



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:12 PM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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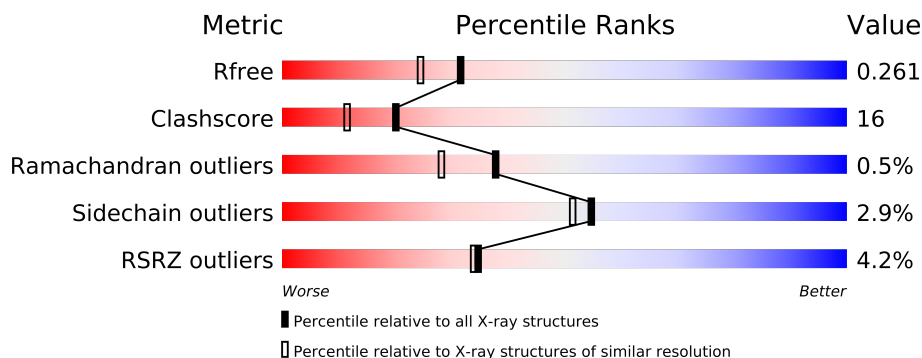
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	196	
1	B	196	
1	C	196	
2	H	210	
2	I	210	
2	J	210	
3	L	211	
3	M	211	
3	N	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	CAC	L	1001	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14872 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	190	Total	C	N	O	S	Se	0	0	0
			1421	899	243	273	2	4			
1	B	190	Total	C	N	O	S	Se	0	0	0
			1421	899	243	273	2	4			
1	C	191	Total	C	N	O	S	Se	0	0	0
			1426	902	244	274	2	4			

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
2	H	210	Total	C	N	O	S	0	0	0
			1578	999	258	316	5			
2	I	210	Total	C	N	O	S	0	0	0
			1578	999	258	316	5			
2	J	210	Total	C	N	O	S	0	0	0
			1578	999	258	316	5			

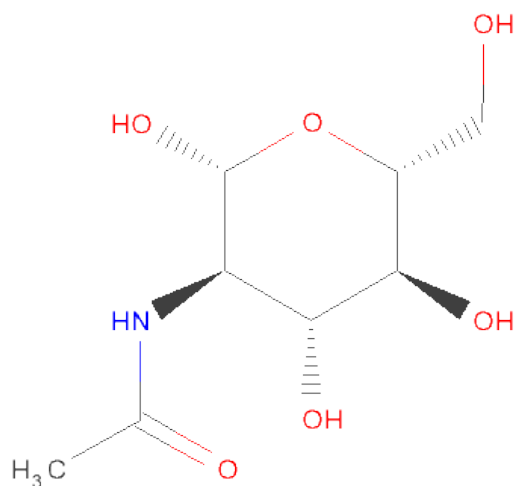
- Molecule 3 is a protein called IMMUNOGLOBULIN IGG RU5.

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

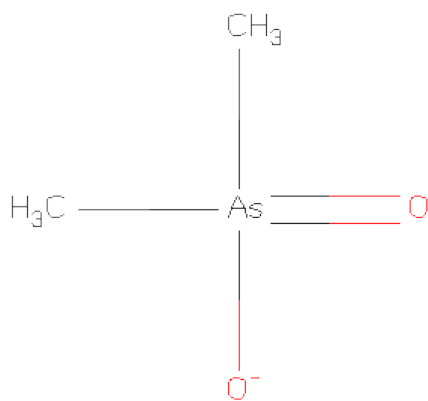
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	2	Total	C	N	O	0	0
			24	14	1	9		
4	I	2	Total	C	N	O	0	0
			24	14	1	9		
4	J	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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



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

- Molecule 7 is water.

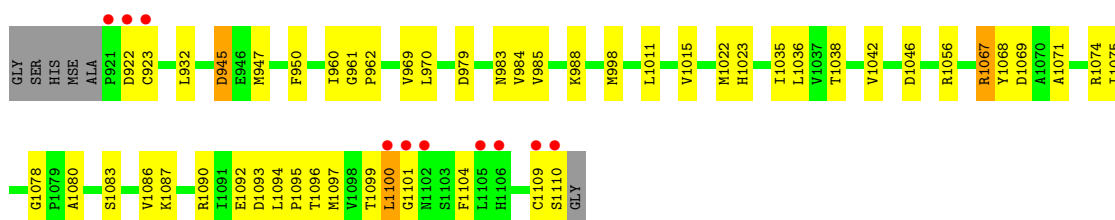
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total 84	O 84	0	0
7	B	79	Total 79	O 79	0	0
7	C	58	Total 58	O 58	0	0
7	H	87	Total 87	O 87	0	0
7	I	107	Total 107	O 107	0	0
7	J	48	Total 48	O 48	0	0
7	L	163	Total 163	O 163	0	0
7	M	139	Total 139	O 139	0	0
7	N	113	Total 113	O 113	0	0

### 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.

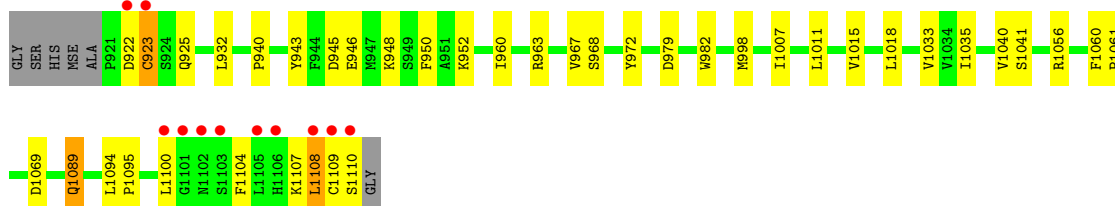
#### • Molecule 1: VON WILLEBRAND FACTOR

Chain A: 



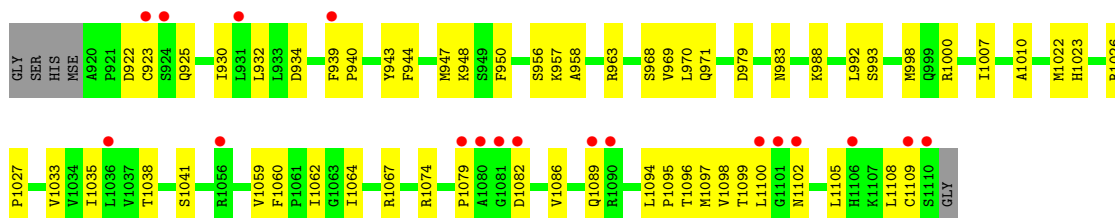
#### • Molecule 1: VON WILLEBRAND FACTOR

Chain B: 



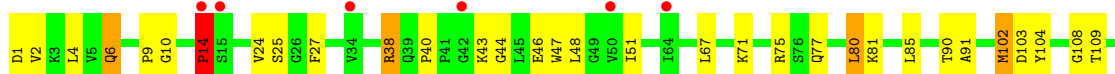
#### • Molecule 1: VON WILLEBRAND FACTOR

Chain C: 



#### • Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain H: 

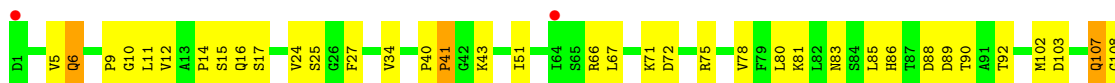






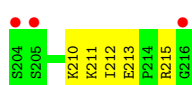
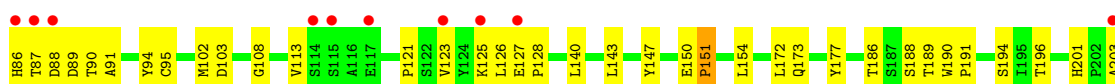
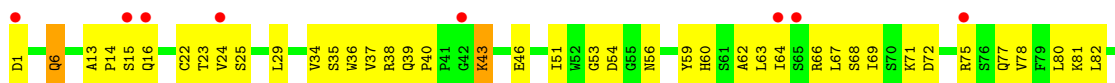
• Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain I:



• Molecule 2: IMMUNOGLOBULIN IGG RU5

Chain J:



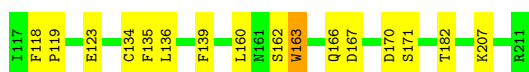
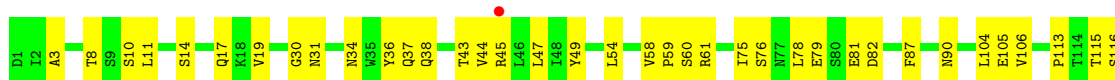
• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain L:



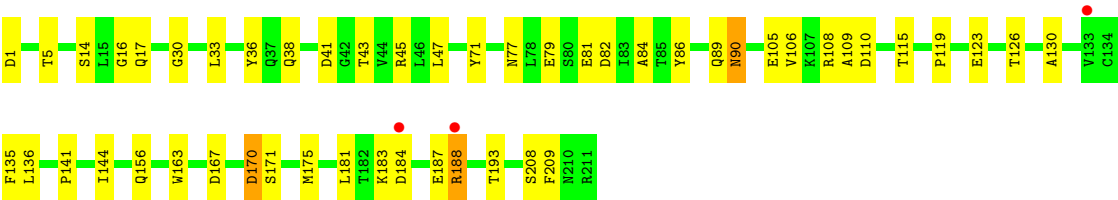
• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain M:



• Molecule 3: IMMUNOGLOBULIN IGG RU5

Chain N:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 85.9 (29.90-2.03)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227 , 0.264 0.225 , 0.261	Depositor DCC
$R_{free}$ test set	7206 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 143245 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 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	0.36	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1578	0	1540	62	0
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	H	24	0	22	8	0
4	I	24	0	22	6	0
4	J	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (439) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H	1:B:1108:LEU:HD23	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:H:552: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
1:C:1062:ILE:HD13	1:C:1097:MSE:HE1	1.64	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:I:551:NAG:H61	4:I:552: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:H:551:NAG:H62	4:H:552:FUC:H3	1.68	0.74
2:I:127:GLU:HG2	2:I:213:GLU:O	1.87	0.73
4:J:551:NAG:H61	4:J:552: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
4:H:551:NAG:H4	5:H:553:NAG:C1	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:I:551:NAG:H61	4:I:552: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
4:I:551:NAG:H4	7:I:584:HOH:O	1.94	0.66
2:H:6:GLN:HE21	2:H:6:GLN:H	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
4:H:551:NAG:O4	5:H:553:NAG:H82	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
3:M:78:LEU:HD11	3:M:104:LEU:HD21	1.80	0.63
1:A:1056:ARG:HG2	1:A:1056:ARG:HH11	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:I:6:GLN:NE2	2:I:108:GLY:H	1.97	0.63
1:B:1040:VAL:HG12	1:B:1069:ASP:HB2	1.79	0.63
2:J:150:GLU:HG3	2:J:151:PRO:CA	2.29	0.63
2:H:6:GLN:HB2	2:H:109:THR:HG23	1.80	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:H:551:NAG:H62	4:H:552: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:HD13	2:H:80:LEU:C	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
2:J:6:GLN:HE22	2:J:108:GLY:H	1.48	0.59
3:M:11:LEU:HD21	7:M:344:HOH:O	2.02	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:125:LYS:HD3	2:H:127:GLU:OE1	2.04	0.58
1:C:956:SER:HA	1:C:988:LYS:HD3	1.85	0.58
2:H:154:LEU:HD23	2:H:155:THR:N	2.19	0.58
1:C:1074:ARG:HG3	1:C:1082:ASP:OD2	2.04	0.58
2:I:173:GLN:HG2	7:I:638:HOH:O	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
4:I:551:NAG:H61	4:I:552:FUC:C5	2.34	0.57
2:H:6:GLN:NE2	2:H:108:GLY:H	2.01	0.57
1:A:1086:VAL:HG21	1:A:1097:MSE:CE	2.35	0.57
3:L:105:GLU:HG2	3:L:106:VAL:N	2.20	0.57
2:H:43:LYS:HB3	7:H:596:HOH:O	2.05	0.57
1:C:943:TYR:O	1:C:947:MSE:HG3	2.05	0.57
1:A:1022:MSE:HG2	7:N:286:HOH:O	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
3:M:43:THR:HA	7:M:277:HOH:O	2.05	0.56
2:I:67:LEU:HD11	2:I:80:LEU:CD2	2.36	0.56
4:H:551:NAG:H62	4:H:552:FUC:C3	2.35	0.56
2:J:186:THR:HG22	2:J:188:SER:H	1.70	0.56
4:I:551:NAG:H61	4:I:552:FUC:C3	2.36	0.56
3:L:151:ASP:HA	3:L:191:SER:OG	2.06	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
2:J:39:GLN:C	2:J:91:ALA:HB1	2.26	0.55
1:C:939:PHE:HB3	1:C:940:PRO:CD	2.35	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:O	3:N:126:THR:HG22	2.07	0.55
2:I:116:ALA:HB3	2:I:148:PHE:CE2	2.42	0.55
1:C:1095:PRO:O	1:C:1099:THR:HG23	2.08	0.54
3:M:31:ASN:HD21	3:N:156:GLN:NE2	2.06	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
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
2:J:6:GLN:N	2:J:6:GLN:HE21	2.03	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1038:THR:HG22	1:C:1064:ILE:HB	1.91	0.53
3:N:108:ARG:HG2	3:N:109:ALA:N	2.22	0.53
1:A:1090:ARG:HG2	1:A:1093:ASP:OD2	2.08	0.53
2:J:80:LEU:HD13	2:J:80:LEU:C	2.29	0.53
1:B:1108:LEU:CD2	1:B:1108:LEU:H	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:N:14:SER:O	3:N:17:GLN:HB2	2.09	0.53
3:M:105:GLU:HG2	3:M:106:VAL:N	2.23	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: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:171:VAL:HG11	3:L:160:LEU:HG	1.92	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
3:M:167:ASP:HB3	3:M:170:ASP:HB3	1.90	0.52
2:H:51:ILE:CD1	2:H:71:LYS:HG2	2.40	0.52
4:H:551:NAG:C6	4:H:552:FUC:H5	2.39	0.51
2:I:90:THR:HG23	2:I:112:THR:HA	1.92	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
2:J:38:ARG:HG2	2:J:40:PRO:HD3	1.93	0.51
3:L:48:ILE:HD13	3:L:54:LEU:HD23	1.92	0.51
3:L:188:ARG:HD3	7:L:1142:HOH:O	2.10	0.51
3:N:181:LEU:HD23	3:N:181:LEU:N	2.26	0.51
2:J:51:ILE:HG23	2:J:51:ILE:O	2.10	0.51
1:B:1007:ILE:HD12	1:B:1041:SER:HB2	1.93	0.51
2:J:6:GLN:H	2:J:6:GLN:NE2	2.07	0.51
7:M:305:HOH:O	2:J:173:GLN:HG3	2.09	0.51
2:I:102:MET:HB2	3:M:36:TYR:CE2	2.45	0.51
4:J:552:FUC:H4	7:J:580:HOH:O	2.11	0.50
3:M:166:GLN:HG2	3:M:171:SER:HA	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:127:GLU:HB2	2:I:215:ARG:HG3	1.92	0.50
3:M:14:SER:HB2	3:M:17:GLN:NE2	2.26	0.50
2:H:24:VAL:HG11	2:H:27:PHE:CE1	2.47	0.50
1:A:1011:LEU:O	1:A:1015:VAL:HG23	2.12	0.50
1:C:957:LYS:HD3	1:C:1098:VAL:HG12	1.93	0.50
3:M:163:TRP:CD1	3:M:163:TRP:N	2.79	0.50
2:H:102:MET:HE1	3:L:96:TRP:CE3	2.46	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:J:90:THR:O	2:J:91:ALA:HB2	2.11	0.50
2:H:38:ARG:HD2	2:H:46:GLU:OE1	2.12	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:J:551:NAG:C8	2.41	0.49
2:J:128:PRO:O	2:J:215:ARG:HD2	2.12	0.49
1:B:1108:LEU:N	1:B:1108:LEU:HD23	2.18	0.49
2:I:12:VAL:HG11	2:I:85:LEU:CD1	2.43	0.49
2:H:102:MET:HE1	3:L:96:TRP:HE3	1.77	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:I:12:VAL:O	2:I:113:VAL:HA	2.11	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
2:J:39:GLN:O	2:J:91:ALA:HB1	2.13	0.48
3:L:125:LEU:O	3:L:183:LYS:HD2	2.13	0.48
1:A:947:MSE:HG2	1:A:1036:LEU:HD23	1.95	0.48
3:M:59:PRO:C	3:M:61:ARG:H	2.15	0.48
2:I:80:LEU:C	2:I:80:LEU:HD13	2.33	0.48
1:A:932:LEU:HD23	1:A:1035:ILE:HD12	1.95	0.48
4:J:551:NAG:H61	4:J:552:FUC:C5	2.40	0.48
1:B:1094:LEU:HB3	1:B:1095:PRO:CD	2.43	0.48
1:B:922:ASP:HB3	1:B:925:GLN:CG	2.43	0.48
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:I:81:LYS:HE3	2:I:83:ASN:OD1	2.13	0.48
2:H:153:THR:OG1	2:H:200:ALA:HB3	2.13	0.48
2:J:37:VAL:HG23	2:J:94:TYR:HB2	1.94	0.48
2:I:128:PRO:O	2:I:215:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:31:ASN:HD21	3:N:156:GLN:HE22	1.62	0.48
2:I:16:GLN:HG2	2:I:17:SER:H	1.79	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: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:H:2:VAL:HG11	2:H:104:TYR:CG	2.48	0.47
2:J:14:PRO:O	2:J:16:GLN:N	2.47	0.47
4:J:551:NAG:C6	4:J:552:FUC:H5	2.42	0.47
3:N:119:PRO:HG3	3:N:209:PHE:CD2	2.49	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:J:87:THR:C	2:J:89:ASP:H	2.15	0.47
2:J:29:LEU:O	2:J:53:GLY:HA2	2.14	0.47
3:M:182:THR:HA	7:M:350:HOH:O	2.15	0.47
3:N:110:ASP:OD1	3:N:141:PRO:HD3	2.15	0.47
2:I:123:VAL:O	2:I:210:LYS:HE3	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
2:J:140:LEU:HD22	2:J:140:LEU:N	2.30	0.46
1:C:1060:PHE:CE1	1:C:1108:LEU:HG	2.49	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
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:90:THR:O	2:H:91:ALA:HB2	2.15	0.46
2:J:56:ASN:ND2	4:J:552:FUC:H61	2.30	0.46
2:H:24:VAL:HG12	2:H:25:SER:N	2.31	0.46
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
3:N:47:LEU:HD11	3:N:86:TYR:HE2	1.81	0.46
2:H:149:PRO:HD2	2:H:203:ALA:CB	2.46	0.46
3:N:79:GLU:HB2	3:N:82:ASP:OD2	2.16	0.46
2:J:6:GLN:N	2:J:6:GLN:NE2	2.63	0.46
1:C:947:MSE:O	1:C:950:PHE:HB3	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:51:ILE:O	2:I:51:ILE:HG23	2.15	0.45
2:I:11:LEU:HD22	2:I:149:PRO:HG3	1.98	0.45
2:J:127:GLU:HG3	2:J:212:ILE:CG2	2.46	0.45
1:C:1007:ILE:HD12	1:C:1041:SER:HB2	1.99	0.45
2:J:87:THR:H	2:J:113:VAL:CG1	2.30	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:C	2:J:89:ASP:N	2.70	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:HH11	1:C:1067:ARG:HG2	1.82	0.45
1:C:944:PHE:O	1:C:948:LYS:HG3	2.17	0.45
4:J:551:NAG:H61	4:J:552:FUC:H3	1.99	0.45
2:H:24:VAL:HG11	2:H:27:PHE:CZ	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
2:I:172:LEU:HB2	2:I:177:TYR:CE1	2.52	0.45
2:J:22:CYS:HB2	2:J:36:TRP:CH2	2.52	0.45
4:I:551:NAG:C6	4:I:552:FUC:H5	2.42	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
2:I:190:TRP:CG	2:I:191:PRO:HA	2.52	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
3:N:45:ARG:HG3	3:N:45:ARG:NH1	2.32	0.44
1:C:971:GLN:HE22	1:C:1000:ARG:HA	1.82	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
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
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:950:PHE:HB2	1:A:1094:LEU:HG	2.00	0.44
1:A:922:ASP:HA	1:A:1110:SER:H	1.82	0.44
2:H:190:TRP:CG	2:H:191:PRO:HA	2.52	0.44
1:A:1068:TYR:OH	1:A:1087:LYS:HD3	2.17	0.44
1:B:972:TYR:HE2	1:B:1035:ILE:HD11	1.81	0.44
3:M:116:SER:O	3:M:134:CYS:HA	2.17	0.44
3:M:113:PRO:HB3	3:M:139:PHE:HB3	2.00	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
3:M:61:ARG:NH1	3:M:82:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:963:ARG:CZ	3:N:30:GLY:HA2	2.47	0.44
2:I:9:PRO:HG2	2:I:10:GLY:H	1.82	0.44
3:N:89:GLN:NE2	3:N:90:ASN:O	2.50	0.44
2:J:13:ALA:O	2:J:16:GLN:HB2	2.18	0.44
2:I:24:VAL:HG12	2:I:25:SER:N	2.33	0.44
3:N:5:THR:HG23	7:N:235:HOH:O	2.18	0.44
1:A:983:ASN:N	1:A:983:ASN:ND2	2.65	0.44
2:J:24:VAL:CG1	2:J:25:SER:N	2.80	0.44
2:J:66:ARG:HH21	2:J:82:LEU:HG	1.83	0.43
3:M:14:SER:CB	3:M:17:GLN:NE2	2.81	0.43
1:B:950:PHE:HB2	1:B:1094:LEU:HG	1.99	0.43
3:N:38:GLN:O	3:N:84:ALA:HB1	2.18	0.43
1:C:1094:LEU:HB3	1:C:1095:PRO:CD	2.47	0.43
2:H:51:ILE:HG23	2:H:51:ILE:O	2.18	0.43
2:H:24:VAL:CG1	2:H:25:SER:N	2.81	0.43
2:I:14:PRO:C	2:I:16:GLN:H	2.21	0.43
1:C:969:VAL:C	1:C:970:LEU:HD12	2.37	0.43
3:M:34:ASN:OD1	3:M:49:TYR:HA	2.18	0.43
1:A:1100:LEU:HG	1:A:1101:GLY:N	2.33	0.43
2:J:59:TYR:HB2	2:J:64:ILE:HG12	2.00	0.43
3:L:10:SER:HA	3:L:103:LYS:O	2.18	0.43
2:J:127:GLU:HG3	2:J:212:ILE:HG23	2.00	0.43
2:H:157:ASN:HA	7:H:628:HOH:O	2.18	0.43
1:A:984:VAL:O	1:A:985:VAL:C	2.56	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
1:A:1046:ASP:OD1	1:A:1075:ILE:HD13	2.18	0.43
2:H:9:PRO:HG2	2:H:10:GLY:H	1.82	0.43
2:J:68:SER:OG	2:J:81:LYS:HB2	2.17	0.43
1:A:1090:ARG:HG3	1:A:1092:GLU:HB2	1.99	0.43
3:N:130:ALA:HB3	3:N:181:LEU:O	2.19	0.43
2:I:66:ARG:HH22	2:I:89:ASP:CG	2.22	0.43
1:B:948:LYS:O	1:B:952:LYS:HG3	2.19	0.43
1:A:1023:HIS:HE1	3:N:81:GLU:OE2	2.02	0.43
2:H:121:PRO:CB	2:H:147:TYR:HB3	2.34	0.43
2:H:6:GLN:HE21	2:H:6:GLN:N	2.12	0.43
1:A:945:ASP:HB3	7:A:509:HOH:O	2.19	0.43
3:M:44:VAL:HG22	7:M:312:HOH:O	2.18	0.43
3:L:14:SER:H	3:L:17:GLN:NE2	2.17	0.43
2:H:75:ARG:O	2:H:77:GLN:HG3	2.19	0.43
2:H:157:ASN:CB	2:H:160:SER:HB3	2.49	0.42
1:A:1080:ALA:O	1:A:1083:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:H:38:ARG:HG3	2:H:46:GLU:HB2	2.01	0.42
1:A:985:VAL:HG11	3:L:96:TRP:HZ2	1.83	0.42
1:C:1067:ARG:O	1:C:1067:ARG:HG3	2.19	0.42
1:C:983:ASN:N	1:C:983:ASN:HD22	2.16	0.42
2:I:189:THR:O	2:I:193:GLN:HB2	2.19	0.42
1:A:969:VAL:C	1:A:970:LEU:HD12	2.40	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:14:PRO:O	2:H:85:LEU:HB2	2.19	0.42
3:L:135:PHE:C	3:L:136:LEU:HD12	2.40	0.42
2:H:129:VAL:HG11	7:L:1160:HOH:O	2.19	0.42
1:C:1026:ARG:HA	1:C:1027:PRO:HD3	1.86	0.42
1:A:962:PRO:HB3	3:L:29:ILE:O	2.19	0.42
1:C:1105:LEU:HD22	1:C:1105:LEU:H	1.84	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
2:H:4:LEU:N	2:H:4:LEU:HD12	2.34	0.42
2:H:121:PRO:HB3	2:H:147:TYR:CB	2.34	0.42
3:M:61:ARG:CG	3:M:76:SER:O	2.68	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: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
1:C:1089:GLN:HG2	7:C:616:HOH:O	2.18	0.42
3:M:118:PHE:HA	3:M:119:PRO:HD3	1.93	0.42
2:I:92:THR:HA	2:I:110:SER:HA	2.01	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
3:M:44:VAL:HG12	3:M:45:ARG:N	2.35	0.41
3:L:14:SER:CB	3:L:17:GLN:NE2	2.83	0.41
2:J:80:LEU:HD22	2:J:81:LYS:H	1.84	0.41
1:B:940:PRO:O	1:B:943:TYR:HB2	2.20	0.41
3:N:41:ASP:OD1	3:N:43:THR:HG23	2.20	0.41
3:M:14:SER:HB2	3:M:17:GLN:HE21	1.85	0.41
2:H:47:TRP:CD1	2:H:102:MET:HE1	2.55	0.41
3:M:37:GLN:HB2	3:M:47:LEU:HD11	2.01	0.41
3:L:175:MET:O	3:L:175:MET:HG3	2.20	0.41
2:J:196:THR:HG23	2:J:210:LYS:C	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:136:LEU:N	3:L:136:LEU:HD12	2.36	0.41
2:J:60:HIS:NE2	3:N:1:ASP:OD2	2.47	0.41
1:B:963:ARG:CZ	3:M:30:GLY:HA2	2.51	0.41
1:A:1069:ASP:OD2	1:A:1071:ALA:HB3	2.20	0.41
3:M:170:ASP:O	3:M:171:SER:HB2	2.20	0.41
3:M:36:TYR:HB2	3:M:87:PHE:CE1	2.55	0.41
2:I:34:VAL:HG21	2:I:78:VAL:HG21	2.02	0.41
3:L:144:ILE:HG22	3:L:163:TRP:CZ3	2.56	0.41
2:J:66:ARG:HH22	2:J:89:ASP:CG	2.22	0.41
2:H:38:ARG:CD	2:H:46:GLU:OE1	2.69	0.41
1:C:1062:ILE:HA	1:C:1086:VAL:O	2.21	0.41
2:H:191:PRO:O	2:H:192:SER:C	2.58	0.41
2:H:145:LYS:HB2	2:H:145:LYS:HE3	1.92	0.41
2:J:34:VAL:HG11	2:J:78:VAL:HG21	2.02	0.41
2:I:14:PRO:O	2:I:15:SER:HB2	2.21	0.41
2:H:201:HIS:HB3	2:H:206:THR:HB	2.03	0.41
3:N:115:THR:HA	3:N:135:PHE:O	2.20	0.41
1:A:1074:ARG:HG2	1:A:1074:ARG:HH11	1.86	0.41
2:H:140:LEU:HG	2:H:212:ILE:HG21	2.03	0.41
2:J:121:PRO:CB	2:J:147:TYR:HB3	2.41	0.41
2:J:127:GLU:HB2	2:J:215:ARG:HG3	2.03	0.41
3:M:54:LEU:CD1	3:M:60:SER:HA	2.48	0.41
3:L:184:ASP:HB3	3:L:188:ARG:NH1	2.34	0.41
2:J:80:LEU:HD13	2:J:81:LYS:N	2.36	0.41
2:J:125:LYS:HE2	3:N:123:GLU:OE2	2.21	0.41
3:M:3:ALA:HB2	7:M:348:HOH:O	2.21	0.41
4:H:551:NAG:H62	4:H:552:FUC:C5	2.49	0.41
3:M:160:LEU:HD12	3:M:160:LEU:HA	1.94	0.41
2:J:56:ASN:HA	4:J:551:NAG:C7	2.51	0.40
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:62:ALA:O	2:J:63:LEU:HD23	2.20	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: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:1096:THR:HA	1:C:1099:THR:OG1	2.21	0.40
1:C:1022:MSE:HE2	7:C:162:HOH:O	2.20	0.40
3:N:167:ASP:OD2	3:N:170:ASP:HB2	2.20	0.40
2:I:24:VAL:HG11	2:I:27:PHE:CE1	2.56	0.40
3:L:29:ILE:HG12	7:L:1009:HOH:O	2.21	0.40
1:A:1069:ASP:OD2	1:A:1071:ALA:N	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:932:LEU:HD21	1:C:1010:ALA:HB1	2.04	0.40
1:C:925:GLN:OE1	1:C:925:GLN:HA	2.21	0.40
3:N:193:THR:OG1	3:N:208:SER:HB3	2.21	0.40
3:N:136:LEU:HD12	3:N:136:LEU:N	2.35	0.40
1:B:1056:ARG:NH1	1:B:1056:ARG:HG2	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	188/196 (96%)	182 (97%)	5 (3%)	1 (0%)	38	28
1	B	188/196 (96%)	180 (96%)	7 (4%)	1 (0%)	38	28
1	C	189/196 (96%)	176 (93%)	10 (5%)	3 (2%)	14	5
2	H	206/210 (98%)	189 (92%)	15 (7%)	2 (1%)	22	12
2	I	206/210 (98%)	194 (94%)	11 (5%)	1 (0%)	38	28
2	J	206/210 (98%)	184 (89%)	21 (10%)	1 (0%)	38	28
3	L	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
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%)	38	28

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

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Mol	Chain	Res	Type
2	H	14	PRO
2	H	203	ALA
1	C	1079	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/155 (101%)	155 (99%)	2 (1%)	80	82
1	B	157/155 (101%)	153 (98%)	4 (2%)	60	58
1	C	157/155 (101%)	155 (99%)	2 (1%)	80	82
2	H	183/183 (100%)	172 (94%)	11 (6%)	27	19
2	I	183/183 (100%)	173 (94%)	10 (6%)	30	22
2	J	183/183 (100%)	177 (97%)	6 (3%)	50	45
3	L	186/186 (100%)	182 (98%)	4 (2%)	64	64
3	M	186/186 (100%)	183 (98%)	3 (2%)	75	76
3	N	186/186 (100%)	182 (98%)	4 (2%)	64	64
All	All	1578/1572 (100%)	1532 (97%)	46 (3%)	55	51

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

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

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

Mol	Chain	Res	Type
1	A	959	ASN
2	H	6	GLN
2	H	173	GLN
3	L	17	GLN

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

6 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	H	551	2,4	12,14,15	0.55	0	15,19,21	0.83	0
4	FUC	H	552	4	9,10,11	0.39	0	10,14,16	0.62	0
4	NAG	I	551	2,4	12,14,15	0.54	0	15,19,21	0.86	1 (6%)
4	FUC	I	552	4	9,10,11	0.40	0	10,14,16	0.38	0
4	NAG	J	551	2,4	12,14,15	0.54	0	15,19,21	0.70	0
4	FUC	J	552	4	9,10,11	0.45	0	10,14,16	0.39	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
4	NAG	H	551	2,4	-	0/6/23/26	0/1/1/1
4	FUC	H	552	4	-	0/0/17/20	0/1/1/1
4	NAG	I	551	2,4	-	0/6/23/26	0/1/1/1
4	FUC	I	552	4	-	0/0/17/20	0/1/1/1
4	NAG	J	551	2,4	-	0/6/23/26	0/1/1/1
4	FUC	J	552	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	551	NAG	C2-N2-C7	-2.03	119.67	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

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	-	12,14,15	0.45	0	15,19,21	0.70	0
5	NAG	I	553	-	12,14,15	0.46	0	15,19,21	0.62	0
6	CAC	L	1001	-	4,4,4	2.61	2 (50%)	6,6,6	11.11	3 (50%)

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	-	-	0/6/23/26	0/1/1/1
5	NAG	I	553	-	-	0/6/23/26	0/1/1/1
6	CAC	L	1001	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1001	CAC	O2-AS	-4.08	1.63	1.68
6	L	1001	CAC	AS-C1	2.63	1.95	1.90

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1001	CAC	O2-AS-O1	-26.62	106.80	112.54
6	L	1001	CAC	O2-AS-C2	-4.51	105.46	109.15
6	L	1001	CAC	O2-AS-C1	-2.67	106.97	109.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	190/196 (96%)	0.06	10 (5%) 25 25	21, 33, 56, 61	0
1	B	190/196 (96%)	0.14	11 (5%) 22 22	24, 35, 56, 61	0
1	C	191/196 (97%)	0.38	18 (9%) 9 8	26, 43, 57, 61	0
2	H	210/210 (100%)	0.21	8 (3%) 38 38	22, 40, 54, 57	0
2	I	210/210 (100%)	0.04	4 (1%) 64 64	24, 36, 48, 59	0
2	J	210/210 (100%)	0.70	21 (10%) 8 7	30, 50, 57, 60	0
3	L	211/211 (100%)	-0.35	0 100 100	18, 28, 46, 53	0
3	M	211/211 (100%)	-0.25	1 (0%) 88 90	23, 33, 45, 55	0
3	N	211/211 (100%)	-0.08	3 (1%) 72 73	25, 37, 52, 56	0
All	All	1834/1851 (99%)	0.09	76 (4%) 35 35	18, 37, 54, 61	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1100	LEU	5.9
2	J	203	ALA	5.2
2	J	1	ASP	4.8
2	I	216	GLY	4.7
1	B	923	CYS	4.7
1	B	1100	LEU	4.3
2	I	1	ASP	4.2
2	J	216	GLY	4.1
1	C	1081	GLY	4.0
2	J	117	GLU	3.9
1	C	1100	LEU	3.9
1	B	1106	HIS	3.8
1	A	1106	HIS	3.8
2	H	216	GLY	3.7
1	A	922	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	J	114	SER	3.4
1	B	1102	ASN	3.4
2	J	64	ILE	3.3
1	C	923	CYS	3.3
1	C	939	PHE	3.1
1	A	921	PRO	3.1
1	C	1036	LEU	2.9
1	A	1101	GLY	2.9
1	B	1105	LEU	2.8
2	J	86	HIS	2.8
2	H	64	ILE	2.8
2	H	127	GLU	2.8
2	J	87	THR	2.8
2	J	15	SER	2.7
1	C	1101	GLY	2.7
1	B	1103	SER	2.7
1	A	1102	ASN	2.6
1	B	1110	SER	2.6
1	C	1110	SER	2.6
2	J	205	SER	2.6
1	B	922	ASP	2.6
1	C	1109	CYS	2.6
2	J	204	SER	2.5
1	C	1080	ALA	2.5
2	J	123	VAL	2.5
1	C	1089	GLN	2.5
2	J	42	GLY	2.5
3	N	184	ASP	2.4
1	B	1108	LEU	2.4
1	C	1106	HIS	2.4
3	N	188	ARG	2.4
1	C	931	LEU	2.4
2	H	50	VAL	2.3
1	B	1101	GLY	2.3
3	N	133	VAL	2.3
1	C	1102	ASN	2.3
2	J	115	SER	2.2
2	H	14	PRO	2.2
2	J	16	GLN	2.2
1	C	924	SER	2.2
2	H	15	SER	2.2
2	I	64	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	45	ARG	2.2
1	A	1105	LEU	2.2
1	C	1056	ARG	2.1
1	A	923	CYS	2.1
1	A	1109	CYS	2.1
1	C	1082	ASP	2.1
1	C	1079	PRO	2.1
2	J	65	SER	2.1
1	C	1090	ARG	2.1
1	A	1110	SER	2.1
2	J	88	ASP	2.1
2	J	24	VAL	2.1
2	I	205	SER	2.1
2	J	75	ARG	2.1
2	J	125	LYS	2.1
1	B	1109	CYS	2.0
2	J	127	GLU	2.0
2	H	42	GLY	2.0
2	H	34	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	J	551	14/15	0.29	54.35	56,57,58,59	0
4	FUC	H	552	10/11	0.32	24.44	55,57,57,57	0
4	FUC	J	552	10/11	0.51	17.33	60,60,61,61	0
4	FUC	I	552	10/11	0.23	7.83	58,58,59,59	0
4	NAG	I	551	14/15	0.22	7.13	47,50,54,56	0
4	NAG	H	551	14/15	0.18	3.75	46,49,53,56	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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	CAC	L	1001	5/5	0.12	0.74	43,44,47,47	0
5	NAG	H	553	14/15	0.37	-	57,58,59,59	0
5	NAG	I	553	14/15	0.39	-	59,60,62,62	0

## 6.5 Other polymers

There are no such residues in this entry.