



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:45 PM GMT

PDB ID : 4DKF  
Title : Crystal Structure of Human Interleukin-34 Bound to FAb2  
Authors : Ma, X.; Chen, Y.; Stawicki, S.; Wu, Y.; Bazan, J.F.; Starovasnik, M.A.  
Deposited on : 2012-02-03  
Resolution : 2.61 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>

---

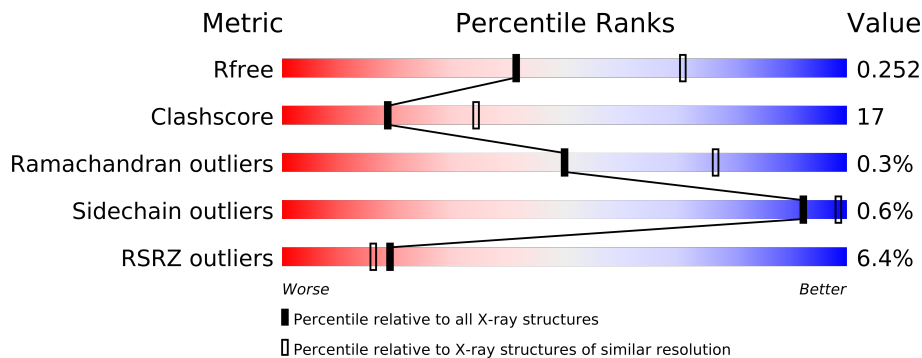
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.61 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	1940 (2.64-2.60)
Clashscore	79885	2404 (2.64-2.60)
Ramachandran outliers	78287	2360 (2.64-2.60)
Sidechain outliers	78261	2360 (2.64-2.60)
RSRZ outliers	66119	1939 (2.64-2.60)

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	190	
1	B	190	
2	H	226	
2	I	226	
3	L	214	
3	M	214	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8977 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 Interleukin-34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1311	837	224	242	8			
1	B	137	Total	C	N	O	S	0	0	0
			1118	722	192	197	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
A	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
A	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
A	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
A	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
A	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
B	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
B	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
B	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4

- Molecule 2 is a protein called FAb2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1577	994	262	315	6			
2	I	206	Total	C	N	O	S	0	0	0
			1515	954	254	301	6			

- Molecule 3 is a protein called FAb2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1625	1017	273	330	5			
3	M	207	Total	C	N	O	S	0	0	0
			1583	990	264	324	5			

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
A	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
A	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
A	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
A	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
A	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
A	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
A	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	18	ALA	-	EXPRESSION TAG	UNP Q6ZMJ4
B	19	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	20	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	194	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	195	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
B	196	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	197	GLY	-	EXPRESSION TAG	UNP Q6ZMJ4
B	198	ASN	-	EXPRESSION TAG	UNP Q6ZMJ4
B	199	SER	-	EXPRESSION TAG	UNP Q6ZMJ4
B	200	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	201	TYR	-	EXPRESSION TAG	UNP Q6ZMJ4
B	202	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4
B	203	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	204	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	205	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	206	ASP	-	EXPRESSION TAG	UNP Q6ZMJ4
B	207	LYS	-	EXPRESSION TAG	UNP Q6ZMJ4

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	14	Total O 14 14	0	0
5	H	22	Total O 22 22	0	0
5	L	42	Total O 42 42	0	0
5	I	21	Total O 21 21	0	0

*Continued on next page...*

*Continued from previous page...*

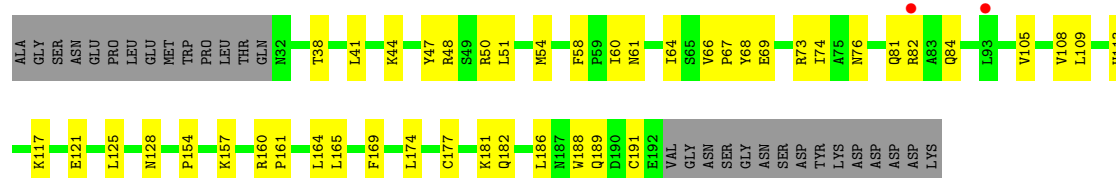
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	20	Total	O	0	0
			20	20		

### 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.

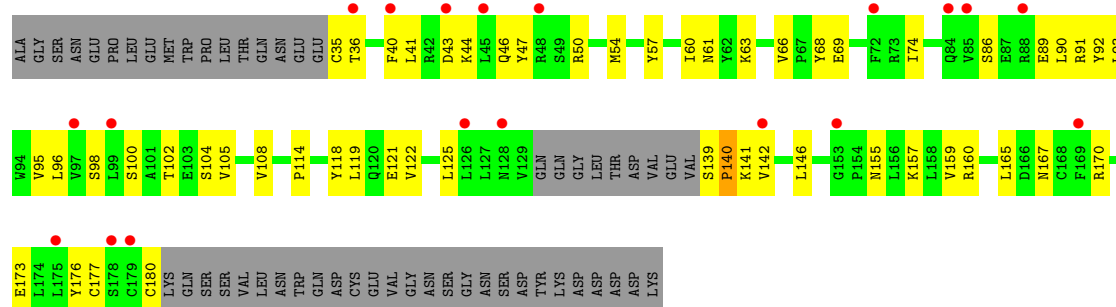
#### • Molecule 1: Interleukin-34

Chain A: 



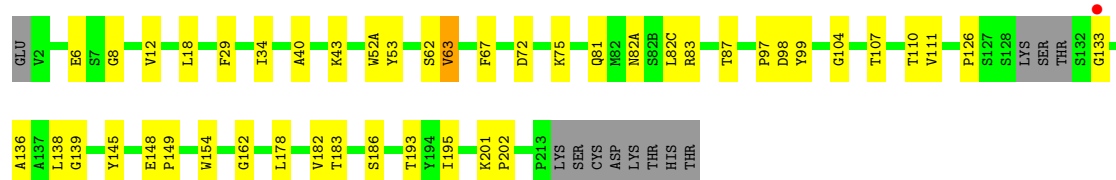
#### • Molecule 1: Interleukin-34

Chain B: 



#### • Molecule 2: FAb2 Heavy Chain

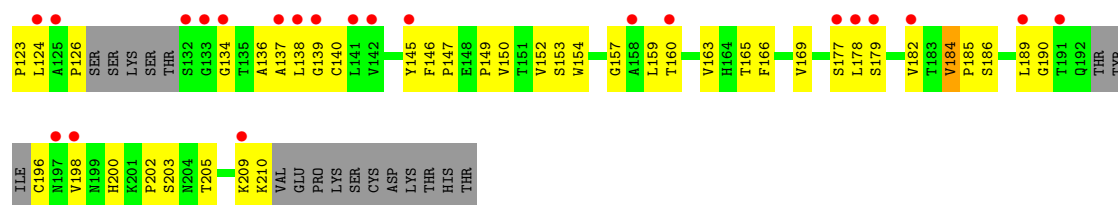
Chain H: 



#### • Molecule 2: FAb2 Heavy Chain

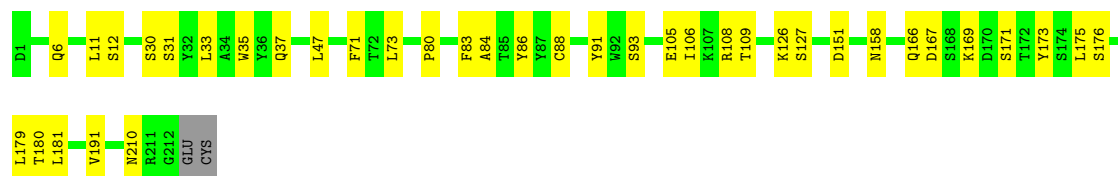
Chain I: 





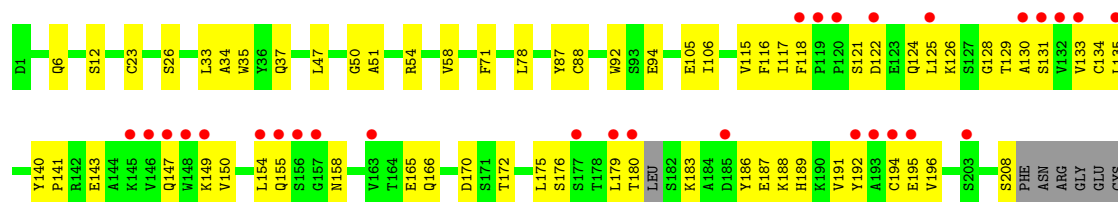
### • Molecule 3: FAb2 Light Chain

Chain L:



### • Molecule 3: FAb2 Light Chain

Chain M:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.92Å 181.82Å 79.25Å 90.00° 118.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 47.70 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-2.61) 98.5 (47.70-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.225 , 0.256 0.224 , 0.252	Depositor DCC
$R_{free}$ test set	2212 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.4	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.0	EDS
Estimated twinning fraction	0.014 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.011 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 44007 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	0/1337	0.45	0/1815
1	B	0.30	0/1141	0.43	0/1547
2	H	0.40	0/1616	0.55	0/2205
2	I	0.33	0/1551	0.49	0/2113
3	L	0.44	0/1661	0.54	0/2255
3	M	0.34	0/1617	0.48	0/2195
All	All	0.37	0/8923	0.50	0/12130

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	1311	0	1320	43	1
1	B	1118	0	1148	49	0
2	H	1577	0	1519	37	0
2	I	1515	0	1459	75	0
3	L	1625	0	1579	35	0
3	M	1583	0	1536	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	61	0	52	5	0
4	B	61	0	52	6	0
5	A	7	0	0	0	0
5	B	14	0	0	0	0
5	H	22	0	0	3	0
5	I	21	0	0	3	0
5	L	42	0	0	3	0
5	M	20	0	0	1	1
All	All	8977	0	8665	292	2

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 17.

All (292) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:85:GLU:HB2	5:I:314:HOH:O	1.52	1.08
2:H:12:VAL:HG21	2:H:18:LEU:HD22	1.34	1.06
1:A:54:MET:HG3	1:A:165:LEU:HD12	1.33	1.04
1:B:170:ARG:NH1	2:I:52(A):TRP:CH2	2.33	0.97
1:B:118:TYR:O	1:B:122:VAL:HG23	1.67	0.95
3:M:192:TYR:HB2	5:M:317:HOH:O	1.68	0.94
2:I:139:GLY:HA2	2:I:154:TRP:HH2	1.35	0.92
2:H:97:PRO:O	3:L:91:TYR:O	1.85	0.92
2:H:63:VAL:HG21	2:H:67:PHE:CD2	2.05	0.90
3:M:124:GLN:HG2	3:M:129:THR:O	1.71	0.90
1:A:60:ILE:HG22	1:A:61:ASN:ND2	1.90	0.86
2:H:63:VAL:CG2	2:H:67:PHE:CD2	2.58	0.85
3:M:115:VAL:HG21	3:M:196:VAL:HG21	1.60	0.84
2:H:63:VAL:HG22	2:H:67:PHE:CG	2.13	0.83
2:H:133:GLY:HA3	5:H:303:HOH:O	1.77	0.83
2:I:139:GLY:HA2	2:I:154:TRP:CH2	2.15	0.82
1:B:170:ARG:NH1	2:I:52(A):TRP:CZ2	2.47	0.81
2:I:51:ILE:HD12	2:I:57:THR:HG22	1.63	0.81
3:M:115:VAL:O	3:M:116:PHE:CD1	2.34	0.80
1:A:54:MET:HG3	1:A:165:LEU:CD1	2.11	0.80
2:I:137:ALA:H	3:M:116:PHE:HE2	1.27	0.80
3:M:125:LEU:HD22	3:M:183:LYS:HG2	1.63	0.80
1:B:105:VAL:O	1:B:108:VAL:HG22	1.82	0.79
2:I:152:VAL:HG12	2:I:153:SER:H	1.48	0.77
3:L:108:ARG:NH1	3:L:109:THR:O	2.18	0.77
2:H:72:ASP:OD2	2:H:75:LYS:HD2	1.86	0.75
2:I:152:VAL:HG12	2:I:153:SER:N	2.02	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:44:LYS:NZ	1:B:121:GLU:OE1	2.20	0.73
3:M:147:GLN:O	3:M:195:GLU:HB3	1.88	0.73
2:H:40:ALA:O	2:H:43:LYS:HB2	1.89	0.72
1:B:160:ARG:NH1	2:I:98:ASP:OD2	2.24	0.70
3:M:115:VAL:C	3:M:116:PHE:HD1	1.95	0.69
2:I:184:VAL:HB	2:I:185:PRO:HD2	1.74	0.69
2:I:200:HIS:CE1	2:I:202:PRO:HB2	2.27	0.69
2:H:63:VAL:CG2	2:H:67:PHE:CG	2.75	0.69
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.28	0.69
3:M:115:VAL:O	3:M:116:PHE:HD1	1.74	0.68
1:A:60:ILE:HD12	1:B:108:VAL:O	1.93	0.68
2:I:122:PHE:CE1	3:M:124:GLN:HA	2.29	0.68
3:M:115:VAL:CG2	3:M:196:VAL:HG21	2.23	0.67
2:I:82:MET:HE2	2:I:82(C):LEU:HD21	1.75	0.67
1:B:61:ASN:HD21	3:M:94:GLU:H	1.43	0.67
3:L:126:LYS:O	5:L:338:HOH:O	2.13	0.66
3:L:175:LEU:HD23	3:L:176:SER:N	2.10	0.66
2:I:137:ALA:HB1	2:I:182:VAL:O	1.97	0.65
3:M:183:LYS:HD3	3:M:183:LYS:O	1.97	0.65
1:A:181:LYS:HE2	1:A:191:CYS:O	1.97	0.65
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.78	0.64
2:I:126:PRO:HG3	2:I:138:LEU:HB3	1.79	0.64
3:M:124:GLN:OE1	3:M:131:SER:N	2.30	0.63
1:A:105:VAL:O	1:A:108:VAL:HG22	1.98	0.63
4:A:302:NAG:O3	4:A:303:MAN:H2	1.98	0.63
1:B:90:LEU:HD12	1:B:91:ARG:N	2.13	0.63
2:I:95:GLY:HA2	2:I:99:TYR:HD2	1.64	0.63
2:I:200:HIS:HE1	2:I:202:PRO:HB2	1.63	0.62
3:M:78:LEU:HD21	3:M:106:ILE:CD1	2.30	0.62
3:L:167:ASP:OD2	3:L:169:LYS:HB2	2.00	0.62
1:B:68:TYR:HD1	4:B:302:NAG:H82	1.63	0.62
3:L:180:THR:C	3:L:181:LEU:HD12	2.20	0.62
3:M:175:LEU:HD23	3:M:176:SER:N	2.15	0.61
1:B:176:TYR:O	1:B:180:CYS:SG	2.59	0.61
3:L:30:SER:OG	3:L:31:SER:N	2.33	0.60
1:B:170:ARG:NH1	2:I:52(A):TRP:CZ3	2.69	0.60
3:M:191:VAL:HG12	3:M:192:TYR:H	1.67	0.60
3:M:155:GLN:HB3	3:M:158:ASN:HD21	1.67	0.60
3:M:23:CYS:HB2	3:M:35:TRP:CH2	2.37	0.60
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.84	0.59
3:M:33:LEU:HD22	3:M:71:PHE:CG	2.36	0.59
3:M:33:LEU:HD22	3:M:71:PHE:CD2	2.38	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:12:VAL:CG2	2:H:18:LEU:HD22	2.23	0.58
3:M:117:ILE:CG2	3:M:194:CYS:HB2	2.33	0.58
2:I:137:ALA:N	3:M:116:PHE:HE2	2.00	0.58
1:B:61:ASN:ND2	3:M:94:GLU:H	2.01	0.57
1:B:54:MET:HG3	1:B:165:LEU:HD12	1.86	0.57
1:A:186:LEU:HA	1:A:189:GLN:HG2	1.86	0.57
2:I:157:GLY:O	2:I:160:THR:HG23	2.04	0.57
3:M:183:LYS:HD3	3:M:183:LYS:C	2.25	0.57
1:A:68:TYR:CE1	4:A:303:MAN:O2	2.58	0.57
1:B:92:TYR:O	1:B:95:VAL:HG12	2.05	0.57
1:A:74:ILE:HG23	1:A:174:LEU:HD22	1.86	0.57
1:A:66:VAL:HG23	1:A:67:PRO:O	2.05	0.56
3:M:149:LYS:HG2	3:M:154:LEU:HD21	1.87	0.56
2:I:139:GLY:CA	2:I:154:TRP:HH2	2.15	0.56
1:B:173:GLU:O	1:B:177:CYS:HB2	2.06	0.56
1:A:47:TYR:HA	1:A:50:ARG:HE	1.69	0.56
2:H:98:ASP:N	5:H:314:HOH:O	1.92	0.56
3:M:150:VAL:CG1	3:M:155:GLN:OE1	2.53	0.56
3:M:50:GLY:O	3:M:51:ALA:HB3	2.06	0.56
1:A:125:LEU:O	1:A:128:ASN:HB2	2.07	0.55
1:B:68:TYR:CD1	4:B:302:NAG:H82	2.42	0.55
3:L:6:GLN:NE2	3:L:86:TYR:O	2.36	0.55
1:A:60:ILE:HG22	1:A:61:ASN:CG	2.25	0.55
3:L:108:ARG:HH11	3:L:108:ARG:HG3	1.72	0.55
2:I:12:VAL:CG2	2:I:18:LEU:HD13	2.37	0.55
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.89	0.55
3:L:83:PHE:O	3:L:84:ALA:HB2	2.06	0.55
1:B:47:TYR:HA	1:B:50:ARG:HE	1.72	0.54
3:L:191:VAL:HG22	3:L:210:ASN:OD1	2.07	0.54
1:B:74:ILE:HG12	2:I:53:TYR:HE1	1.73	0.54
1:A:47:TYR:HB2	1:A:50:ARG:HH21	1.73	0.54
2:H:83:ARG:HD3	5:H:311:HOH:O	2.06	0.54
2:H:145:TYR:OH	2:H:148:GLU:OE2	2.10	0.54
2:I:166:PHE:O	2:I:178:LEU:CD2	2.55	0.53
3:M:140:TYR:CD1	3:M:141:PRO:HA	2.43	0.53
2:I:152:VAL:CG1	2:I:153:SER:H	2.19	0.53
3:M:150:VAL:HG23	3:M:192:TYR:CE2	2.44	0.53
2:H:148:GLU:OE1	2:H:149:PRO:HA	2.08	0.52
2:H:162:GLY:O	2:H:182:VAL:HA	2.10	0.52
1:A:44:LYS:NZ	1:A:121:GLU:OE1	2.36	0.52
3:M:155:GLN:CB	3:M:179:LEU:HD11	2.40	0.52
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:TYR:CD2	1:B:114:PRO:HB2	2.44	0.52
3:M:150:VAL:CG2	3:M:192:TYR:CE2	2.92	0.52
1:B:90:LEU:HD12	1:B:91:ARG:HG3	1.92	0.52
3:M:191:VAL:HG12	3:M:192:TYR:N	2.25	0.52
2:I:16:GLY:O	2:I:82(C):LEU:HD12	2.09	0.52
2:I:150:VAL:HG11	2:I:198:VAL:CG1	2.40	0.52
3:M:187:GLU:O	3:M:188:LYS:C	2.49	0.51
2:H:87:THR:HG23	2:H:110:THR:HA	1.93	0.51
3:L:166:GLN:HG3	3:L:173:TYR:OH	2.11	0.51
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.46	0.51
3:M:115:VAL:C	3:M:116:PHE:CD1	2.78	0.51
2:I:152:VAL:CG1	2:I:153:SER:N	2.72	0.51
1:B:47:TYR:CA	1:B:50:ARG:HH21	2.24	0.51
2:H:52(A):TRP:CE3	2:H:53:TYR:N	2.79	0.51
1:B:86:SER:HB2	1:B:89:GLU:HB2	1.92	0.51
3:M:115:VAL:CG1	3:M:116:PHE:N	2.74	0.50
1:A:64:ILE:HD11	1:A:164:LEU:CD1	2.41	0.50
2:I:33:GLY:C	2:I:34:ILE:HD12	2.31	0.50
3:M:78:LEU:HD21	3:M:106:ILE:HD13	1.94	0.50
3:L:33:LEU:HD22	3:L:71:PHE:CD2	2.45	0.50
2:H:193:THR:HG22	2:H:195:ILE:CD1	2.41	0.50
4:A:302:NAG:O3	4:A:303:MAN:C2	2.60	0.49
1:B:90:LEU:HD12	1:B:91:ARG:H	1.75	0.49
1:B:105:VAL:HG11	1:B:119:LEU:HD11	1.94	0.49
1:A:47:TYR:CA	1:A:50:ARG:HH21	2.25	0.49
2:I:178:LEU:HD13	2:I:178:LEU:C	2.32	0.49
3:M:117:ILE:HG22	3:M:194:CYS:HB2	1.95	0.49
1:A:64:ILE:HD11	1:A:164:LEU:HD12	1.94	0.49
3:M:116:PHE:HB2	3:M:135:LEU:HB3	1.94	0.49
1:B:98:SER:O	1:B:102:THR:HG23	2.11	0.49
3:L:175:LEU:HD23	3:L:175:LEU:C	2.32	0.49
3:M:158:ASN:HB2	3:M:180:THR:O	2.12	0.49
1:A:73:ARG:O	1:A:74:ILE:C	2.51	0.49
2:I:38:ARG:HD3	2:I:48:VAL:HG21	1.95	0.49
2:I:6:GLU:OE2	2:I:106:GLY:HA2	2.12	0.49
1:B:66:VAL:O	1:B:155:ASN:HB3	2.13	0.48
3:M:140:TYR:CG	3:M:141:PRO:HA	2.48	0.48
1:A:69:GLU:O	4:A:301:NAG:H83	2.14	0.48
3:M:133:VAL:HG22	3:M:134:CYS:N	2.28	0.48
1:A:61:ASN:ND2	3:L:93:SER:OG	2.47	0.48
3:M:6:GLN:OE1	3:M:87:TYR:HA	2.14	0.48
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:2:VAL:HA	2:I:25:SER:O	2.14	0.48
2:H:136:ALA:O	2:H:183:THR:HA	2.14	0.48
1:A:108:VAL:O	1:B:60:ILE:HG12	2.14	0.47
3:L:179:LEU:HG	3:L:181:LEU:CD1	2.44	0.47
1:B:96:LEU:HD13	1:B:146:LEU:HD22	1.95	0.47
3:M:54:ARG:HD3	3:M:58:VAL:O	2.13	0.47
1:B:41:LEU:HD21	1:B:125:LEU:HB3	1.96	0.47
1:A:47:TYR:CE2	1:A:51:LEU:HD22	2.49	0.47
3:L:166:GLN:CG	3:L:173:TYR:CZ	2.98	0.47
3:L:106:ILE:HD12	3:L:106:ILE:N	2.30	0.47
2:H:18:LEU:HD23	2:H:82(C):LEU:CD1	2.45	0.47
2:I:178:LEU:HD13	2:I:179:SER:N	2.30	0.47
2:I:48:VAL:HG13	2:I:63:VAL:HG21	1.96	0.47
2:I:6:GLU:H	2:I:105:GLN:HE22	1.61	0.47
3:M:33:LEU:HG	3:M:34:ALA:N	2.29	0.47
2:I:209:LYS:CG	2:I:210:LYS:N	2.78	0.47
2:I:169:VAL:HG23	2:I:177:SER:OG	2.15	0.47
2:H:178:LEU:C	2:H:178:LEU:HD12	2.36	0.47
3:M:126:LYS:C	3:M:128:GLY:N	2.67	0.47
1:A:109:LEU:HD22	1:A:113:HIS:CG	2.50	0.46
2:H:81:GLN:NE2	2:H:82(A):ASN:OD1	2.48	0.46
3:M:125:LEU:CD2	3:M:130:ALA:HB2	2.44	0.46
3:L:11:LEU:HD12	3:L:11:LEU:C	2.36	0.46
4:B:303:MAN:O6	4:B:304:BMA:H4	2.16	0.46
2:I:189:LEU:HD12	2:I:190:GLY:N	2.30	0.46
4:B:303:MAN:H3	4:B:305:MAN:H2	1.65	0.46
2:I:12:VAL:HG22	2:I:18:LEU:CD1	2.45	0.46
3:M:158:ASN:O	3:M:179:LEU:HG	2.16	0.46
3:L:127:SER:HA	5:L:338:HOH:O	2.15	0.46
1:B:41:LEU:CD2	1:B:125:LEU:HB3	2.46	0.46
2:I:12:VAL:HG21	2:I:18:LEU:HD13	1.97	0.46
1:A:160:ARG:O	1:A:161:PRO:C	2.55	0.46
1:B:93:LEU:HD13	1:B:142:VAL:HG13	1.98	0.46
1:A:154:PRO:HA	3:M:26:SER:O	2.16	0.46
2:H:107:THR:HG23	2:H:107:THR:O	2.16	0.46
3:M:170:ASP:OD1	3:M:172:THR:HG23	2.16	0.46
2:I:163:VAL:HB	2:I:182:VAL:HG12	1.97	0.45
1:A:61:ASN:ND2	3:L:93:SER:CB	2.79	0.45
1:B:47:TYR:HB2	1:B:50:ARG:HH21	1.81	0.45
1:B:35:CYS:SG	1:B:35:CYS:O	2.75	0.45
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.15	0.45
2:H:98:ASP:C	2:H:99:TYR:CD2	2.89	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:193:THR:HG22	2:H:195:ILE:HD12	1.98	0.45
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.98	0.45
1:A:177:CYS:O	1:A:181:LYS:N	2.48	0.45
2:I:209:LYS:HG2	2:I:210:LYS:N	2.32	0.45
1:A:54:MET:HA	1:A:54:MET:HE2	1.99	0.45
2:I:124:LEU:HD12	2:I:139:GLY:C	2.37	0.45
1:A:66:VAL:O	1:A:157:LYS:HB3	2.17	0.45
1:B:121:GLU:O	1:B:125:LEU:HD13	2.16	0.45
1:A:182:GLN:OE1	1:A:182:GLN:N	2.50	0.45
3:M:186:TYR:O	3:M:192:TYR:OH	2.34	0.45
2:H:52(A):TRP:CE3	2:H:53:TYR:HA	2.52	0.45
1:B:89:GLU:HG2	1:B:142:VAL:HG21	1.99	0.45
3:L:80:PRO:HA	3:L:106:ILE:HG12	1.99	0.45
1:B:43:ASP:O	1:B:46:GLN:HG2	2.17	0.45
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.51	0.45
1:B:100:SER:O	1:B:104:SER:HB2	2.16	0.45
2:I:67:PHE:CD1	2:I:67:PHE:N	2.85	0.44
3:M:116:PHE:HB3	3:M:118:PHE:HE2	1.82	0.44
1:A:117:LYS:HE3	1:A:117:LYS:HB3	1.80	0.44
2:I:134:GLY:O	2:I:186:SER:N	2.37	0.44
2:I:124:LEU:HB3	3:M:118:PHE:CE1	2.53	0.44
1:A:50:ARG:NH1	1:A:169:PHE:CD2	2.85	0.44
1:A:54:MET:HE2	1:A:58:PHE:HE1	1.81	0.44
2:I:124:LEU:HB2	2:I:139:GLY:H	1.83	0.44
2:I:159:LEU:C	2:I:159:LEU:HD23	2.38	0.44
2:I:205:THR:HG21	5:I:312:HOH:O	2.18	0.44
3:M:115:VAL:HG12	3:M:116:PHE:N	2.33	0.43
2:I:146:PHE:CE1	2:I:147:PRO:HB3	2.53	0.43
2:I:12:VAL:HG22	2:I:18:LEU:HD12	2.00	0.43
1:B:47:TYR:HA	1:B:50:ARG:HH21	1.83	0.43
3:M:187:GLU:C	3:M:189:HIS:N	2.68	0.43
3:M:105:GLU:HG2	3:M:166:GLN:NE2	2.33	0.43
2:H:29:PHE:CD1	2:H:34:ILE:HD11	2.53	0.43
1:B:167:ASN:HA	2:I:53:TYR:OH	2.18	0.43
2:I:94:ARG:O	2:I:100(A):MET:HA	2.19	0.43
1:A:73:ARG:O	1:A:76:ASN:N	2.51	0.43
1:A:160:ARG:HD2	2:H:98:ASP:OD2	2.19	0.43
1:B:139:SER:OG	1:B:140:PRO:HD2	2.19	0.43
1:A:54:MET:CG	1:A:165:LEU:CD1	2.90	0.43
3:L:108:ARG:HD2	3:L:171:SER:CB	2.49	0.43
2:I:196:CYS:N	5:I:319:HOH:O	2.52	0.43
1:A:58:PHE:CZ	1:A:109:LEU:HD21	2.54	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:51:ILE:CD1	2:I:57:THR:HG22	2.40	0.43
2:I:67:PHE:HD1	2:I:67:PHE:N	2.17	0.43
3:L:12:SER:HA	3:L:105:GLU:O	2.19	0.43
3:L:181:LEU:N	3:L:181:LEU:HD12	2.34	0.43
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.54	0.42
1:A:38:THR:OG1	1:A:188:TRP:NE1	2.49	0.42
2:I:124:LEU:HD21	3:M:133:VAL:HG11	2.01	0.42
1:B:141:LYS:HG3	1:B:141:LYS:H	1.64	0.42
1:A:82:ARG:C	1:A:84:GLN:H	2.21	0.42
2:I:196:CYS:N	2:I:209:LYS:O	2.53	0.42
3:L:151:ASP:HB2	5:L:318:HOH:O	2.20	0.42
2:H:8:GLY:O	2:H:18:LEU:HD12	2.20	0.42
1:B:159:VAL:HG22	1:B:160:ARG:N	2.34	0.42
1:B:41:LEU:HD21	1:B:125:LEU:CB	2.50	0.42
1:A:81:GLN:O	1:A:84:GLN:N	2.50	0.42
3:M:122:ASP:C	3:M:124:GLN:H	2.22	0.42
1:A:47:TYR:CB	1:A:50:ARG:HH21	2.33	0.42
2:I:147:PRO:HD2	2:I:202:PRO:CB	2.50	0.42
2:I:124:LEU:HD12	2:I:140:CYS:N	2.35	0.41
2:I:200:HIS:ND1	2:I:203:SER:HB3	2.34	0.41
1:B:96:LEU:CD1	1:B:146:LEU:HD22	2.50	0.41
3:M:12:SER:HA	3:M:105:GLU:O	2.20	0.41
2:I:4:LEU:HD21	2:I:27:PHE:HZ	1.85	0.41
3:M:150:VAL:HG12	3:M:155:GLN:OE1	2.20	0.41
3:M:155:GLN:HB3	3:M:179:LEU:HD11	2.01	0.41
1:B:63:LYS:HG3	3:M:92:TRP:CH2	2.55	0.41
2:I:150:VAL:HG11	2:I:198:VAL:HG13	2.02	0.41
1:B:36:THR:HG22	1:B:40:PHE:HE2	1.86	0.41
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.55	0.41
3:M:165:GLU:O	3:M:166:GLN:C	2.59	0.41
1:B:69:GLU:O	4:B:301:NAG:H83	2.20	0.41
2:I:119:PRO:HA	2:I:145:TYR:HB3	2.02	0.41
3:M:122:ASP:C	3:M:124:GLN:N	2.74	0.41
4:A:303:MAN:H3	4:A:305:MAN:H2	1.31	0.41
1:A:41:LEU:HD13	1:A:125:LEU:HB2	2.03	0.41
3:M:78:LEU:HD21	3:M:106:ILE:HD12	2.02	0.41
3:L:179:LEU:HG	3:L:181:LEU:HD11	2.02	0.41
2:I:97:PRO:O	2:I:98:ASP:HB2	2.20	0.41
2:I:12:VAL:HG11	2:I:82(C):LEU:HD13	2.01	0.41
3:M:149:LYS:HG2	3:M:154:LEU:CD2	2.51	0.41
2:H:99:TYR:CD2	2:H:99:TYR:N	2.88	0.41
2:I:30:THR:HA	2:I:52(A):TRP:CE3	2.56	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:12:VAL:CG2	2:I:18:LEU:CD1	2.99	0.41
2:H:12:VAL:O	2:H:111:VAL:HA	2.21	0.40
3:M:117:ILE:CD1	3:M:208:SER:HA	2.51	0.40
2:H:52(A):TRP:HE3	2:H:53:TYR:N	2.19	0.40
2:I:123:PRO:HD2	3:M:121:SER:CB	2.52	0.40
2:I:136:ALA:O	2:I:184:VAL:O	2.39	0.40
2:I:150:VAL:CG1	2:I:198:VAL:CG1	2.99	0.40
3:L:158:ASN:OD1	3:L:158:ASN:N	2.53	0.40
1:B:157:LYS:CE	4:B:302:NAG:H81	2.51	0.40
2:H:67:PHE:HA	2:H:81:GLN:O	2.22	0.40
3:L:108:ARG:NH1	3:L:108:ARG:HG3	2.34	0.40
2:I:99:TYR:OH	2:I:101:ASP:OD2	2.13	0.40
2:I:34:ILE:HD12	2:I:34:ILE:N	2.37	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:303:HOH:O	5:M:319:HOH:O[2_555]	1.98	0.22
1:A:48:ARG:NH1	1:A:48:ARG:NH1[2_656]	1.99	0.21

## 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	159/190 (84%)	150 (94%)	9 (6%)	0	100	100
1	B	133/190 (70%)	126 (95%)	6 (4%)	1 (1%)	27	52
2	H	210/226 (93%)	201 (96%)	8 (4%)	1 (0%)	38	66
2	I	200/226 (88%)	187 (94%)	12 (6%)	1 (0%)	38	66
3	L	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
3	M	203/214 (95%)	186 (92%)	17 (8%)	0	100	100
All	All	1115/1260 (88%)	1053 (94%)	59 (5%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	62	SER
1	B	140	PRO
2	I	149	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	151/176 (86%)	151 (100%)	0	100	100
1	B	128/176 (73%)	128 (100%)	0	100	100
2	H	174/186 (94%)	172 (99%)	2 (1%)	84	96
2	I	166/186 (89%)	163 (98%)	3 (2%)	71	91
3	L	185/187 (99%)	185 (100%)	0	100	100
3	M	181/187 (97%)	180 (99%)	1 (1%)	92	98
All	All	985/1098 (90%)	979 (99%)	6 (1%)	92	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	63	VAL
2	H	186	SER
2	I	31	SER
2	I	165	THR
2	I	184	VAL
3	M	143	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	61	ASN
2	I	155	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 ⓘ

10 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	A	301	1,4	12,14,15	0.84	1 (8%)	15,19,21	1.45	3 (20%)
4	NAG	A	302	4	12,14,15	0.76	1 (8%)	15,19,21	1.05	1 (6%)
4	MAN	A	303	4	10,11,12	0.66	0	11,15,17	3.21	4 (36%)
4	BMA	A	304	4	10,11,12	1.00	1 (10%)	11,15,17	1.50	2 (18%)
4	MAN	A	305	4	10,11,12	0.68	0	11,15,17	0.91	0
4	NAG	B	301	1,4	12,14,15	0.63	0	15,19,21	0.85	1 (6%)
4	NAG	B	302	4	12,14,15	0.60	0	15,19,21	0.99	1 (6%)
4	MAN	B	303	4	10,11,12	0.70	0	11,15,17	1.96	3 (27%)
4	BMA	B	304	4	10,11,12	0.78	0	11,15,17	1.21	1 (9%)
4	MAN	B	305	4	10,11,12	0.77	0	11,15,17	0.88	1 (9%)

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	A	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	302	4	-	0/6/23/26	0/1/1/1
4	MAN	A	303	4	-	0/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	304	4	-	0/2/19/22	0/1/1/1
4	MAN	A	305	4	-	0/2/19/22	0/1/1/1
4	NAG	B	301	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	302	4	-	0/6/23/26	0/1/1/1
4	MAN	B	303	4	-	0/2/19/22	0/1/1/1
4	BMA	B	304	4	-	0/2/19/22	0/1/1/1
4	MAN	B	305	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	304	BMA	O5-C5	-2.68	1.40	1.45
4	A	301	NAG	O5-C5	-2.38	1.41	1.45
4	A	302	NAG	O5-C5	-2.17	1.41	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	MAN	C3-C4-C5	-7.05	97.62	110.20
4	A	303	MAN	O5-C5-C6	5.08	112.31	106.98
4	B	303	MAN	O5-C5-C6	4.37	111.57	106.98
4	A	303	MAN	C4-C3-C2	-3.60	105.67	110.50
4	A	303	MAN	O5-C5-C4	-3.36	106.39	110.65
4	B	304	BMA	O5-C5-C6	3.33	110.48	106.98
4	A	301	NAG	O5-C5-C4	-3.33	106.43	110.65
4	A	304	BMA	C4-C3-C2	3.31	114.95	110.50
4	A	301	NAG	O5-C5-C6	2.98	110.11	106.98
4	B	303	MAN	C3-C4-C5	-2.86	105.09	110.20
4	A	301	NAG	C3-C2-N2	-2.76	107.56	111.76
4	A	304	BMA	O5-C5-C4	-2.57	107.39	110.65
4	A	302	NAG	O5-C5-C4	-2.47	107.52	110.65
4	B	303	MAN	O5-C5-C4	-2.44	107.56	110.65
4	B	301	NAG	O5-C5-C6	2.26	109.35	106.98
4	B	302	NAG	C3-C2-N2	-2.20	108.41	111.76
4	B	305	MAN	O5-C5-C6	2.03	109.11	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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	161/190 (84%)	0.15	2 (1%) 75 77	44, 62, 87, 91	0
1	B	137/190 (72%)	0.84	19 (13%) 4 2	58, 83, 104, 106	0
2	H	214/226 (94%)	0.04	1 (0%) 88 90	35, 55, 65, 70	0
2	I	206/226 (91%)	0.53	22 (10%) 6 5	45, 64, 105, 111	0
3	L	212/214 (99%)	0.01	0 100 100	26, 40, 57, 61	0
3	M	207/214 (96%)	0.64	29 (14%) 3 2	38, 59, 118, 125	0
All	All	1137/1260 (90%)	0.34	73 (6%) 19 16	26, 58, 106, 125	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	138	LEU	6.4
2	I	197	ASN	5.1
1	B	175	LEU	4.8
3	M	192	TYR	4.6
3	M	133	VAL	4.5
1	B	40	PHE	4.4
3	M	149	LYS	4.4
1	B	126	LEU	4.3
3	M	147	GLN	4.2
3	M	145	LYS	4.2
3	M	193	ALA	3.6
2	I	191	THR	3.6
1	B	178	SER	3.4
2	I	177	SER	3.4
1	B	85	VAL	3.4
3	M	118	PHE	3.4
3	M	157	GLY	3.4
3	M	119	PRO	3.3
1	B	97	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	141	LEU	3.2
1	B	88	ARG	3.2
1	B	169	PHE	3.2
3	M	146	VAL	3.2
1	A	82	ARG	3.2
3	M	122	ASP	3.2
2	I	125	ALA	3.1
1	B	72	PHE	3.1
2	I	198	VAL	3.0
1	B	84	GLN	2.9
3	M	135	LEU	2.9
2	I	137	ALA	2.9
2	I	158	ALA	2.8
2	I	182	VAL	2.7
3	M	195	GLU	2.7
3	M	120	PRO	2.7
3	M	203	SER	2.7
2	I	139	GLY	2.7
3	M	131	SER	2.6
2	I	179	SER	2.5
3	M	148	TRP	2.5
1	B	36	THR	2.5
1	B	48	ARG	2.5
3	M	155	GLN	2.5
3	M	177	SER	2.4
2	I	133	GLY	2.4
1	B	128	ASN	2.4
2	I	132	SER	2.4
2	H	133	GLY	2.3
2	I	124	LEU	2.3
3	M	132	VAL	2.3
3	M	130	ALA	2.3
2	I	145	TYR	2.3
1	A	93	LEU	2.3
3	M	179	LEU	2.3
2	I	189	LEU	2.3
1	B	43	ASP	2.2
3	M	156	SER	2.2
3	M	180	THR	2.2
1	B	142	VAL	2.2
1	B	99	LEU	2.2
3	M	163	VAL	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	45	LEU	2.1
2	I	178	LEU	2.1
3	M	125	LEU	2.1
3	M	154	LEU	2.1
3	M	185	ASP	2.1
2	I	160	THR	2.1
1	B	153	GLY	2.1
1	B	179	CYS	2.0
2	I	209	LYS	2.0
2	I	142	VAL	2.0
2	I	134	GLY	2.0
3	M	194	CYS	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	B	302	14/15	0.18	-	84,89,91,94	0
4	NAG	A	302	14/15	0.13	-	68,76,81,84	0
4	BMA	A	304	11/12	0.21	-	88,99,103,105	0
4	MAN	A	303	11/12	0.14	-	80,85,88,89	0
4	NAG	A	301	14/15	0.13	-	65,71,75,76	0
4	MAN	B	305	11/12	0.14	-	91,97,104,106	0
4	MAN	B	303	11/12	0.19	-	92,97,102,104	0
4	BMA	B	304	11/12	0.24	-	101,107,112,113	0
4	MAN	A	305	11/12	0.13	-	76,84,88,92	0
4	NAG	B	301	14/15	0.13	-	82,87,90,91	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.