W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 04:39 AM BST

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 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 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	:	2.13.1
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)	:	2.13.1

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 2.61 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.
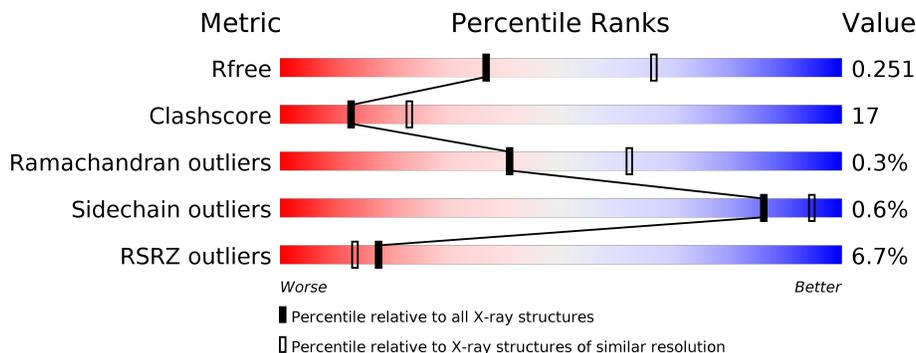
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 >=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	190	2% 61% 24% 15%
1	B	190	11% 44% 28% • 28%
2	H	226	75% 19% 5%
2	I	226	10% 58% 33% 9%
3	L	214	81% 18% •
3	M	214	14% 66% 30% •

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Mol	Chain	Length	Quality of chain
4	C	5	40% 60%
4	D	5	40% 60%

2   Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8977 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Interleukin-34.

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

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

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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 1577	C 994	N 262	O 315	S 6	0	0	0
2	I	206	Total 1515	C 954	N 254	O 301	S 6	0	0	0

- Molecule 3 is a protein called FAb2 Light Chain.

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

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyrano se-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.
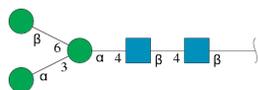
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	5	Total 61	C 34	N 2	O 25	0	0	0
4	D	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	14	Total 14	O 14	0	0
5	H	22	Total 22	O 22	0	0
5	L	42	Total 42	O 42	0	0
5	I	21	Total 21	O 21	0	0
5	M	20	Total 20	O 20	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: Interleukin-34
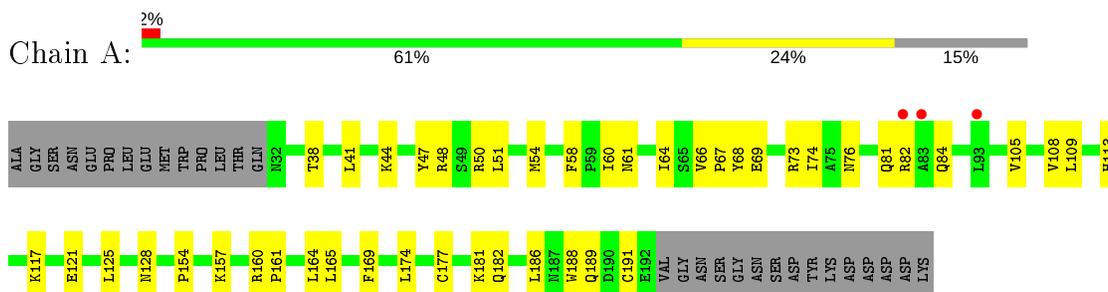
Chain A:

- Molecule 1: Interleukin-34

Chain B:
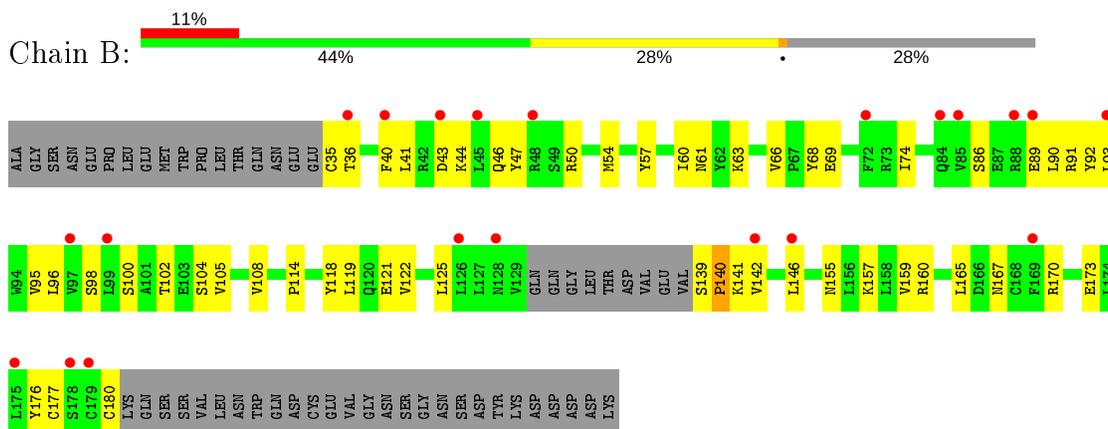
- Molecule 2: FAb2 Heavy Chain
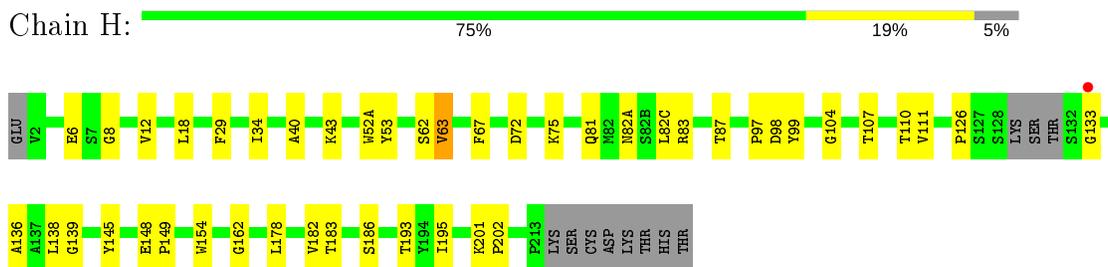
Chain H:

- Molecule 2: FAb2 Heavy Chain
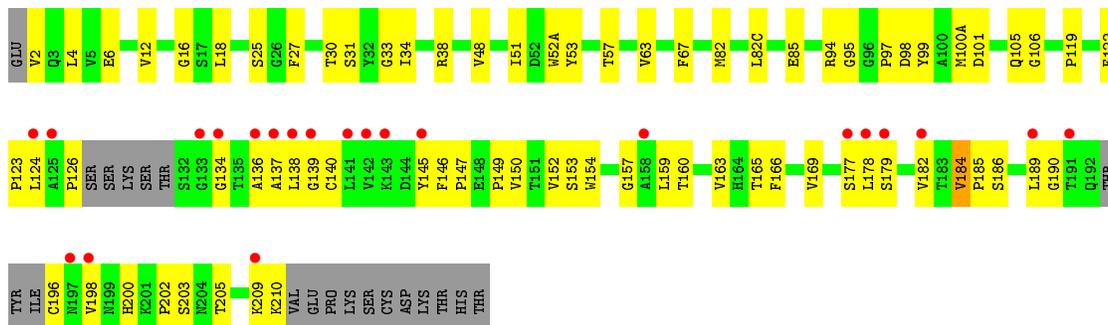
Chain I:

• Molecule 3: FAb2 Light Chain
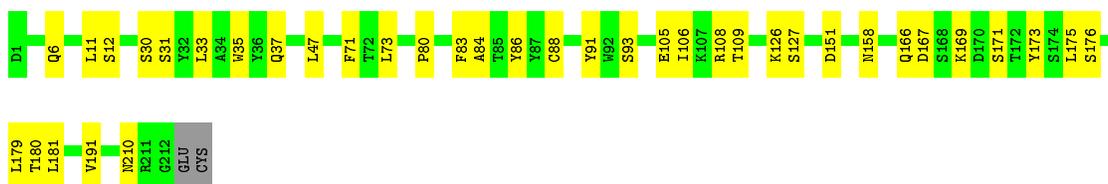
Chain L:

• Molecule 3: FAb2 Light Chain

Chain M:
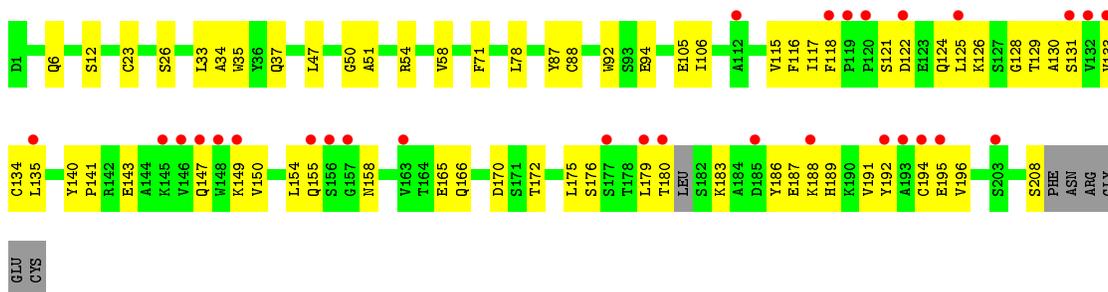
• Molecule 4: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain C:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]alpha-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain D:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.70 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.225 , 0.256 0.223 , 0.251	Depositor DCC
R_{free} test set	2213 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
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
F_o,F_c correlation	0.94	EDS
Total number of atoms	8977	wwPDB-VP
Average B, all atoms (Å^2)	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.*

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[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: 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 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	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
4	C	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	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

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 17.

All (292) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:152:VAL:HG12	2:I:153:SER:N	2.02	0.74
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
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
3:M:115:VAL:C	3:M:116:PHE:HD1	1.95	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:C:2:NAG:O3	4:C:3: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:D:2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:186:LEU:HA	1:A:189:GLN:HG2	1.86	0.57
1:B:54:MET:HG3	1:B:165:LEU:HD12	1.86	0.57
2:I:157:GLY:O	2:I:160:THR:HG23	2.04	0.57
1:B:61:ASN:ND2	3:M:94:GLU:H	2.01	0.57
1:A:68:TYR:CE1	4:C:3:MAN:O2	2.58	0.57
1:B:92:TYR:O	1:B:95:VAL:HG12	2.05	0.57
3:M:183:LYS:HD3	3:M:183:LYS:C	2.25	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
1:A:47:TYR:HA	1:A:50:ARG:HE	1.69	0.56
1:B:173:GLU:O	1:B:177:CYS:HB2	2.06	0.56
2:I:139:GLY:CA	2:I:154:TRP:HH2	2.15	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:D:2: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:NZ	1:A:121:GLU:OE1	2.36	0.52
1:B:57:TYR:CD2	1:B:114:PRO:HB2	2.44	0.52
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.92	0.52
3:M:155:GLN:CB	3:M:179:LEU:HD11	2.40	0.52
1:B:90:LEU:HD12	1:B:91:ARG:HG3	1.92	0.52
3:M:150:VAL:CG2	3:M:192:TYR:CE2	2.92	0.52
2:I:150:VAL:HG11	2:I:198:VAL:CG1	2.40	0.52
2:I:16:GLY:O	2:I:82(C):LEU:HD12	2.09	0.52
3:M:191:VAL:HG12	3:M:192:TYR:N	2.25	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
2:I:152:VAL:CG1	2:I:153:SER:N	2.72	0.51
3:M:115:VAL:C	3:M:116:PHE:CD1	2.78	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
1:B:90:LEU:HD12	1:B:91:ARG:H	1.75	0.49
4:C:2:NAG:O3	4:C:3:MAN:C2	2.60	0.49
1:A:47:TYR:CA	1:A:50:ARG:HH21	2.25	0.49
1:B:105:VAL:HG11	1:B:119:LEU:HD11	1.94	0.49
2:I:178:LEU:HD13	2:I:178:LEU:C	2.32	0.49
1:A:64:ILE:HD11	1:A:164:LEU:HD12	1.94	0.49
3:M:117:ILE:HG22	3:M:194:CYS:HB2	1.95	0.49
1:B:98:SER:O	1:B:102:THR:HG23	2.11	0.49
3:M:116:PHE:HB2	3:M:135:LEU:HB3	1.94	0.49
3:L:175:LEU:HD23	3:L:175:LEU:C	2.32	0.49
1:A:73:ARG:O	1:A:74:ILE:C	2.51	0.49
2:I:6:GLU:OE2	2:I:106:GLY:HA2	2.12	0.49
2:I:38:ARG:HD3	2:I:48:VAL:HG21	1.95	0.49
3:M:158:ASN:HB2	3:M:180:THR:O	2.12	0.49
1:B:66:VAL:O	1:B:155:ASN:HB3	2.13	0.48
1:A:69:GLU:O	4:C:1:NAG:H83	2.14	0.48
3:M:140:TYR:CG	3:M:141:PRO:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASN:ND2	3:L:93:SER:OG	2.47	0.48
3:M:133:VAL:HG22	3:M:134:CYS:N	2.28	0.48
3:M:6:GLN:OE1	3:M:87:TYR:HA	2.14	0.48
2:H:136:ALA:O	2:H:183:THR:HA	2.14	0.48
2:I:2:VAL:HA	2:I:25:SER:O	2.14	0.48
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.48	0.48
1:A:108:VAL:O	1:B:60:ILE:HG12	2.14	0.47
1:B:96:LEU:HD13	1:B:146:LEU:HD22	1.95	0.47
3:L:179:LEU:HG	3:L:181:LEU:CD1	2.44	0.47
3:M:54:ARG:HD3	3:M:58:VAL:O	2.13	0.47
1:A:47:TYR:CE2	1:A:51:LEU:HD22	2.49	0.47
1:B:41:LEU:HD21	1:B:125:LEU:HB3	1.96	0.47
3:L:106:ILE:HD12	3:L:106:ILE:N	2.30	0.47
3:L:166:GLN:CG	3:L:173:TYR:CZ	2.98	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:169:VAL:HG23	2:I:177:SER:OG	2.15	0.47
2:I:209:LYS:CG	2:I:210:LYS:N	2.78	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
4:D:3:MAN:O6	4:D:5:BMA:H4	2.16	0.46
2:I:189:LEU:HD12	2:I:190:GLY:N	2.30	0.46
3:L:11:LEU:HD12	3:L:11:LEU:C	2.36	0.46
3:M:125:LEU:CD2	3:M:130:ALA:HB2	2.44	0.46
4:D:3:MAN:H3	4:D:4:MAN:H2	1.65	0.46
2:I:12:VAL:HG22	2:I:18:LEU:CD1	2.45	0.46
3:L:127:SER:HA	5:L:338:HOH:O	2.15	0.46
3:M:158:ASN:O	3:M:179:LEU:HG	2.16	0.46
1:A:160:ARG:O	1:A:161:PRO:C	2.55	0.46
1:B:41:LEU:CD2	1:B:125:LEU:HB3	2.46	0.46
1:B:93:LEU:HD13	1:B:142:VAL:HG13	1.98	0.46
2:I:12:VAL:HG21	2:I:18:LEU:HD13	1.97	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
1:A:61:ASN:ND2	3:L:93:SER:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:CYS:SG	1:B:35:CYS:O	2.75	0.45
1:B:47:TYR:HB2	1:B:50:ARG:HH21	1.81	0.45
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.15	0.45
2:I:163:VAL:HB	2:I:182:VAL:HG12	1.97	0.45
2:H:193:THR:HG22	2:H:195:ILE:HD12	1.98	0.45
2:H:98:ASP:C	2:H:99:TYR:CD2	2.89	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:66:VAL:O	1:A:157:LYS:HB3	2.17	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:182:GLN:OE1	1:A:182:GLN:N	2.50	0.45
1:B:121:GLU:O	1:B:125:LEU:HD13	2.16	0.45
1:B:100:SER:O	1:B:104:SER:HB2	2.16	0.45
1:B:43:ASP:O	1:B:46:GLN:HG2	2.17	0.45
1:B:89:GLU:HG2	1:B:142:VAL:HG21	1.99	0.45
2:H:52(A):TRP:CE3	2:H:53:TYR:HA	2.52	0.45
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.51	0.45
3:L:80:PRO:HA	3:L:106:ILE:HG12	1.99	0.45
3:M:186:TYR:O	3:M:192:TYR:OH	2.34	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
1:A:50:ARG:NH1	1:A:169:PHE:CD2	2.85	0.44
2:I:124:LEU:HB3	3:M:118:PHE:CE1	2.53	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
1:B:47:TYR:HA	1:B:50:ARG:HH21	1.83	0.43
2:H:29:PHE:CD1	2:H:34:ILE:HD11	2.53	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
3:M:105:GLU:HG2	3:M:166:GLN:NE2	2.33	0.43
3:M:187:GLU:C	3:M:189:HIS:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:196:CYS:N	5:I:319:HOH:O	2.52	0.43
3:L:108:ARG:HD2	3:L:171:SER:CB	2.49	0.43
1:A:58:PHE:CZ	1:A:109:LEU:HD21	2.54	0.43
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
1:A:38:THR:OG1	1:A:188:TRP:NE1	2.49	0.42
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.54	0.42
1:A:82:ARG:C	1:A:84:GLN:H	2.21	0.42
1:B:141:LYS:HG3	1:B:141:LYS:H	1.64	0.42
2:I:124:LEU:HD21	3:M:133:VAL:HG11	2.01	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
1:B:159:VAL:HG22	1:B:160:ARG:N	2.34	0.42
2:H:8:GLY:O	2:H:18:LEU:HD12	2.20	0.42
1:A:81:GLN:O	1:A:84:GLN:N	2.50	0.42
1:B:41:LEU:HD21	1:B:125:LEU:CB	2.50	0.42
1:A:47:TYR:CB	1:A:50:ARG:HH21	2.33	0.42
3:M:122:ASP:C	3:M:124:GLN:H	2.22	0.42
2:I:147:PRO:HD2	2:I:202:PRO:CB	2.50	0.42
1:B:96:LEU:CD1	1:B:146:LEU:HD22	2.50	0.41
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
2:I:4:LEU:HD21	2:I:27:PHE:HZ	1.85	0.41
3:M:12:SER:HA	3:M:105:GLU:O	2.20	0.41
1:B:63:LYS:HG3	3:M:92:TRP:CH2	2.55	0.41
3:M:155:GLN:HB3	3:M:179:LEU:HD11	2.01	0.41
3:M:150:VAL:HG12	3:M:155:GLN:OE1	2.20	0.41
1:B:36:THR:HG22	1:B:40:PHE:HE2	1.86	0.41
2:I:150:VAL:HG11	2:I:198:VAL:HG13	2.02	0.41
1:B:69:GLU:O	4:D:1:NAG:H83	2.20	0.41
2:I:119:PRO:HA	2:I:145:TYR:HB3	2.02	0.41
3:M:165:GLU:O	3:M:166:GLN:C	2.59	0.41
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.55	0.41
1:A:41:LEU:HD13	1:A:125:LEU:HB2	2.03	0.41
4:C:3:MAN:H3	4:C:4:MAN:H2	1.31	0.41
3:M:122:ASP:C	3:M:124:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:179:LEU:HG	3:L:181:LEU:HD11	2.02	0.41
3:M:78:LEU:HD21	3:M:106:ILE:HD12	2.02	0.41
2:I:97:PRO:O	2:I:98:ASP:HB2	2.20	0.41
2:H:99:TYR:CD2	2:H:99:TYR:N	2.88	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:I:12:VAL:CG2	2:I:18:LEU:CD1	2.99	0.41
2:I:30:THR:HA	2:I:52(A):TRP:CE3	2.56	0.41
2:H:12:VAL:O	2:H:111:VAL:HA	2.21	0.40
2:H:52(A):TRP:HE3	2:H:53:TYR:N	2.19	0.40
3:M:117:ILE:CD1	3:M:208:SER:HA	2.51	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:D:2:NAG:H81	2.51	0.40
2:H:67:PHE:HA	2:H:81:GLN:O	2.22	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
3:L:108:ARG:NH1	3:L:108:ARG:HG3	2.34	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	Interatomic distance (Å)	Clash overlap (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 (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	159/190 (84%)	150 (94%)	9 (6%)	0	100	100
1	B	133/190 (70%)	126 (95%)	6 (4%)	1 (1%)	19	36
2	H	210/226 (93%)	201 (96%)	8 (4%)	1 (0%)	29	50
2	I	200/226 (88%)	187 (94%)	12 (6%)	1 (0%)	29	50
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%)	41	62

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 (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	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%)	73	88
2	I	166/186 (89%)	163 (98%)	3 (2%)	59	79
3	L	185/187 (99%)	185 (100%)	0	100	100
3	M	181/187 (97%)	180 (99%)	1 (1%)	86	94
All	All	985/1098 (90%)	979 (99%)	6 (1%)	86	94

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

Mol	Chain	Res	Type
2	H	63	VAL
2	H	186	SER

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Mol	Chain	Res	Type
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 (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)

10 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	C	1	1,4	14,14,15	0.68	0	17,19,21	0.98	1 (5%)
4	NAG	C	2	4	14,14,15	0.56	0	17,19,21	0.87	0
4	MAN	C	3	4	11,11,12	0.53	0	15,15,17	3.06	5 (33%)
4	MAN	C	4	4	11,11,12	0.56	0	15,15,17	1.07	2 (13%)
4	BMA	C	5	4	11,11,12	0.81	0	15,15,17	1.01	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.50	0	17,19,21	0.75	0
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	MAN	D	3	4	11,11,12	0.67	0	15,15,17	1.74	3 (20%)
4	MAN	D	4	4	11,11,12	0.59	0	15,15,17	1.14	1 (6%)
4	BMA	D	5	4	11,11,12	0.56	0	15,15,17	0.82	1 (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
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	MAN	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	1/1/1/1
4	BMA	C	5	4	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	MAN	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	BMA	D	5	4	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3	MAN	C3-C4-C5	-7.07	97.62	110.24
4	C	3	MAN	C1-C2-C3	5.75	116.74	109.67
4	C	3	MAN	O5-C1-C2	4.43	117.61	110.77
4	D	3	MAN	C1-C2-C3	4.26	114.90	109.67
4	D	4	MAN	C1-C2-C3	3.27	113.69	109.67
4	C	3	MAN	O5-C5-C6	3.26	112.31	107.20
4	C	3	MAN	C2-C3-C4	-3.02	105.67	110.89
4	D	3	MAN	C3-C4-C5	-2.89	105.09	110.24
4	D	3	MAN	O5-C5-C6	2.78	111.57	107.20
4	C	4	MAN	C1-O5-C5	2.52	115.61	112.19
4	C	5	BMA	C2-C3-C4	2.34	114.95	110.89
4	D	5	BMA	O5-C5-C6	2.09	110.48	107.20
4	C	4	MAN	C1-C2-C3	2.06	112.20	109.67
4	C	1	NAG	C1-O5-C5	-2.02	109.46	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4	MAN	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	C	5	BMA	O5-C5-C6-O6
4	C	5	BMA	C4-C5-C6-O6
4	C	4	MAN	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	MAN	C4-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
4	D	5	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	5	BMA	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4	MAN	C1-C2-C3-C4-C5-O5
4	D	5	BMA	C1-C2-C3-C4-C5-O5

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	2	0
4	D	2	NAG	3	0
4	D	3	MAN	2	0
4	D	4	MAN	1	0
4	C	4	MAN	1	0
4	C	3	MAN	4	0
4	D	5	BMA	1	0
4	C	1	NAG	1	0
4	D	1	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	161/190 (84%)	0.12	3 (1%)	66	62	44, 62, 87, 91	0
1	B	137/190 (72%)	0.85	21 (15%)	2	1	58, 83, 104, 106	0
2	H	214/226 (94%)	0.01	1 (0%)	91	89	35, 55, 65, 70	0
2	I	206/226 (91%)	0.52	22 (10%)	6	4	45, 64, 105, 111	0
3	L	212/214 (99%)	-0.00	0	100	100	26, 40, 57, 61	0
3	M	207/214 (96%)	0.64	29 (14%)	2	1	38, 59, 118, 125	0
All	All	1137/1260 (90%)	0.33	76 (6%)	17	13	26, 58, 106, 125	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	138	LEU	6.0
2	I	197	ASN	5.2
1	B	126	LEU	4.7
3	M	145	LYS	4.6
1	B	40	PHE	4.3
3	M	149	LYS	4.2
3	M	192	TYR	4.2
2	I	177	SER	4.2
3	M	147	GLN	4.0
1	B	175	LEU	4.0
3	M	157	GLY	3.9
3	M	133	VAL	3.8
2	I	191	THR	3.7
1	B	178	SER	3.7
3	M	122	ASP	3.6
1	B	97	VAL	3.6
1	A	82	ARG	3.5
3	M	119	PRO	3.5
1	B	85	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	M	193	ALA	3.4
3	M	118	PHE	3.3
2	I	125	ALA	3.2
2	I	141	LEU	3.2
1	B	88	ARG	3.2
1	B	84	GLN	3.1
3	M	135	LEU	3.0
2	I	139	GLY	3.0
1	B	169	PHE	3.0
1	B	72	PHE	2.9
2	I	182	VAL	2.9
2	I	198	VAL	2.9
3	M	146	VAL	2.9
3	M	156	SER	2.7
3	M	120	PRO	2.7
2	I	158	ALA	2.7
2	I	137	ALA	2.7
3	M	203	SER	2.7
3	M	155	GLN	2.6
2	I	189	LEU	2.6
3	M	125	LEU	2.6
3	M	195	GLU	2.5
3	M	185	ASP	2.5
1	B	142	VAL	2.5
1	B	128	ASN	2.5
2	I	178	LEU	2.4
2	I	124	LEU	2.4
3	M	177	SER	2.4
2	H	133	GLY	2.4
3	M	179	LEU	2.4
3	M	148	TRP	2.4
1	B	43	ASP	2.4
3	M	163	VAL	2.4
3	M	194	CYS	2.4
1	A	93	LEU	2.3
2	I	145	TYR	2.3
2	I	179	SER	2.3
1	B	36	THR	2.3
3	M	131	SER	2.2
3	M	112	ALA	2.2
1	B	179	CYS	2.2
1	B	48	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	136	ALA	2.2
3	M	180	THR	2.1
2	I	133	GLY	2.1
2	I	134	GLY	2.1
1	A	83	ALA	2.1
1	B	45	LEU	2.1
1	B	89	GLU	2.1
1	B	99	LEU	2.1
2	I	142	VAL	2.0
2	I	143	LYS	2.0
2	I	209	LYS	2.0
1	B	93	LEU	2.0
1	B	146	LEU	2.0
3	M	188	LYS	2.0
3	M	132	VAL	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	MAN	D	3	11/12	0.69	0.18	92,97,102,104	0
4	BMA	D	5	11/12	0.72	0.22	101,107,112,113	0
4	BMA	C	5	11/12	0.79	0.21	88,99,103,105	0
4	MAN	C	4	11/12	0.82	0.14	76,84,88,92	0
4	MAN	C	3	11/12	0.85	0.15	80,85,88,89	0
4	MAN	D	4	11/12	0.85	0.16	91,97,104,106	0
4	NAG	D	2	14/15	0.92	0.21	84,89,91,94	0
4	NAG	C	1	14/15	0.93	0.15	65,71,75,76	0
4	NAG	C	2	14/15	0.94	0.14	68,76,81,84	0
4	NAG	D	1	14/15	0.94	0.14	82,87,90,91	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.