Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:29 PM EDT

PDB ID	:	1FE8
Title	:	CRYSTAL STRUCTURE OF THE VON WILLEBRAND FACTOR A3 DOMAIN IN COMPLEX WITH A FAB FRAGMENT OF IGG RU5 THAT INHIBITS COLLAGEN BINDING
Authors	:	Bouma, B.; Huizinga, E.G.; Schiphorst, M.E.; Sixma, J.J.; Kroon, J.; Gros, P.
Deposited on	:	2000-07-21
Resolution	:	2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

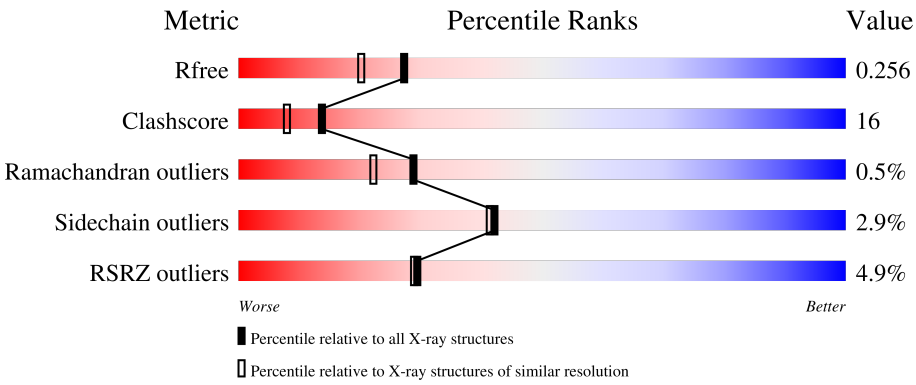
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	196	6% 71% 24%
1	B	196	8% 77% 19%
1	C	196	11% 67% 30%
2	H	210	5% 67% 29%
2	I	210	2% 68% 29%

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Mol	Chain	Length	Quality of chain
2	J	210	11% 61% 38%
3	L	211	83% 15%
3	M	211	75% 25%
3	N	211	2% 76% 22%
4	D	2	50% 50%
4	E	2	50% 50%
4	F	2	50% 50%

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	NAG	D	1	-	-	X	-
4	FUC	D	2	-	-	X	-
4	FUC	F	2	-	-	X	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14872 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 VON WILLEBRAND FACTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	190	1421	899	243	273	2	4	0	0	0
1	B	190	1421	899	243	273	2	4	0	0	0
1	C	191	1426	902	244	274	2	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	916	GLY	-	cloning artifact	? P04275
A	917	SER	-	cloning artifact	? P04275
A	918	HIS	-	cloning artifact	? P04275
A	919	MSE	-	cloning artifact	? P04275
A	947	MSE	MET	modified residue	? P04275
A	998	MSE	MET	modified residue	? P04275
A	1022	MSE	MET	modified residue	? P04275
A	1097	MSE	MET	modified residue	? P04275
B	916	GLY	-	cloning artifact	? P04275
B	917	SER	-	cloning artifact	? P04275
B	918	HIS	-	cloning artifact	? P04275
B	919	MSE	-	cloning artifact	? P04275
B	947	MSE	MET	modified residue	? P04275
B	998	MSE	MET	modified residue	? P04275
B	1022	MSE	MET	modified residue	? P04275
B	1097	MSE	MET	modified residue	? P04275
C	916	GLY	-	cloning artifact	? P04275
C	917	SER	-	cloning artifact	? P04275
C	918	HIS	-	cloning artifact	? P04275
C	919	MSE	-	cloning artifact	? P04275
C	947	MSE	MET	modified residue	? P04275
C	998	MSE	MET	modified residue	? P04275
C	1022	MSE	MET	modified residue	? P04275

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1097	MSE	MET	modified residue	? P04275

- Molecule 2 is a protein called IMMUNOGLOBULIN IGG RU5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	210	1578	999	258	316	5	0	0	0
2	I	210	1578	999	258	316	5	0	0	0
2	J	210	1578	999	258	316	5	0	0	0

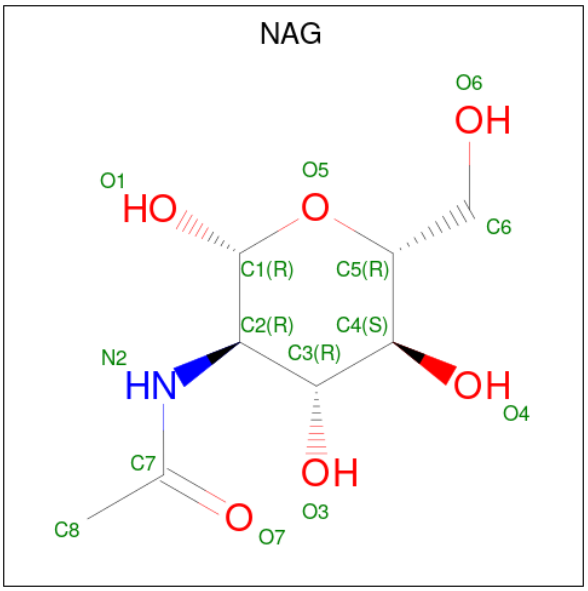
- Molecule 3 is a protein called IMMUNOGLOBULIN IGG RU5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	1629	1009	277	337	6	0	0	0
3	M	211	1629	1009	277	337	6	0	0	0
3	N	211	1629	1009	277	337	6	0	0	0

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

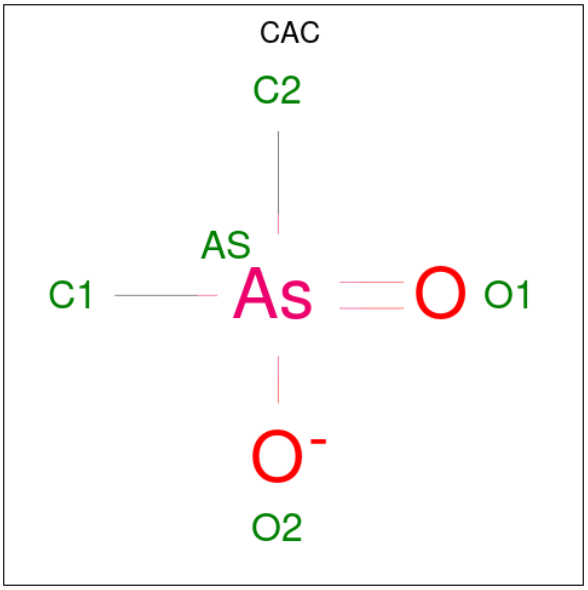
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	24	14	1	9	0	0	0
4	E	2	24	14	1	9	0	0	0
4	F	2	24	14	1	9	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
6	L	1	5	1	2	2	0	0

- Molecule 7 is water.

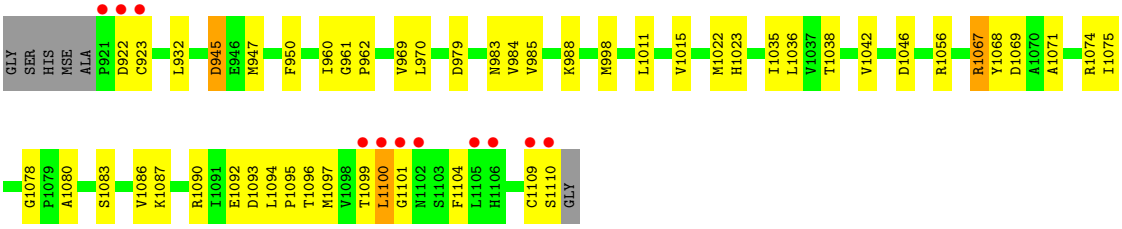
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	84	84	84	0	0
			Total	O		
7	H	87	87	87	0	0
			Total	O		
7	L	163	163	163	0	0
			Total	O		
7	B	79	79	79	0	0
			Total	O		
7	I	107	107	107	0	0
			Total	O		
7	M	139	139	139	0	0
			Total	O		
7	C	58	58	58	0	0
			Total	O		
7	J	48	48	48	0	0
			Total	O		
7	N	113	113	113	0	0

3 Residue-property plots (i)

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

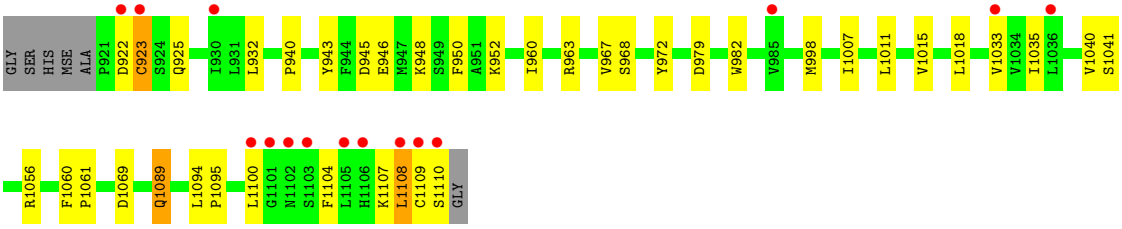
• Molecule 1: VON WILLEBRAND FACTOR

Chain A:



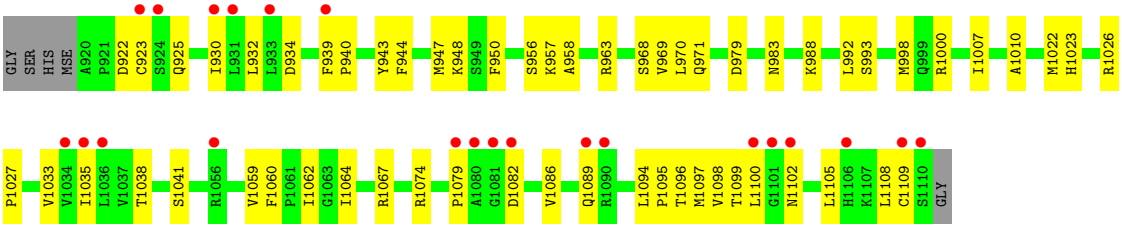
• Molecule 1: VON WILLEBRAND FACTOR

Chain B:



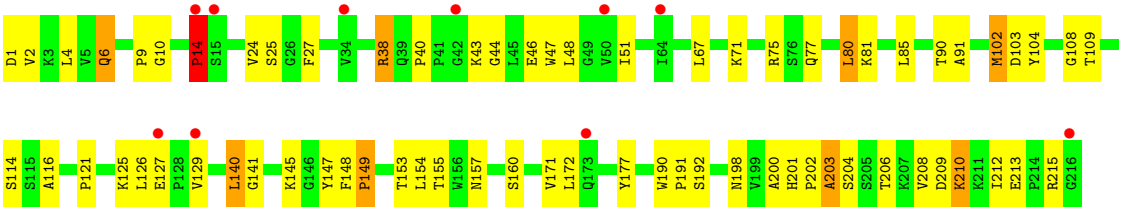
• Molecule 1: VON WILLEBRAND FACTOR

Chain C:



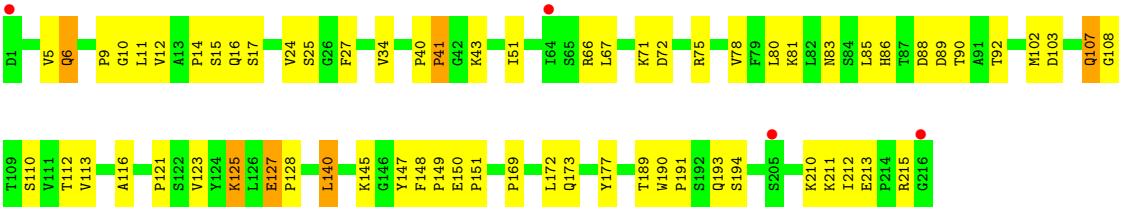
• Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain H:



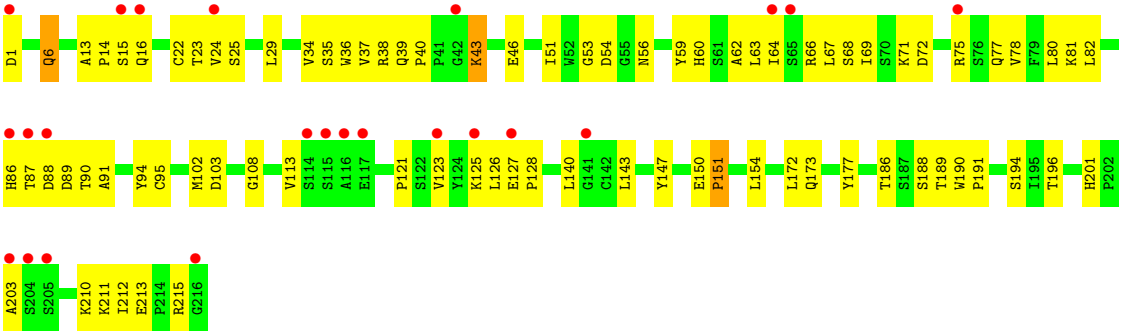
• Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain I:



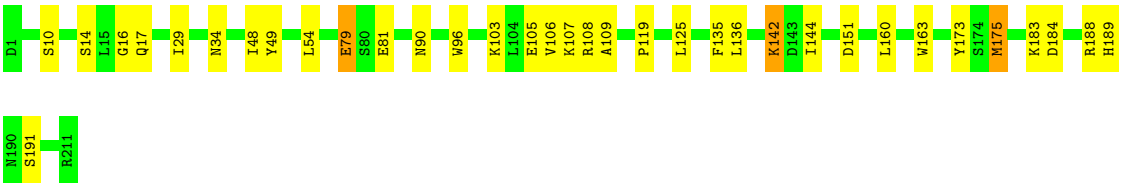
• Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain J:



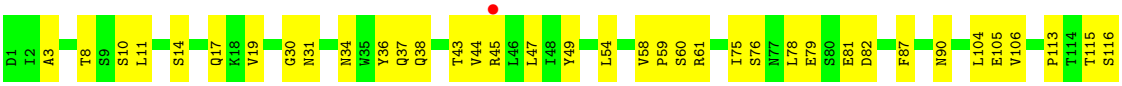
• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain L:



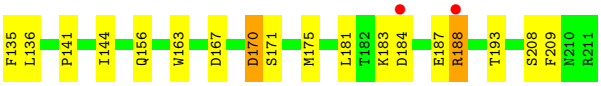
• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain M:



• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain N:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.80Å 183.60Å 131.80Å 90.00° 116.20° 90.00°	Depositor
Resolution (Å)	29.90 – 2.03 29.90 – 2.03	Depositor EDS
% Data completeness (in resolution range)	85.9 (29.90-2.03) 85.8 (29.90-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.264 0.220 , 0.256	Depositor DCC
R_{free} test set	7206 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14872	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, CAC

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	0.36	0/1443	0.63	0/1956
1	B	0.34	0/1443	0.62	0/1956
1	C	0.32	0/1448	0.59	0/1964
2	H	0.35	0/1618	0.66	0/2215
2	I	0.34	0/1618	0.69	0/2215
2	J	0.31	0/1618	0.62	0/2215
3	L	0.39	0/1664	0.67	0/2260
3	M	0.37	0/1664	0.65	0/2260
3	N	0.34	0/1664	0.62	0/2260
All	All	0.35	0/14180	0.64	0/19301

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	1421	0	1433	40	0
1	B	1421	0	1433	29	0
1	C	1426	0	1437	49	0
2	H	1578	0	1540	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1578	0	1540	53	0
2	J	1578	0	1540	89	0
3	L	1629	0	1554	35	0
3	M	1629	0	1554	45	0
3	N	1629	0	1554	39	0
4	D	24	0	22	8	0
4	E	24	0	22	6	0
4	F	24	0	22	8	0
5	H	14	0	13	2	0
5	I	14	0	13	1	0
6	L	5	0	0	0	0
7	A	84	0	0	3	0
7	B	79	0	0	1	0
7	C	58	0	0	2	0
7	H	87	0	0	2	0
7	I	107	0	0	5	0
7	J	48	0	0	2	0
7	L	163	0	0	8	0
7	M	139	0	0	9	0
7	N	113	0	0	2	0
All	All	14872	0	13677	439	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 16.

All (439) 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:944:PHE:HA	1:C:947:MSE:HE3	1.31	1.06
2:J:90:THR:HG22	2:J:113:VAL:H	1.22	1.04
2:H:121:PRO:HB3	2:H:147:TYR:HB3	1.48	0.96
2:J:150:GLU:HG3	2:J:151:PRO:HA	1.52	0.92
1:B:1108:LEU:HD23	1:B:1108:LEU:H	1.36	0.91
2:I:40:PRO:HG2	2:I:43:LYS:HB2	1.58	0.85
2:I:121:PRO:HB3	2:I:147:TYR:HB3	1.59	0.83
1:B:1035:ILE:HG23	1:B:1061:PRO:HA	1.62	0.82
1:A:988:LYS:HB2	4:D:2:FUC:H4	1.60	0.82
2:H:38:ARG:HG2	2:H:48:LEU:HD21	1.61	0.81
2:I:6:GLN:H	2:I:107:GLN:HE22	1.29	0.81
2:I:125:LYS:HZ3	2:I:213:GLU:H	1.29	0.79
2:H:127:GLU:HG2	2:H:213:GLU:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1062:ILE:HD13	1:C:1097:MSE:HE1	1.64	0.78
2:J:90:THR:HG22	2:J:113:VAL:N	1.99	0.78
2:J:43:LYS:HE3	2:J:43:LYS:HA	1.65	0.77
2:J:121:PRO:HB3	2:J:147:TYR:HB3	1.67	0.76
4:E:1:NAG:H61	4:E:2:FUC:H5	1.68	0.76
1:A:1097:MSE:HE2	1:A:1104:PHE:CD1	2.21	0.76
1:C:993:SER:HB2	2:J:54:ASP:HB2	1.68	0.75
3:L:142:LYS:HB2	7:L:1058:HOH:O	1.85	0.75
3:M:38:GLN:HG3	7:M:312:HOH:O	1.87	0.75
4:D:1:NAG:H62	4:D:2:FUC:H3	1.68	0.74
2:I:127:GLU:HG2	2:I:213:GLU:O	1.87	0.73
4:F:1:NAG:H61	4:F:2:FUC:H5	1.69	0.73
2:J:127:GLU:HG2	2:J:213:GLU:O	1.88	0.73
2:J:6:GLN:H	2:J:6:GLN:HE21	1.37	0.73
5:H:553:NAG:C1	4:D:1:NAG:H4	2.19	0.73
2:J:40:PRO:HB2	2:J:43:LYS:HB2	1.69	0.72
1:C:944:PHE:CA	1:C:947:MSE:HE3	2.16	0.72
1:C:944:PHE:HA	1:C:947:MSE:CE	2.16	0.72
2:J:90:THR:CG2	2:J:113:VAL:H	2.01	0.71
3:N:183:LYS:O	3:N:187:GLU:HG2	1.91	0.70
2:J:6:GLN:NE2	2:J:108:GLY:H	1.89	0.70
3:M:79:GLU:HG2	3:M:81:GLU:H	1.57	0.69
3:M:167:ASP:OD2	3:M:170:ASP:HB2	1.93	0.69
2:H:51:ILE:HD13	2:H:71:LYS:HG2	1.73	0.69
4:E:1:NAG:H61	4:E:2:FUC:H3	1.73	0.69
2:I:125:LYS:NZ	2:I:213:GLU:H	1.91	0.68
1:A:1094:LEU:HB3	1:A:1095:PRO:HD3	1.76	0.68
2:H:125:LYS:HE3	2:H:210:LYS:HD2	1.75	0.67
3:M:54:LEU:HD11	3:M:60:SER:HA	1.75	0.67
3:N:108:ARG:HG2	3:N:108:ARG:HH11	1.59	0.67
2:I:6:GLN:NE2	2:I:107:GLN:NE2	2.42	0.67
3:N:184:ASP:HB3	3:N:188:ARG:NH1	2.09	0.67
7:I:584:HOH:O	4:E:1:NAG:H4	1.94	0.66
2:H:6:GLN:H	2:H:6:GLN:HE21	1.43	0.65
2:I:72:ASP:OD1	2:I:75:ARG:HD3	1.95	0.65
3:L:108:ARG:HG2	3:L:109:ALA:N	2.11	0.65
2:J:87:THR:O	2:J:90:THR:HG23	1.96	0.65
5:H:553:NAG:H82	4:D:1:NAG:O4	1.97	0.65
2:J:86:HIS:C	2:J:88:ASP:H	1.99	0.64
3:L:14:SER:HB2	3:L:17:GLN:HE21	1.62	0.64
2:I:145:LYS:HE2	7:I:582:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:ARG:HG2	1:A:1056:ARG:HH11	1.63	0.63
3:M:78:LEU:HD11	3:M:104:LEU:HD21	1.80	0.63
3:L:105:GLU:HG3	3:L:173:TYR:OH	1.98	0.63
3:N:105:GLU:HG2	3:N:106:VAL:N	2.14	0.63
1:B:932:LEU:HD23	1:B:1035:ILE:HD13	1.81	0.63
1:B:1040:VAL:HG12	1:B:1069:ASP:HB2	1.79	0.63
2:I:6:GLN:NE2	2:I:108:GLY:H	1.97	0.63
2:H:6:GLN:HB2	2:H:109:THR:HG23	1.80	0.63
2:J:150:GLU:HG3	2:J:151:PRO:CA	2.29	0.63
1:B:923:CYS:HB2	1:B:1110:SER:O	1.99	0.62
2:J:23:THR:HG22	2:J:77:GLN:HG2	1.80	0.62
2:I:194:SER:HB2	2:I:211:LYS:HE2	1.81	0.62
3:L:183:LYS:HE3	7:L:1112:HOH:O	1.98	0.62
2:J:87:THR:H	2:J:113:VAL:HG11	1.65	0.62
1:B:945:ASP:HB2	7:B:488:HOH:O	2.00	0.62
3:M:10:SER:HB2	7:M:276:HOH:O	2.00	0.62
2:H:172:LEU:HB2	2:H:177:TYR:CE1	2.34	0.61
3:L:184:ASP:HB3	3:L:188:ARG:HH12	1.65	0.61
1:C:934:ASP:O	1:C:947:MSE:HE1	2.00	0.61
4:D:1:NAG:H62	4:D:2:FUC:H5	1.82	0.61
2:J:38:ARG:HD2	2:J:46:GLU:OE1	2.01	0.61
1:A:979:ASP:OD2	1:A:998:MSE:HE3	1.99	0.61
1:C:1062:ILE:CD1	1:C:1097:MSE:HE1	2.30	0.60
2:J:140:LEU:HD12	2:J:212:ILE:HG21	1.83	0.60
2:J:86:HIS:O	2:J:88:ASP:N	2.34	0.60
3:L:79:GLU:OE2	1:C:1023:HIS:HE1	1.83	0.60
2:H:80:LEU:C	2:H:80:LEU:HD13	2.22	0.60
2:H:6:GLN:HE22	2:H:108:GLY:H	1.49	0.60
2:I:5:VAL:HA	2:I:107:GLN:HE21	1.67	0.59
1:C:1007:ILE:HG23	1:C:1035:ILE:HD11	1.83	0.59
2:J:67:LEU:HD11	2:J:80:LEU:HD21	1.84	0.59
2:J:87:THR:HA	2:J:113:VAL:HB	1.84	0.59
2:H:44:GLY:HA3	7:L:1065:HOH:O	2.03	0.59
2:J:67:LEU:HD11	2:J:80:LEU:CD2	2.32	0.59
2:I:6:GLN:H	2:I:6:GLN:HE21	1.49	0.59
3:M:11:LEU:HD21	7:M:344:HOH:O	2.02	0.59
2:J:6:GLN:HE22	2:J:108:GLY:H	1.48	0.59
1:B:1104:PHE:O	1:B:1107:LYS:HB2	2.03	0.59
1:B:979:ASP:OD2	1:B:998:MSE:HE3	2.03	0.58
2:I:6:GLN:NE2	2:I:107:GLN:HE22	2.00	0.58
1:C:988:LYS:O	1:C:992:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:16:GLY:O	3:N:77:ASN:HA	2.03	0.58
2:H:210:LYS:HB2	2:H:210:LYS:NZ	2.19	0.58
3:M:54:LEU:HD22	3:M:58:VAL:HB	1.85	0.58
2:H:125:LYS:HD3	2:H:127:GLU:OE1	2.04	0.58
2:H:154:LEU:HD23	2:H:155:THR:N	2.19	0.58
2:I:173:GLN:HG2	7:I:638:HOH:O	2.04	0.58
1:C:956:SER:HA	1:C:988:LYS:HD3	1.85	0.58
1:C:1074:ARG:HG3	1:C:1082:ASP:OD2	2.04	0.58
2:H:116:ALA:HB3	2:H:148:PHE:CE2	2.39	0.58
2:J:186:THR:HB	2:J:189:THR:HG23	1.85	0.57
2:H:208:VAL:HG12	2:H:209:ASP:N	2.19	0.57
2:H:6:GLN:NE2	2:H:108:GLY:H	2.01	0.57
4:E:1:NAG:H61	4:E:2:FUC:C5	2.34	0.57
1:A:1086:VAL:HG21	1:A:1097:MSE:CE	2.35	0.57
2:H:43:LYS:HB3	7:H:596:HOH:O	2.05	0.57
3:L:105:GLU:HG2	3:L:106:VAL:N	2.20	0.57
1:A:1022:MSE:HG2	7:N:286:HOH:O	2.05	0.57
1:C:943:TYR:O	1:C:947:MSE:HG3	2.05	0.57
2:I:6:GLN:HE21	2:I:107:GLN:HE22	1.51	0.57
2:J:38:ARG:HD3	2:J:40:PRO:HG3	1.87	0.56
3:L:16:GLY:N	1:C:1022:MSE:HE1	2.21	0.56
2:I:67:LEU:HD11	2:I:80:LEU:CD2	2.36	0.56
3:M:43:THR:HA	7:M:277:HOH:O	2.05	0.56
2:J:186:THR:HG22	2:J:188:SER:H	1.70	0.56
4:D:1:NAG:H62	4:D:2:FUC:C3	2.35	0.56
3:L:151:ASP:HA	3:L:191:SER:OG	2.06	0.56
4:E:1:NAG:H61	4:E:2:FUC:C3	2.36	0.56
2:I:5:VAL:HA	2:I:107:GLN:NE2	2.20	0.56
2:I:140:LEU:HG	2:I:212:ILE:HG21	1.88	0.56
1:C:939:PHE:HB3	1:C:940:PRO:CD	2.35	0.55
2:J:39:GLN:C	2:J:91:ALA:HB1	2.26	0.55
2:J:16:GLN:HG2	7:J:567:HOH:O	2.06	0.55
2:H:157:ASN:HB3	2:H:160:SER:HB3	1.88	0.55
2:J:201:HIS:CE1	2:J:203:ALA:HB3	2.41	0.55
3:N:126:THR:HG22	3:N:126:THR:O	2.07	0.55
2:I:116:ALA:HB3	2:I:148:PHE:CE2	2.42	0.55
3:M:31:ASN:HD21	3:N:156:GLN:NE2	2.06	0.54
1:C:1095:PRO:O	1:C:1099:THR:HG23	2.08	0.54
3:L:81:GLU:HG2	7:L:1051:HOH:O	2.06	0.54
2:I:51:ILE:HD13	2:I:71:LYS:HG2	1.90	0.54
1:B:1011:LEU:O	1:B:1015:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:19:VAL:HG22	3:M:75:ILE:HB	1.89	0.53
3:N:144:ILE:HG22	3:N:163:TRP:CZ3	2.43	0.53
2:I:6:GLN:H	2:I:6:GLN:NE2	2.06	0.53
1:C:1038:THR:HG22	1:C:1064:ILE:HB	1.91	0.53
2:J:6:GLN:HE21	2:J:6:GLN:N	2.03	0.53
1:A:1090:ARG:HG2	1:A:1093:ASP:OD2	2.08	0.53
3:N:108:ARG:HG2	3:N:109:ALA:N	2.22	0.53
2:J:80:LEU:C	2:J:80:LEU:HD13	2.29	0.53
1:B:1108:LEU:H	1:B:1108:LEU:CD2	2.16	0.53
2:I:6:GLN:HE22	2:I:108:GLY:H	1.56	0.53
1:C:1098:VAL:HG13	1:C:1105:LEU:HD21	1.90	0.53
2:J:59:TYR:HE2	2:J:69:ILE:HG13	1.74	0.53
2:I:86:HIS:O	2:I:113:VAL:HG11	2.09	0.53
3:M:105:GLU:HG2	3:M:106:VAL:N	2.23	0.53
3:N:14:SER:O	3:N:17:GLN:HB2	2.09	0.53
2:J:40:PRO:HA	2:J:91:ALA:HB2	1.90	0.52
1:C:922:ASP:OD2	1:C:925:GLN:HG2	2.08	0.52
1:A:1104:PHE:HB3	7:A:750:HOH:O	2.09	0.52
3:L:107:LYS:HB2	3:L:107:LYS:NZ	2.24	0.52
2:J:14:PRO:C	2:J:16:GLN:H	2.12	0.52
1:B:972:TYR:CE2	1:B:1035:ILE:HD11	2.44	0.52
2:H:171:VAL:HG11	3:L:160:LEU:HG	1.92	0.52
2:I:125:LYS:HD3	3:M:123:GLU:OE1	2.09	0.52
3:M:136:LEU:HD12	3:M:136:LEU:N	2.24	0.52
2:H:80:LEU:HD22	2:H:81:LYS:N	2.23	0.52
2:H:215:ARG:CZ	3:L:119:PRO:HG2	2.40	0.52
2:I:125:LYS:HZ2	2:I:127:GLU:CG	2.22	0.52
2:H:51:ILE:CD1	2:H:71:LYS:HG2	2.40	0.52
3:M:167:ASP:HB3	3:M:170:ASP:HB3	1.90	0.52
2:I:90:THR:HG23	2:I:112:THR:HA	1.92	0.51
4:D:1:NAG:C6	4:D:2:FUC:H5	2.39	0.51
3:L:14:SER:CB	3:L:17:GLN:HE21	2.23	0.51
1:A:1056:ARG:HG2	1:A:1056:ARG:NH1	2.24	0.51
1:A:1042:VAL:HA	2:J:189:THR:HG21	1.93	0.51
1:A:1078:GLY:HA2	7:A:459:HOH:O	2.10	0.51
3:L:48:ILE:HD13	3:L:54:LEU:HD23	1.92	0.51
2:J:38:ARG:HG2	2:J:40:PRO:HD3	1.93	0.51
3:L:188:ARG:HD3	7:L:1142:HOH:O	2.10	0.51
1:B:1007:ILE:HD12	1:B:1041:SER:HB2	1.93	0.51
2:J:51:ILE:HG23	2:J:51:ILE:O	2.10	0.51
3:N:181:LEU:HD23	3:N:181:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:305:HOH:O	2:J:173:GLN:HG3	2.09	0.51
2:J:6:GLN:H	2:J:6:GLN:NE2	2.07	0.51
2:I:102:MET:HB2	3:M:36:TYR:CE2	2.45	0.51
3:M:166:GLN:HG2	3:M:171:SER:HA	1.93	0.50
7:J:580:HOH:O	4:F:2:FUC:H4	2.11	0.50
2:I:127:GLU:HB2	2:I:215:ARG:HG3	1.92	0.50
2:H:24:VAL:HG11	2:H:27:PHE:CE1	2.47	0.50
3:M:14:SER:HB2	3:M:17:GLN:NE2	2.26	0.50
1:A:1011:LEU:O	1:A:1015:VAL:HG23	2.12	0.50
2:H:102:MET:HE1	3:L:96:TRP:CE3	2.46	0.50
3:M:163:TRP:N	3:M:163:TRP:CD1	2.79	0.50
1:C:957:LYS:HD3	1:C:1098:VAL:HG12	1.93	0.50
2:J:86:HIS:C	2:J:88:ASP:N	2.65	0.50
2:J:190:TRP:CG	2:J:191:PRO:HA	2.47	0.50
2:H:38:ARG:HD2	2:H:46:GLU:OE1	2.12	0.50
2:J:90:THR:O	2:J:91:ALA:HB2	2.11	0.50
2:J:90:THR:HG22	2:J:113:VAL:HB	1.94	0.49
2:J:172:LEU:HB2	2:J:177:TYR:CE1	2.47	0.49
2:J:56:ASN:HA	4:F:1:NAG:C8	2.41	0.49
2:J:128:PRO:O	2:J:215:ARG:HD2	2.12	0.49
2:H:102:MET:HE1	3:L:96:TRP:HE3	1.77	0.49
1:B:1108:LEU:HD23	1:B:1108:LEU:N	2.18	0.49
2:I:12:VAL:HG11	2:I:85:LEU:CD1	2.43	0.49
2:I:12:VAL:O	2:I:113:VAL:HA	2.11	0.49
3:N:108:ARG:HG2	3:N:108:ARG:NH1	2.26	0.49
3:N:163:TRP:N	3:N:163:TRP:CD1	2.81	0.49
2:H:126:LEU:HB2	2:H:141:GLY:CA	2.43	0.49
1:B:943:TYR:O	1:B:946:GLU:HB2	2.13	0.49
1:A:923:CYS:N	1:A:1109:CYS:HB2	2.28	0.49
2:J:72:ASP:HB3	2:J:75:ARG:HB2	1.95	0.49
1:C:950:PHE:HB2	1:C:1094:LEU:HG	1.94	0.49
1:C:1086:VAL:HG11	1:C:1097:MSE:SE	2.62	0.49
1:A:947:MSE:HG2	1:A:1036:LEU:HD23	1.95	0.48
3:L:125:LEU:O	3:L:183:LYS:HD2	2.13	0.48
3:M:59:PRO:C	3:M:61:ARG:H	2.15	0.48
2:J:39:GLN:O	2:J:91:ALA:HB1	2.13	0.48
1:A:932:LEU:HD23	1:A:1035:ILE:HD12	1.95	0.48
2:I:80:LEU:HD13	2:I:80:LEU:C	2.33	0.48
1:B:922:ASP:HB3	1:B:925:GLN:CG	2.43	0.48
1:B:1094:LEU:HB3	1:B:1095:PRO:CD	2.43	0.48
4:F:1:NAG:H61	4:F:2:FUC:C5	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:123:VAL:HG23	2:J:123:VAL:O	2.13	0.48
3:L:14:SER:HB2	3:L:17:GLN:NE2	2.28	0.48
2:H:153:THR:OG1	2:H:200:ALA:HB3	2.13	0.48
2:I:81:LYS:HE3	2:I:83:ASN:OD1	2.13	0.48
2:J:37:VAL:HG23	2:J:94:TYR:HB2	1.94	0.48
2:I:16:GLN:HG2	2:I:17:SER:H	1.79	0.48
2:I:128:PRO:O	2:I:215:ARG:HD2	2.13	0.48
3:M:31:ASN:HD21	3:N:156:GLN:HE22	1.62	0.48
2:J:43:LYS:HA	2:J:43:LYS:CE	2.38	0.48
2:I:107:GLN:HG3	7:I:560:HOH:O	2.14	0.47
2:H:2:VAL:HG11	2:H:104:TYR:CG	2.48	0.47
2:H:40:PRO:HB2	2:H:43:LYS:HE2	1.95	0.47
3:L:34:ASN:OD1	3:L:49:TYR:HA	2.15	0.47
2:J:14:PRO:O	2:J:16:GLN:N	2.47	0.47
3:N:119:PRO:HG3	3:N:209:PHE:CD2	2.49	0.47
4:F:1:NAG:C6	4:F:2:FUC:H5	2.42	0.47
1:C:958:ALA:O	1:C:988:LYS:NZ	2.48	0.47
1:C:1105:LEU:N	1:C:1105:LEU:HD22	2.29	0.47
1:B:968:SER:HB2	1:B:982:TRP:CE3	2.49	0.47
2:I:123:VAL:O	2:I:210:LYS:HE3	2.15	0.47
3:M:182:THR:HA	7:M:350:HOH:O	2.15	0.47
2:J:29:LEU:O	2:J:53:GLY:HA2	2.14	0.47
2:J:87:THR:C	2:J:89:ASP:H	2.15	0.47
3:N:110:ASP:OD1	3:N:141:PRO:HD3	2.15	0.47
1:A:1038:THR:O	1:A:1067:ARG:HB2	2.15	0.47
1:C:930:ILE:HG12	1:C:968:SER:OG	2.14	0.47
1:C:979:ASP:OD2	1:C:998:MSE:HE3	2.15	0.47
2:J:194:SER:HB2	2:J:211:LYS:HE3	1.97	0.47
2:J:196:THR:HG23	2:J:210:LYS:O	2.15	0.47
2:J:102:MET:HB2	3:N:36:TYR:CE2	2.50	0.46
1:C:1074:ARG:HH11	1:C:1074:ARG:HG2	1.79	0.46
3:N:170:ASP:O	3:N:171:SER:HB2	2.14	0.46
1:C:1060:PHE:CE1	1:C:1108:LEU:HG	2.49	0.46
2:J:140:LEU:N	2:J:140:LEU:HD22	2.30	0.46
1:A:1086:VAL:HG21	1:A:1097:MSE:HE3	1.96	0.46
2:H:80:LEU:HD22	2:H:81:LYS:H	1.81	0.46
2:H:90:THR:O	2:H:91:ALA:HB2	2.15	0.46
3:M:36:TYR:HB2	3:M:87:PHE:CZ	2.50	0.46
2:J:53:GLY:HA2	2:J:71:LYS:NZ	2.31	0.46
2:H:24:VAL:HG12	2:H:25:SER:N	2.31	0.46
2:J:56:ASN:ND2	4:F:2:FUC:H61	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:128:PRO:HD3	2:J:140:LEU:HD13	1.98	0.46
2:J:154:LEU:C	2:J:154:LEU:HD23	2.36	0.46
2:H:149:PRO:HD2	2:H:203:ALA:CB	2.46	0.46
3:N:47:LEU:HD11	3:N:86:TYR:HE2	1.81	0.46
3:N:79:GLU:HB2	3:N:82:ASP:OD2	2.16	0.46
2:J:6:GLN:NE2	2:J:6:GLN:N	2.63	0.46
2:I:11:LEU:HD22	2:I:149:PRO:HG3	1.98	0.45
2:I:51:ILE:HG23	2:I:51:ILE:O	2.15	0.45
1:C:947:MSE:O	1:C:950:PHE:HB3	2.15	0.45
1:C:1007:ILE:HD12	1:C:1041:SER:HB2	1.99	0.45
2:J:127:GLU:HG3	2:J:212:ILE:CG2	2.46	0.45
1:A:1022:MSE:HE3	7:L:1103:HOH:O	2.17	0.45
2:I:169:PRO:HD2	3:M:162:SER:OG	2.16	0.45
2:J:87:THR:H	2:J:113:VAL:CG1	2.30	0.45
3:L:151:ASP:OD2	3:L:189:HIS:HD2	2.00	0.45
1:B:1056:ARG:HH11	1:B:1056:ARG:HG2	1.82	0.45
1:C:1067:ARG:HG2	1:C:1067:ARG:HH11	1.82	0.45
2:J:87:THR:C	2:J:89:ASP:N	2.70	0.45
2:H:24:VAL:HG11	2:H:27:PHE:CZ	2.52	0.45
2:I:172:LEU:HB2	2:I:177:TYR:CE1	2.52	0.45
1:C:944:PHE:O	1:C:948:LYS:HG3	2.17	0.45
2:J:22:CYS:HB2	2:J:36:TRP:CH2	2.52	0.45
2:J:37:VAL:CG2	2:J:94:TYR:HB2	2.47	0.45
2:J:125:LYS:O	2:J:126:LEU:HD23	2.17	0.45
4:F:1:NAG:H61	4:F:2:FUC:H3	1.99	0.45
2:I:190:TRP:CG	2:I:191:PRO:HA	2.52	0.45
3:M:43:THR:C	7:M:312:HOH:O	2.55	0.45
3:N:47:LEU:HD11	3:N:86:TYR:CE2	2.51	0.45
4:E:1:NAG:C6	4:E:2:FUC:H5	2.42	0.45
1:A:1086:VAL:HG21	1:A:1097:MSE:HE1	2.00	0.45
5:I:553:NAG:H62	7:I:629:HOH:O	2.16	0.45
1:C:971:GLN:HE22	1:C:1000:ARG:HA	1.82	0.44
3:N:45:ARG:HG3	3:N:45:ARG:NH1	2.32	0.44
1:A:960:ILE:HG22	1:A:961:GLY:N	2.31	0.44
1:B:960:ILE:HD11	1:B:967:VAL:HG23	1.99	0.44
1:B:1060:PHE:CE1	1:B:1108:LEU:HB3	2.52	0.44
1:C:983:ASN:N	1:C:983:ASN:ND2	2.65	0.44
3:M:59:PRO:C	3:M:61:ARG:N	2.71	0.44
3:N:45:ARG:HG3	3:N:45:ARG:HH11	1.82	0.44
1:A:922:ASP:HA	1:A:1110:SER:H	1.82	0.44
1:A:950:PHE:HB2	1:A:1094:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:TYR:OH	1:A:1087:LYS:HD3	2.17	0.44
2:H:190:TRP:CG	2:H:191:PRO:HA	2.52	0.44
1:B:972:TYR:HE2	1:B:1035:ILE:HD11	1.81	0.44
3:M:113:PRO:HB3	3:M:139:PHE:HB3	2.00	0.44
3:M:116:SER:O	3:M:134:CYS:HA	2.17	0.44
3:N:33:LEU:HG	3:N:71:TYR:CG	2.53	0.44
3:L:108:ARG:HG2	3:L:109:ALA:H	1.79	0.44
2:I:9:PRO:HG2	2:I:10:GLY:H	1.82	0.44
3:M:61:ARG:NH1	3:M:82:ASP:OD2	2.50	0.44
1:C:963:ARG:CZ	3:N:30:GLY:HA2	2.47	0.44
3:N:89:GLN:NE2	3:N:90:ASN:O	2.50	0.44
1:A:983:ASN:ND2	1:A:983:ASN:N	2.65	0.44
2:I:24:VAL:HG12	2:I:25:SER:N	2.33	0.44
2:J:13:ALA:O	2:J:16:GLN:HB2	2.18	0.44
2:J:24:VAL:CG1	2:J:25:SER:N	2.80	0.44
3:N:5:THR:HG23	7:N:235:HOH:O	2.18	0.44
1:B:950:PHE:HB2	1:B:1094:LEU:HG	1.99	0.43
3:M:14:SER:CB	3:M:17:GLN:NE2	2.81	0.43
2:J:66:ARG:HH21	2:J:82:LEU:HG	1.83	0.43
3:N:38:GLN:O	3:N:84:ALA:HB1	2.18	0.43
1:A:1100:LEU:HG	1:A:1101:GLY:N	2.33	0.43
2:H:24:VAL:CG1	2:H:25:SER:N	2.81	0.43
2:H:51:ILE:HG23	2:H:51:ILE:O	2.18	0.43
2:I:14:PRO:C	2:I:16:GLN:H	2.21	0.43
3:M:34:ASN:OD1	3:M:49:TYR:HA	2.18	0.43
1:C:969:VAL:C	1:C:970:LEU:HD12	2.37	0.43
1:C:1094:LEU:HB3	1:C:1095:PRO:CD	2.47	0.43
3:L:10:SER:HA	3:L:103:LYS:O	2.18	0.43
2:J:59:TYR:HB2	2:J:64:ILE:HG12	2.00	0.43
2:J:127:GLU:HG3	2:J:212:ILE:HG23	2.00	0.43
1:A:984:VAL:O	1:A:985:VAL:C	2.56	0.43
1:A:1046:ASP:OD1	1:A:1075:ILE:HD13	2.18	0.43
2:H:157:ASN:HA	7:H:628:HOH:O	2.18	0.43
2:I:24:VAL:CG1	2:I:25:SER:N	2.81	0.43
2:J:35:SER:O	2:J:95:CYS:HA	2.19	0.43
2:H:9:PRO:HG2	2:H:10:GLY:H	1.82	0.43
1:A:1023:HIS:HE1	3:N:81:GLU:OE2	2.02	0.43
1:A:1090:ARG:HG3	1:A:1092:GLU:HB2	1.99	0.43
1:B:948:LYS:O	1:B:952:LYS:HG3	2.19	0.43
2:I:66:ARG:HH22	2:I:89:ASP:CG	2.22	0.43
2:J:68:SER:OG	2:J:81:LYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:130:ALA:HB3	3:N:181:LEU:O	2.19	0.43
1:A:945:ASP:HB3	7:A:509:HOH:O	2.19	0.43
2:H:6:GLN:HE21	2:H:6:GLN:N	2.12	0.43
2:H:121:PRO:CB	2:H:147:TYR:HB3	2.34	0.43
2:H:75:ARG:O	2:H:77:GLN:HG3	2.19	0.43
3:L:14:SER:H	3:L:17:GLN:NE2	2.17	0.43
3:M:44:VAL:HG22	7:M:312:HOH:O	2.18	0.43
1:A:1080:ALA:O	1:A:1083:SER:HB2	2.19	0.42
2:H:157:ASN:CB	2:H:160:SER:HB3	2.49	0.42
2:H:208:VAL:CG1	2:H:209:ASP:N	2.81	0.42
3:N:181:LEU:HD23	3:N:181:LEU:H	1.83	0.42
3:M:115:THR:HA	3:M:135:PHE:O	2.20	0.42
1:A:969:VAL:C	1:A:970:LEU:HD12	2.40	0.42
1:A:985:VAL:HG11	3:L:96:TRP:HZ2	1.83	0.42
2:H:38:ARG:HG3	2:H:46:GLU:HB2	2.01	0.42
2:I:189:THR:O	2:I:193:GLN:HB2	2.19	0.42
1:C:983:ASN:N	1:C:983:ASN:HD22	2.16	0.42
1:C:1067:ARG:O	1:C:1067:ARG:HG3	2.19	0.42
1:A:962:PRO:HB3	3:L:29:ILE:O	2.19	0.42
2:H:14:PRO:O	2:H:85:LEU:HB2	2.19	0.42
2:H:129:VAL:HG11	7:L:1160:HOH:O	2.19	0.42
3:L:135:PHE:C	3:L:136:LEU:HD12	2.40	0.42
1:C:1026:ARG:HA	1:C:1027:PRO:HD3	1.86	0.42
2:J:121:PRO:HB3	2:J:147:TYR:CB	2.42	0.42
3:N:119:PRO:HG3	3:N:209:PHE:CE2	2.54	0.42
2:H:4:LEU:N	2:H:4:LEU:HD12	2.34	0.42
2:H:149:PRO:HD2	2:H:203:ALA:HB1	2.00	0.42
2:H:202:PRO:O	2:H:204:SER:N	2.53	0.42
1:C:1105:LEU:HD22	1:C:1105:LEU:H	1.84	0.42
2:H:121:PRO:HB3	2:H:147:TYR:CB	2.34	0.42
1:B:968:SER:HB2	1:B:982:TRP:CZ3	2.54	0.42
1:B:1018:LEU:HD11	1:B:1033:VAL:CG2	2.50	0.42
1:B:1089:GLN:HE21	1:B:1089:GLN:HB3	1.56	0.42
3:M:61:ARG:CG	3:M:76:SER:O	2.68	0.42
3:M:207:LYS:HD3	3:M:207:LYS:HA	1.89	0.42
2:H:127:GLU:HG3	2:H:212:ILE:HG23	2.02	0.42
2:I:92:THR:HA	2:I:110:SER:HA	2.01	0.42
3:M:118:PHE:HA	3:M:119:PRO:HD3	1.93	0.42
1:C:1089:GLN:HG2	7:C:616:HOH:O	2.18	0.42
1:A:1096:THR:HA	1:A:1099:THR:OG1	2.19	0.42
2:H:67:LEU:HD11	2:H:80:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:14:SER:CB	3:L:17:GLN:NE2	2.83	0.41
1:B:940:PRO:O	1:B:943:TYR:HB2	2.20	0.41
3:M:44:VAL:HG12	3:M:45:ARG:N	2.35	0.41
2:J:80:LEU:HD22	2:J:81:LYS:H	1.84	0.41
3:N:41:ASP:OD1	3:N:43:THR:HG23	2.20	0.41
2:H:47:TRP:CD1	2:H:102:MET:HE1	2.55	0.41
3:L:175:MET:O	3:L:175:MET:HG3	2.20	0.41
3:M:14:SER:HB2	3:M:17:GLN:HE21	1.85	0.41
3:M:37:GLN:HB2	3:M:47:LEU:HD11	2.01	0.41
1:A:1069:ASP:OD2	1:A:1071:ALA:HB3	2.20	0.41
3:L:136:LEU:HD12	3:L:136:LEU:N	2.36	0.41
1:B:963:ARG:CZ	3:M:30:GLY:HA2	2.51	0.41
2:J:60:HIS:NE2	3:N:1:ASP:OD2	2.47	0.41
2:J:196:THR:HG23	2:J:210:LYS:C	2.40	0.41
3:L:144:ILE:HG22	3:L:163:TRP:CZ3	2.56	0.41
2:I:34:VAL:HG21	2:I:78:VAL:HG21	2.02	0.41
3:M:36:TYR:HB2	3:M:87:PHE:CE1	2.55	0.41
3:M:170:ASP:O	3:M:171:SER:HB2	2.20	0.41
2:H:38:ARG:CD	2:H:46:GLU:OE1	2.69	0.41
2:H:145:LYS:HE3	2:H:145:LYS:HB2	1.92	0.41
2:H:191:PRO:O	2:H:192:SER:C	2.58	0.41
1:C:1062:ILE:HA	1:C:1086:VAL:O	2.21	0.41
2:J:34:VAL:HG11	2:J:78:VAL:HG21	2.02	0.41
2:J:66:ARG:HH22	2:J:89:ASP:CG	2.22	0.41
2:H:201:HIS:HB3	2:H:206:THR:HB	2.03	0.41
2:I:14:PRO:O	2:I:15:SER:HB2	2.21	0.41
1:A:1074:ARG:HH11	1:A:1074:ARG:HG2	1.86	0.41
3:N:115:THR:HA	3:N:135:PHE:O	2.20	0.41
2:H:140:LEU:HG	2:H:212:ILE:HG21	2.03	0.41
3:L:184:ASP:HB3	3:L:188:ARG:NH1	2.34	0.41
3:M:3:ALA:HB2	7:M:348:HOH:O	2.21	0.41
3:M:54:LEU:CD1	3:M:60:SER:HA	2.48	0.41
2:J:80:LEU:HD13	2:J:81:LYS:N	2.36	0.41
2:J:121:PRO:CB	2:J:147:TYR:HB3	2.41	0.41
2:J:125:LYS:HE2	3:N:123:GLU:OE2	2.21	0.41
2:J:127:GLU:HB2	2:J:215:ARG:HG3	2.03	0.41
3:M:160:LEU:HD12	3:M:160:LEU:HA	1.94	0.41
4:D:1:NAG:H62	4:D:2:FUC:C5	2.49	0.41
2:I:12:VAL:HG11	2:I:85:LEU:HD12	2.04	0.40
1:C:1033:VAL:CG1	1:C:1059:VAL:HG22	2.52	0.40
2:J:56:ASN:HA	4:F:1:NAG:C7	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:ALA:O	2:J:63:LEU:HD23	2.20	0.40
1:A:983:ASN:N	1:A:983:ASN:HD22	2.18	0.40
2:H:14:PRO:HD3	2:H:114:SER:C	2.41	0.40
1:C:944:PHE:CD1	1:C:947:MSE:HE3	2.56	0.40
2:J:72:ASP:CG	2:J:75:ARG:HB2	2.42	0.40
1:A:1069:ASP:OD2	1:A:1071:ALA:N	2.50	0.40
3:L:29:ILE:HG12	7:L:1009:HOH:O	2.21	0.40
2:I:24:VAL:HG11	2:I:27:PHE:CE1	2.56	0.40
1:C:932:LEU:HD21	1:C:1010:ALA:HB1	2.04	0.40
1:C:1022:MSE:HE2	7:C:162:HOH:O	2.20	0.40
1:C:1096:THR:HA	1:C:1099:THR:OG1	2.21	0.40
3:N:167:ASP:OD2	3:N:170:ASP:HB2	2.20	0.40
1:C:925:GLN:OE1	1:C:925:GLN:HA	2.21	0.40
3:N:136:LEU:N	3:N:136:LEU:HD12	2.35	0.40
3:N:193:THR:OG1	3:N:208:SER:HB3	2.21	0.40
1:B:1056:ARG:HG2	1:B:1056:ARG:NH1	2.36	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	188/196 (96%)	182 (97%)	5 (3%)	1 (0%)	29	22
1	B	188/196 (96%)	180 (96%)	7 (4%)	1 (0%)	29	22
1	C	189/196 (96%)	176 (93%)	10 (5%)	3 (2%)	9	4
2	H	206/210 (98%)	189 (92%)	15 (7%)	2 (1%)	15	9
2	I	206/210 (98%)	194 (94%)	11 (5%)	1 (0%)	29	22
2	J	206/210 (98%)	184 (89%)	21 (10%)	1 (0%)	29	22
3	L	209/211 (99%)	204 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	209/211 (99%)	206 (99%)	3 (1%)	0	100	100
3	N	209/211 (99%)	202 (97%)	7 (3%)	0	100	100
All	All	1810/1851 (98%)	1717 (95%)	84 (5%)	9 (0%)	29	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1100	LEU
1	C	1102	ASN
2	J	15	SER
1	B	1100	LEU
2	I	41	PRO
1	C	1100	LEU
2	H	14	PRO
2	H	203	ALA
1	C	1079	PRO

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	157/155 (101%)	155 (99%)	2 (1%)	69	72
1	B	157/155 (101%)	153 (98%)	4 (2%)	47	48
1	C	157/155 (101%)	155 (99%)	2 (1%)	69	72
2	H	183/183 (100%)	172 (94%)	11 (6%)	19	14
2	I	183/183 (100%)	173 (94%)	10 (6%)	21	16
2	J	183/183 (100%)	177 (97%)	6 (3%)	38	36
3	L	186/186 (100%)	182 (98%)	4 (2%)	52	53
3	M	186/186 (100%)	183 (98%)	3 (2%)	62	66
3	N	186/186 (100%)	182 (98%)	4 (2%)	52	53
All	All	1578/1572 (100%)	1532 (97%)	46 (3%)	42	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	945	ASP
1	A	1067	ARG
2	H	1	ASP
2	H	6	GLN
2	H	14	PRO
2	H	38	ARG
2	H	80	LEU
2	H	102	MET
2	H	103	ASP
2	H	140	LEU
2	H	149	PRO
2	H	198	ASN
2	H	210	LYS
3	L	79	GLU
3	L	90	ASN
3	L	142	LYS
3	L	175	MET
1	B	923	CYS
1	B	1089	GLN
1	B	1108	LEU
1	B	1109	CYS
2	I	6	GLN
2	I	41	PRO
2	I	88	ASP
2	I	103	ASP
2	I	107	GLN
2	I	125	LYS
2	I	127	GLU
2	I	140	LEU
2	I	150	GLU
2	I	151	PRO
3	M	8	THR
3	M	90	ASN
3	M	163	TRP
1	C	923	CYS
1	C	1109	CYS
2	J	1	ASP
2	J	6	GLN
2	J	43	LYS
2	J	103	ASP
2	J	143	LEU
2	J	151	PRO

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Mol	Chain	Res	Type
3	N	90	ASN
3	N	170	ASP
3	N	175	MET
3	N	188	ARG

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

Mol	Chain	Res	Type
1	A	959	ASN
2	H	6	GLN
2	H	173	GLN
3	L	17	GLN
3	L	77	ASN
3	L	94	ASN
3	L	137	ASN
3	L	189	HIS
3	L	190	ASN
1	B	1006	GLN
1	B	1089	GLN
2	I	6	GLN
2	I	107	GLN
3	M	17	GLN
3	M	137	ASN
3	M	145	ASN
3	M	156	GLN
3	M	189	HIS
1	C	959	ASN
1	C	971	GLN
1	C	1023	HIS
1	C	1084	ASN
2	J	6	GLN
2	J	77	GLN
2	J	173	GLN
3	N	55	HIS
3	N	137	ASN
3	N	156	GLN
3	N	210	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

6 monosaccharides 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	D	1	2,4	14,14,15	0.58	0	17,19,21	0.79	0
4	FUC	D	2	4	10,10,11	0.59	0	14,14,16	0.85	1 (7%)
4	NAG	E	1	2,4	14,14,15	0.61	0	17,19,21	0.87	1 (5%)
4	FUC	E	2	4	10,10,11	0.66	0	14,14,16	0.74	0
4	NAG	F	1	2,4	14,14,15	0.57	0	17,19,21	0.70	0
4	FUC	F	2	4	10,10,11	0.72	0	14,14,16	0.85	1 (7%)

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	D	1	2,4	-	1/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1
4	NAG	E	1	2,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	NAG	F	1	2,4	-	0/6/23/26	0/1/1/1
4	FUC	F	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1	NAG	C2-N2-C7	-2.27	119.67	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2	FUC	C1-C2-C3	2.16	112.32	109.67
4	D	2	FUC	C1-C2-C3	2.05	112.18	109.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6

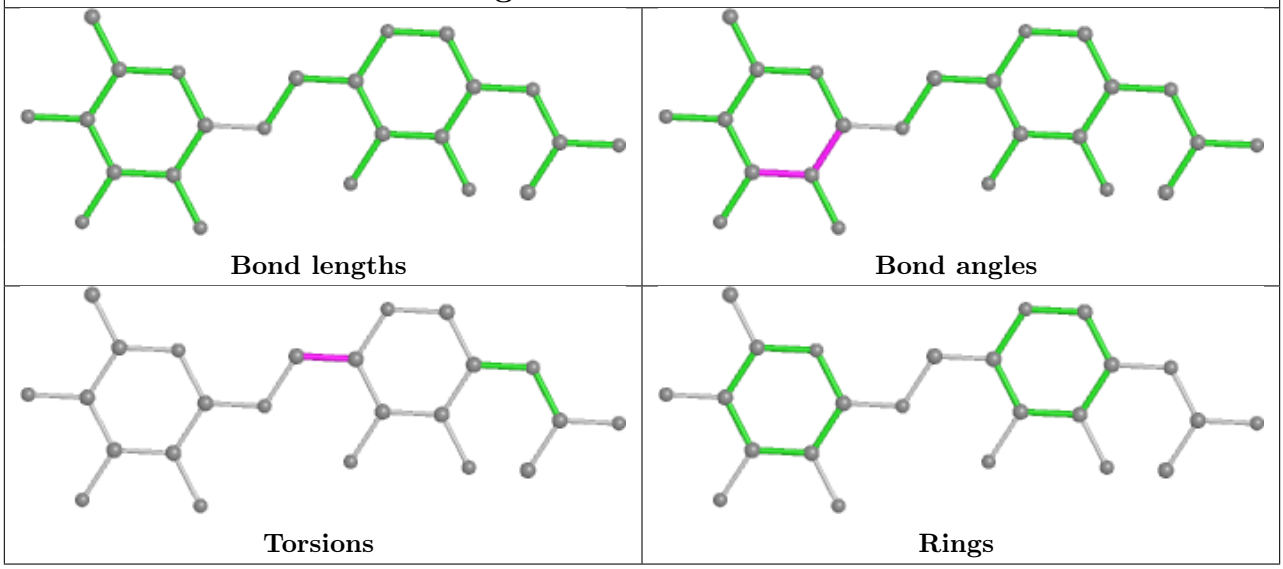
There are no ring outliers.

6 monomers are involved in 22 short contacts:

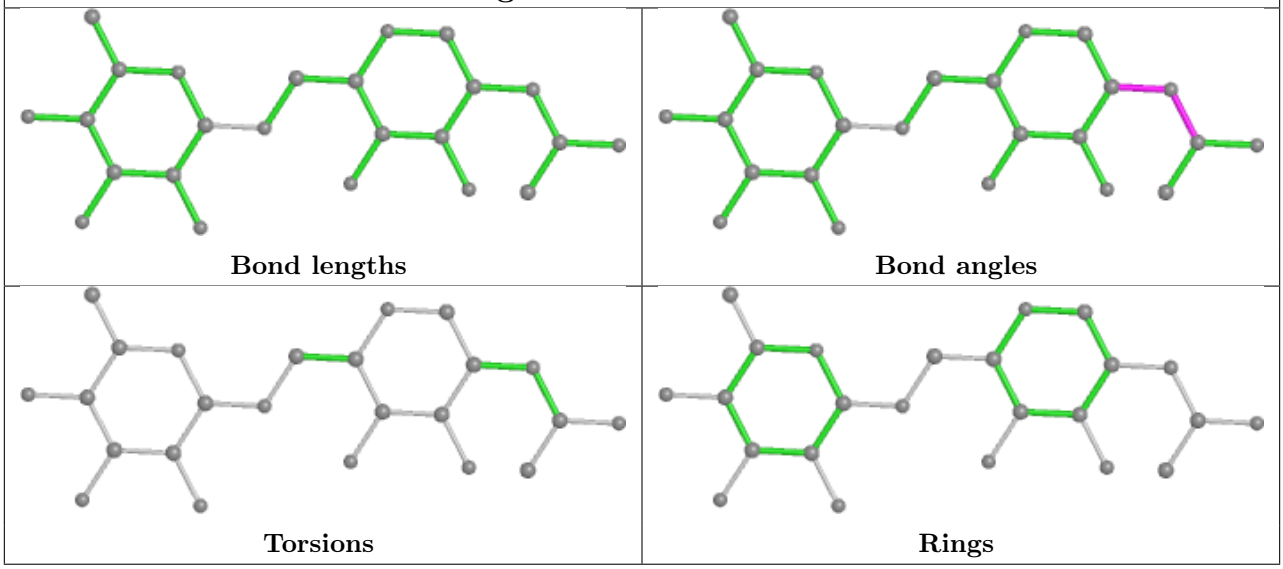
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	6	0
4	D	2	FUC	6	0
4	E	1	NAG	6	0
4	F	2	FUC	6	0
4	D	1	NAG	7	0
4	E	2	FUC	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

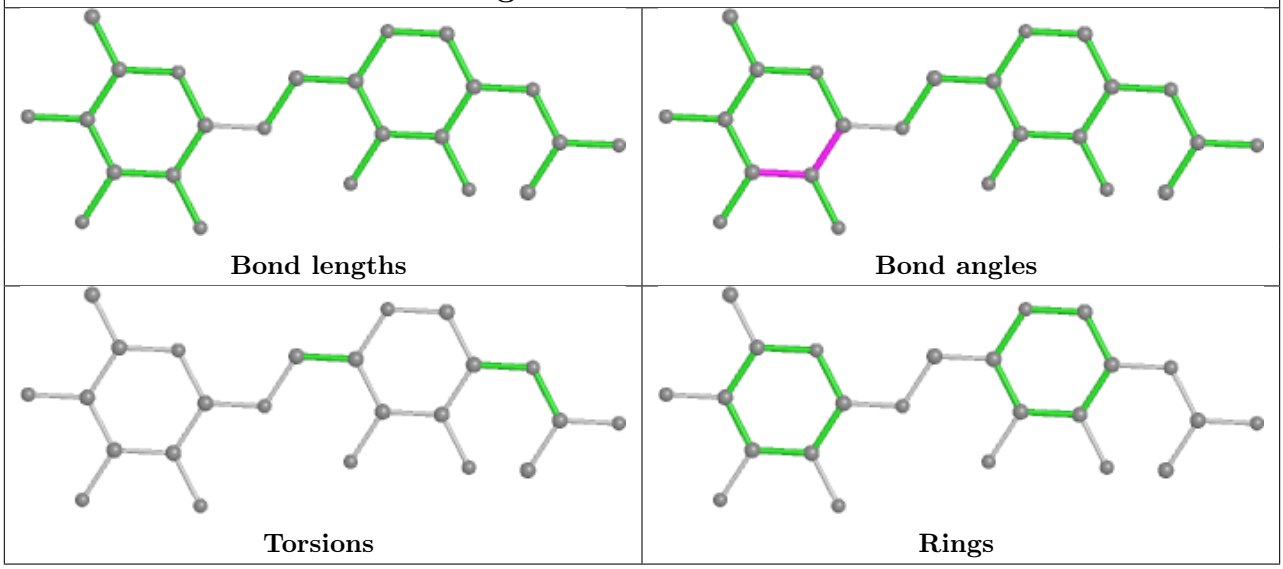
Oligosaccharide Chain D



Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

3 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	H	553	-	14,14,15	0.61	0	17,19,21	0.61	0
5	NAG	I	553	-	14,14,15	0.57	0	17,19,21	0.66	0
6	CAC	L	1001	-	0,4,4	-	-	0,6,6	-	-

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	H	553	-	-	2/6/23/26	0/1/1/1
5	NAG	I	553	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	553	NAG	C8-C7-N2-C2
5	H	553	NAG	O7-C7-N2-C2
5	I	553	NAG	C3-C2-N2-C7
5	I	553	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	553	NAG	2	0
5	I	553	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	J	1
2	H	1
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	129:VAL	C	136:SER	N	14.08
1	H	129:VAL	C	136:SER	N	14.07
1	I	129:VAL	C	136:SER	N	13.60

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	186/196 (94%)	0.11	11 (5%) 22 21	21, 33, 56, 61	0
1	B	186/196 (94%)	0.18	15 (8%) 12 11	24, 35, 56, 61	0
1	C	187/196 (95%)	0.44	22 (11%) 4 4	26, 43, 56, 61	0
2	H	210/210 (100%)	0.24	10 (4%) 30 30	22, 40, 54, 57	0
2	I	210/210 (100%)	0.04	4 (1%) 66 66	24, 36, 48, 59	0
2	J	210/210 (100%)	0.75	23 (10%) 5 5	30, 50, 57, 60	0
3	L	211/211 (100%)	-0.34	0 100 100	18, 28, 46, 53	0
3	M	211/211 (100%)	-0.27	1 (0%) 91 91	23, 33, 45, 55	0
3	N	211/211 (100%)	-0.08	4 (1%) 66 66	25, 37, 52, 56	0
All	All	1822/1851 (98%)	0.11	90 (4%) 29 29	18, 37, 54, 61	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1100	LEU	6.8
2	J	203	ALA	5.4
1	B	923	CYS	5.3
2	I	216	GLY	5.1
2	J	1	ASP	5.0
1	B	1100	LEU	4.6
1	A	1106	HIS	4.5
1	B	1106	HIS	4.5
1	C	1100	LEU	4.4
2	J	117	GLU	4.3
1	C	923	CYS	4.2
1	A	922	ASP	4.2
2	I	1	ASP	4.2
2	J	216	GLY	4.1
1	C	1081	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	216	GLY	4.0
2	J	114	SER	4.0
1	A	1101	GLY	3.9
1	B	1102	ASN	3.9
1	B	1105	LEU	3.7
1	A	921	PRO	3.7
1	C	939	PHE	3.3
2	J	86	HIS	3.2
1	C	1036	LEU	3.2
2	J	64	ILE	3.2
1	C	1109	CYS	3.1
2	J	87	THR	3.0
1	B	1103	SER	2.9
1	C	931	LEU	2.9
1	C	1101	GLY	2.9
2	J	205	SER	2.9
1	B	1101	GLY	2.9
1	B	922	ASP	2.9
1	C	1106	HIS	2.8
3	N	184	ASP	2.8
2	H	64	ILE	2.8
1	A	1102	ASN	2.8
2	H	127	GLU	2.8
2	J	15	SER	2.7
1	B	1109	CYS	2.7
3	N	133	VAL	2.6
1	C	1080	ALA	2.6
1	A	1109	CYS	2.6
1	B	1110	SER	2.5
2	I	205	SER	2.5
2	H	50	VAL	2.5
2	I	64	ILE	2.5
3	N	188	ARG	2.5
1	C	1035	ILE	2.5
1	A	1105	LEU	2.5
1	C	1090	ARG	2.5
1	C	1110	SER	2.5
1	C	1082	ASP	2.5
2	J	42	GLY	2.5
1	C	1102	ASN	2.4
3	N	126	THR	2.4
1	A	923	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	924	SER	2.4
2	J	204	SER	2.4
1	C	1089	GLN	2.3
2	H	14	PRO	2.3
1	B	930	ILE	2.3
1	C	930	ILE	2.3
2	J	123	VAL	2.3
2	J	75	ARG	2.3
2	J	16	GLN	2.3
2	J	24	VAL	2.3
2	H	15	SER	2.3
1	B	1033	VAL	2.2
1	B	1108	LEU	2.2
1	C	1056	ARG	2.2
2	J	65	SER	2.2
1	C	1034	VAL	2.2
1	C	1079	PRO	2.2
2	J	115	SER	2.2
1	B	985	VAL	2.2
2	J	116	ALA	2.2
2	H	34	VAL	2.1
2	J	125	LYS	2.1
1	A	1099	THR	2.1
3	M	45	ARG	2.1
2	J	88	ASP	2.1
2	H	129	VAL	2.1
2	J	127	GLU	2.1
1	A	1110	SER	2.1
2	H	173	GLN	2.1
1	B	1036	LEU	2.0
2	H	42	GLY	2.0
1	C	933	LEU	2.0
2	J	141	GLY	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)

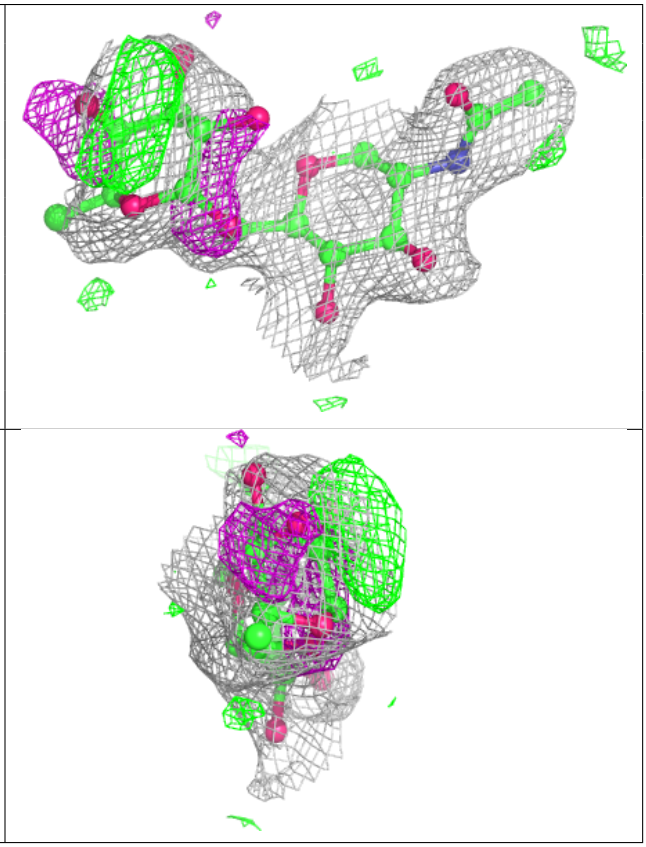
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	F	2	10/11	0.68	0.49	60,60,61,61	0
4	NAG	F	1	14/15	0.70	0.31	56,57,58,59	0
4	FUC	D	2	10/11	0.71	0.33	55,57,57,57	0
4	NAG	D	1	14/15	0.73	0.19	46,49,53,56	0
4	NAG	E	1	14/15	0.80	0.22	47,50,54,56	0
4	FUC	E	2	10/11	0.81	0.23	58,58,59,59	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

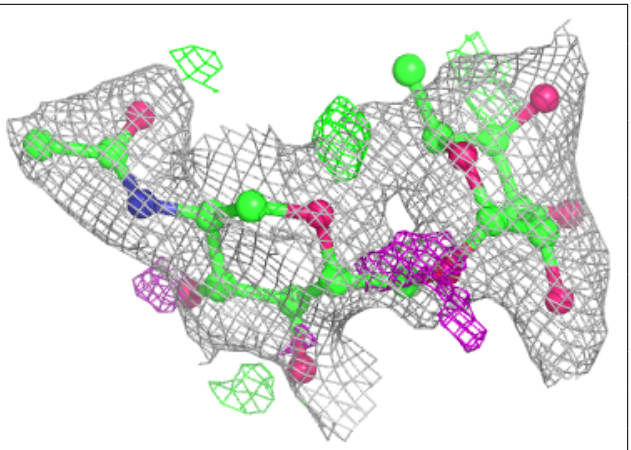
Electron density around Chain D:

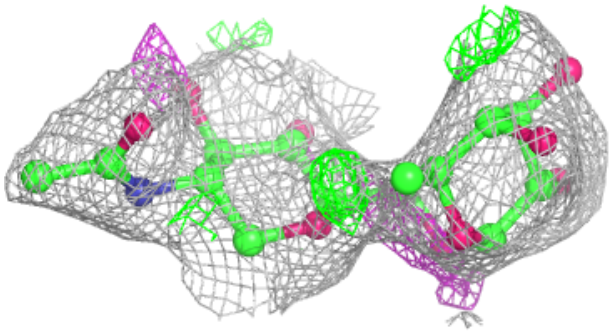
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

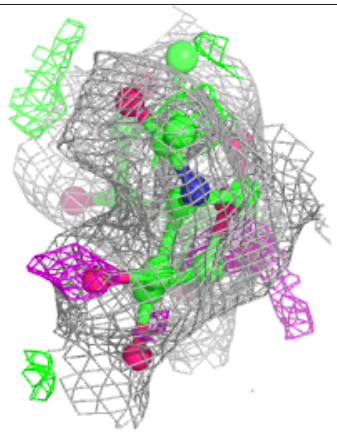


Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

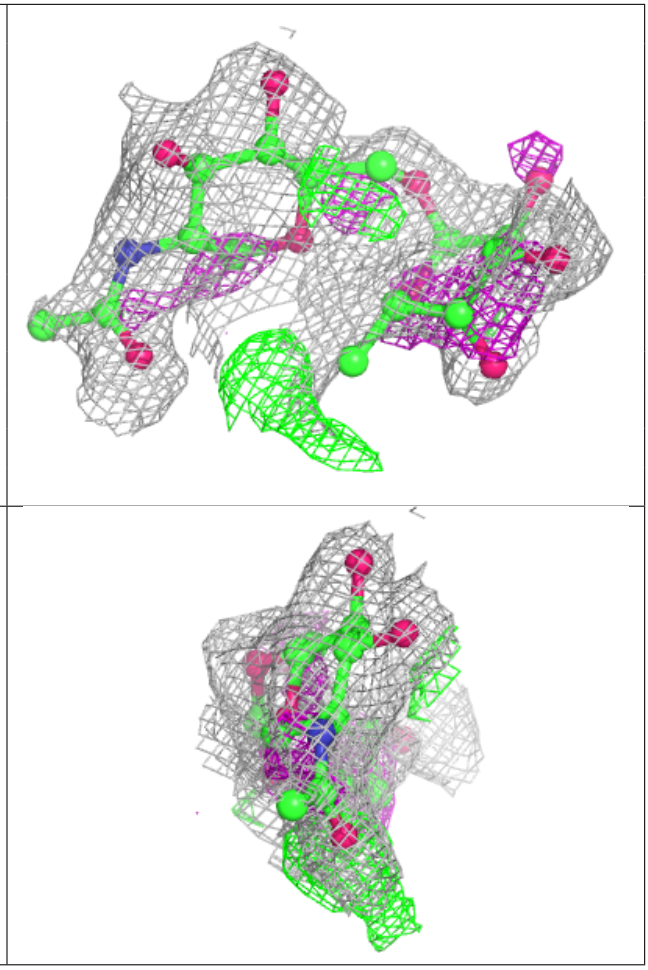






Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	I	553	14/15	0.62	0.38	59,60,62,62	0
5	NAG	H	553	14/15	0.71	0.39	57,58,59,59	0
6	CAC	L	1001	5/5	0.97	0.12	43,44,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.