)	21	51

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	35	LYS
1	C	46	ASN

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Mol	Chain	Res	Type
1	C	47	VAL
1	C	55	ASP
1	C	57	ASP
1	C	74	SER
1	C	170	SER
1	C	174	SER
1	C	179	SER
1	C	262	LEU
1	C	263	ASN
1	C	275	GLU
1	C	277	VAL
1	D	27	ILE
1	D	40	THR
1	D	55	ASP
1	D	68	CYS
1	D	87	ASN
1	D	91	SER
1	D	169	ILE
1	D	176	SER
1	D	179	SER
1	D	195	THR
1	D	197	LYS
1	D	199	VAL
1	D	213	THR
1	D	233	ARG
1	D	250	THR
1	D	255	ASP
1	D	257	THR
1	D	269	VAL
1	D	276	ARG
1	D	281	LEU
2	A	43	LYS
2	A	54	SER
2	A	65	LYS
2	A	79	THR
2	A	82	GLN
2	A	85	SER
2	A	119	SER
2	A	127	SER
2	A	151	ASP
2	A	156	PRO
2	A	157	VAL

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Mol	Chain	Res	Type
2	A	168	SER
2	A	198	THR
2	A	200	THR
2	A	203	CYS
3	B	1	ASP
3	B	69	SER
3	B	100	TYR
3	B	128	ASP
3	B	142	LEU
3	B	149	GLU
3	B	156	VAL
3	B	186	THR
3	B	203	THR
2	H	7	SER
2	H	40	MET
2	H	45	LEU
2	H	54	SER
2	H	59	PHE
2	H	69	THR
2	H	82	GLN
2	H	98	ARG
2	H	122	SER
2	H	158	THR
2	H	167	THR
3	L	5	THR
3	L	18	ARG
3	L	26	SER
3	L	53	LEU
3	L	78	THR
3	L	80	THR
3	L	103	THR
3	L	133	SER
3	L	135	THR
3	L	143	ASN
3	L	203	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	37	GLN
1	C	44	ASN
1	C	46	ASN

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Mol	Chain	Res	Type
1	C	224	HIS
1	D	99	ASN
1	D	109	ASN
2	A	67	GLN
2	A	178	GLN
3	L	27	GLN
3	L	31	ASN
3	L	35	GLN
3	L	143	ASN
3	L	144	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

15 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	$\#\|Z\|>2$
4	NAG	C	401	1,4	14,14,15	1.15	1 (7%)	15,19,21	2.30	6 (40%)
4	FUL	C	402	4	10,10,11	0.59	0	13,14,16	1.86	4 (30%)
4	NAG	C	403	4	14,14,15	0.77	0	15,19,21	1.12	2 (13%)
4	BMA	C	404	4	11,11,12	0.70	0	15,15,17	1.15	1 (6%)
4	MAN	C	405	4	11,11,12	0.59	0	15,15,17	1.46	4 (26%)
4	MAN	C	406	4	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
4	FUL	C	407	4	10,10,11	0.83	0	13,14,16	3.10	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	D	401	1,6	14,14,15	0.90	0	15,19,21	5.63	8 (53%)
6	NAG	D	402	6	14,14,15	1.79	5 (35%)	15,19,21	3.47	7 (46%)
6	BMA	D	403	6	11,11,12	0.76	0	15,15,17	1.55	3 (20%)
6	FUL	D	404	6	10,10,11	0.31	0	13,14,16	0.78	0
6	FUL	D	405	6	10,10,11	0.49	0	13,14,16	0.87	0
7	FUL	D	406	7	10,10,11	0.86	1 (10%)	13,14,16	2.30	4 (30%)
7	NAG	D	407	1,7	14,14,15	0.44	0	15,19,21	1.64	3 (20%)
7	FUC	D	408	7	10,10,11	0.77	0	13,14,16	1.40	2 (15%)

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	C	401	1,4	-	0/6/23/26	0/1/1/1
4	FUL	C	402	4	-	0/0/17/20	0/1/1/1
4	NAG	C	403	4	-	0/6/23/26	0/1/1/1
4	BMA	C	404	4	-	0/2/19/22	0/1/1/1
4	MAN	C	405	4	-	0/2/19/22	0/1/1/1
4	MAN	C	406	4	-	0/2/19/22	0/1/1/1
4	FUL	C	407	4	-	0/0/17/20	0/1/1/1
6	NAG	D	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	402	6	-	0/6/23/26	0/1/1/1
6	BMA	D	403	6	-	0/2/19/22	0/1/1/1
6	FUL	D	404	6	-	0/0/17/20	0/1/1/1
6	FUL	D	405	6	-	0/0/17/20	0/1/1/1
7	FUL	D	406	7	-	0/0/17/20	0/1/1/1
7	NAG	D	407	1,7	-	0/6/23/26	0/1/1/1
7	FUC	D	408	7	-	0/0/17/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	402	NAG	C2-N2	-3.14	1.40	1.46
6	D	402	NAG	C3-C2	-2.64	1.46	1.52
6	D	402	NAG	C1-C2	-2.49	1.48	1.52
6	D	402	NAG	O5-C1	-2.39	1.39	1.43
4	C	401	NAG	C1-C2	-2.25	1.49	1.52
6	D	402	NAG	O7-C7	-2.09	1.18	1.23
7	D	406	FUL	C2-C3	2.04	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	401	NAG	C4-C3-C2	-14.40	88.99	111.34
6	D	401	NAG	C3-C4-C5	-10.22	92.01	110.23
4	C	407	FUL	C1-C2-C3	-9.37	98.20	109.55
6	D	402	NAG	O4-C4-C3	-9.11	89.80	110.36
6	D	401	NAG	C2-N2-C7	-8.16	112.49	123.11
6	D	402	NAG	C2-N2-C7	-6.57	114.56	123.11
6	D	402	NAG	C3-C4-C5	-4.78	101.70	110.23
4	C	401	NAG	O5-C5-C4	-4.51	102.67	110.13
7	D	407	NAG	C3-C4-C5	-3.73	103.57	110.23
7	D	408	FUC	O5-C1-C2	-2.63	106.70	110.89
6	D	403	BMA	C1-O5-C5	-2.60	108.32	112.14
4	C	403	NAG	O4-C4-C3	-2.42	104.91	110.36
4	C	407	FUL	O5-C1-C2	-2.32	107.19	110.89
6	D	402	NAG	O7-C7-N2	-2.11	117.54	121.84
6	D	401	NAG	O6-C6-C5	-2.06	104.41	111.30
4	C	403	NAG	C2-N2-C7	-2.04	120.45	123.11
6	D	402	NAG	O5-C5-C4	2.04	113.51	110.13
6	D	402	NAG	C1-O5-C5	2.04	115.14	112.14
4	C	407	FUL	O2-C2-C3	2.05	114.31	110.19
7	D	406	FUL	O5-C5-C6	2.07	109.98	106.28
4	C	402	FUL	C1-C2-C3	2.09	112.09	109.55
4	C	405	MAN	O5-C5-C4	2.15	113.69	110.13
4	C	405	MAN	C3-C4-C5	2.16	114.07	110.23
4	C	405	MAN	O2-C2-C1	2.16	113.56	109.23
4	C	401	NAG	O4-C4-C3	2.18	115.28	110.36
7	D	407	NAG	O3-C3-C4	2.23	115.39	110.36
6	D	403	BMA	C1-C2-C3	2.24	112.26	109.55
7	D	408	FUC	C3-C4-C5	2.40	113.25	109.66
4	C	406	MAN	C1-O5-C5	2.63	116.00	112.14
4	C	402	FUL	C2-C3-C4	2.66	115.69	111.05
7	D	406	FUL	C2-C3-C4	2.68	115.72	111.05
4	C	402	FUL	C3-C4-C5	2.69	113.67	109.66
4	C	407	FUL	O5-C5-C4	2.71	114.27	109.58
7	D	406	FUL	O5-C1-C2	2.72	115.24	110.89
4	C	406	MAN	C3-C4-C5	2.76	115.14	110.23
4	C	404	BMA	C1-C2-C3	2.89	113.05	109.55
4	C	401	NAG	O6-C6-C5	2.92	121.05	111.30
7	D	407	NAG	O5-C5-C6	2.95	113.66	107.34
6	D	402	NAG	O7-C7-C8	2.99	127.58	122.07
4	C	401	NAG	O4-C4-C5	3.13	117.47	109.23
4	C	401	NAG	C6-C5-C4	3.14	120.85	112.99
6	D	403	BMA	C2-C3-C4	3.17	116.58	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	405	MAN	C1-O5-C5	3.25	116.92	112.14
4	C	402	FUL	O5-C5-C6	3.32	112.23	106.28
4	C	407	FUL	C3-C4-C5	3.65	115.11	109.66
6	D	401	NAG	O5-C5-C4	3.68	116.23	110.13
4	C	401	NAG	C1-O5-C5	3.84	117.79	112.14
6	D	401	NAG	O3-C3-C4	3.86	119.06	110.36
6	D	401	NAG	O4-C4-C3	5.06	121.76	110.36
6	D	401	NAG	C1-O5-C5	5.35	120.01	112.14
7	D	406	FUL	C1-C2-C3	6.76	117.74	109.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	NAG	4	0
4	C	402	FUL	2	0
4	C	404	BMA	2	0
4	C	405	MAN	3	0
6	D	401	NAG	26	0
6	D	402	NAG	17	0
6	D	404	FUL	5	0
6	D	405	FUL	10	0
7	D	407	NAG	10	0

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
5	NAG	C	408	1	14,14,15	0.71	1 (7%)	15,19,21	1.49	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	D	409	-	14,14,15	0.69	0	15,19,21	1.10	1 (6%)
8	GOL	D	410	-	5,5,5	0.31	0	5,5,5	0.43	0
8	GOL	H	301	-	5,5,5	0.40	0	5,5,5	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	408	1	-	0/6/23/26	0/1/1/1
5	NAG	D	409	-	-	0/6/23/26	0/1/1/1
8	GOL	D	410	-	-	0/4/4/4	0/0/0/0
8	GOL	H	301	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	408	NAG	C1-C2	2.19	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	408	NAG	C3-C4-C5	-2.78	105.27	110.23
5	D	409	NAG	C3-C4-C5	2.80	115.22	110.23
5	C	408	NAG	C1-O5-C5	2.94	116.46	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	408	NAG	2	0
5	D	409	NAG	2	0
8	D	410	GOL	1	0
8	H	301	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	C	250/287 (87%)	0.61	28 (11%) 7 3	21, 38, 93, 116	0
1	D	251/287 (87%)	0.59	28 (11%) 7 3	29, 57, 96, 113	0
2	A	214/221 (96%)	0.22	5 (2%) 64 52	32, 50, 78, 94	0
2	H	215/221 (97%)	-0.09	1 (0%) 91 88	22, 38, 59, 77	0
3	B	219/220 (99%)	0.24	8 (3%) 45 33	23, 45, 90, 102	0
3	L	219/220 (99%)	0.04	3 (1%) 78 69	22, 42, 67, 87	0
All	All	1368/1456 (93%)	0.28	73 (5%) 30 20	21, 45, 87, 116	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	ALA	6.1
1	D	268	THR	5.7
1	C	251	GLU	5.6
1	D	290	PHE	5.4
1	D	267	TYR	5.1
1	C	250	THR	5.1
1	C	239	LEU	5.1
1	D	239	LEU	5.0
1	C	214	ALA	4.8
3	B	215	PHE	4.8
1	D	269	VAL	4.7
1	D	288	GLN	4.6
1	C	249	ILE	4.4
3	B	198	TYR	4.3
1	C	269	VAL	4.2
3	B	160	LEU	4.2
1	D	241	ILE	4.2
1	C	222	PHE	4.2
1	C	252	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	289	ARG	3.8
1	C	270	GLN	3.7
1	D	223	MET	3.6
1	C	212	MET	3.6
3	B	200	CYS	3.4
1	D	212	MET	3.4
1	D	221	SER	3.4
1	C	254	ARG	3.3
1	D	261	LEU	3.2
1	C	248	VAL	3.2
1	C	215	LYS	3.2
1	C	240	GLN	3.2
1	D	63	VAL	3.1
1	D	43	LEU	3.1
1	D	255	ASP	3.1
1	C	223	MET	3.0
1	C	221	SER	3.0
1	D	64	ASN	3.0
1	D	27	ILE	3.0
3	B	197	VAL	2.9
1	D	242	GLN	2.9
1	C	225	TRP	2.9
1	C	253	VAL	2.8
1	C	258	SER	2.8
1	C	271	ILE	2.7
1	C	260	GLN	2.6
1	C	261	LEU	2.6
1	D	249	ILE	2.6
1	C	238	GLU	2.6
1	C	241	ILE	2.5
3	B	155	LYS	2.5
1	C	48	THR	2.5
2	H	27	TYR	2.5
3	L	53	LEU	2.5
2	A	72	ALA	2.5
1	C	288	GLN	2.4
2	A	27	TYR	2.4
2	A	196	LEU	2.3
3	B	152	VAL	2.3
1	D	47	VAL	2.3
1	D	41	TRP	2.2
1	D	98	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	259	PHE	2.2
3	B	192	TYR	2.2
1	D	30	LEU	2.1
3	L	191	ASP	2.1
1	D	222	PHE	2.1
2	A	101	LEU	2.1
3	L	79	LEU	2.1
1	C	224	HIS	2.1
1	D	104	TRP	2.0
1	D	48	THR	2.0
1	D	254	ARG	2.0
2	A	133	PRO	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, 95^{th} 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
4	FUL	C	402	10/11	0.92	0.36	2.98	62,70,79,84	0
6	FUL	D	404	10/11	0.72	0.30	1.65	57,58,58,58	0
4	NAG	C	403	14/15	0.94	0.20	1.62	60,69,74,82	0
6	NAG	D	402	14/15	0.81	0.22	1.01	27,29,30,30	0
7	NAG	D	407	14/15	0.86	0.19	-0.43	88,94,103,116	0
4	BMA	C	404	11/12	0.89	0.14	-	85,93,105,108	0
7	FUL	D	406	10/11	0.92	0.18	-	104,112,116,119	0
4	MAN	C	406	11/12	0.77	0.21	-	108,116,121,121	0
7	FUC	D	408	10/11	0.84	0.29	-	112,122,131,133	0
6	NAG	D	401	14/15	0.58	0.23	-	70,70,71,71	0
4	NAG	C	401	14/15	0.88	0.17	-	46,47,48,48	0
6	FUL	D	405	10/11	0.76	0.31	-	20,20,20,20	0
6	BMA	D	403	11/12	0.75	0.18	-	91,103,107,109	0
4	FUL	C	407	10/11	0.82	0.27	-	79,95,101,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MAN	C	405	11/12	0.90	0.18	-	83,94,96,101	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, 95^{th} 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
8	GOL	H	301	6/6	0.75	0.54	9.68	47,47,47,47	0
5	NAG	C	408	14/15	0.74	0.23	-	105,120,134,135	0
5	NAG	D	409	14/15	0.90	0.22	-	81,81,81,81	0
8	GOL	D	410	6/6	0.79	0.24	-	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.