



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DKE
Title : Crystal Structure of Human Interleukin-34 Bound to FAb1.1
Authors : Ma, X.; Chen, Y.; Stawicki, S.; Wu, Y.; Bazan, J.F.; Starovasnik, M.A.
Deposited on : 2012-02-03
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

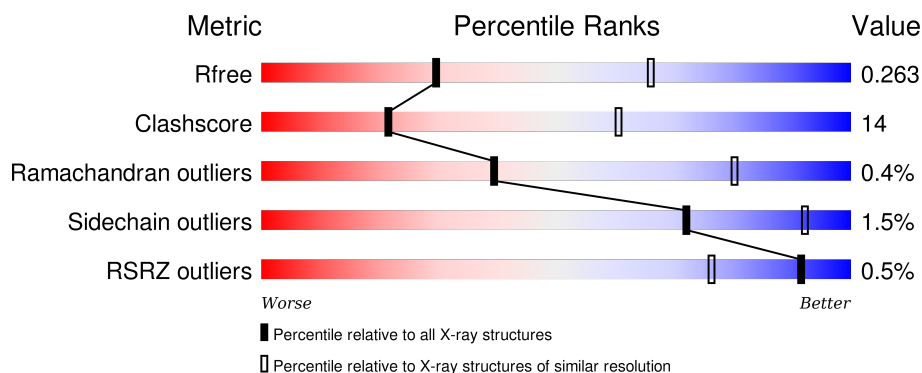
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>62%</div> <div>21%</div> <div>•</div> <div>17%</div> </div>
1	B	190	<div> <div>46%</div> <div>26%</div> <div>28%</div> </div>
2	H	230	<div> <div>77%</div> <div>18%</div> <div>•</div> </div>
2	I	230	<div> <div>66%</div> <div>27%</div> <div>•</div> <div>6%</div> </div>
3	L	214	<div> <div>75%</div> <div>23%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	214	 <div>70% 29%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	302	-	-	X	-
4	MAN	A	303	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9109 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	157	Total	C	N	O	S	0	0	0
			1279	819	218	234	8			
1	B	137	Total	C	N	O	S	0	0	0
			1126	724	193	202	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

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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 FAb1.1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1645	1041	277	320	7			
2	I	216	Total	C	N	O	S	0	0	0
			1623	1030	273	314	6			

- Molecule 3 is a protein called FAb1.1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1645	1033	272	334	6			
3	M	212	Total	C	N	O	S	0	0	0
			1630	1025	270	330	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		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	4	Total	C	N	O	0	0
			50	28	2	20		

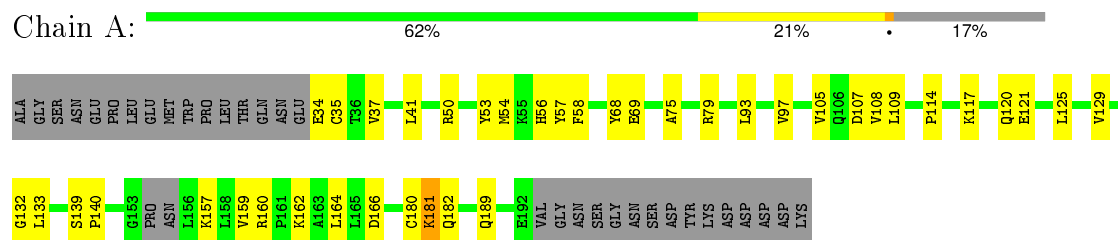
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total 10	O 10	0	0
6	B	9	Total 9	O 9	0	0
6	H	9	Total 9	O 9	0	0
6	L	6	Total 6	O 6	0	0
6	I	7	Total 7	O 7	0	0
6	M	9	Total 9	O 9	0	0

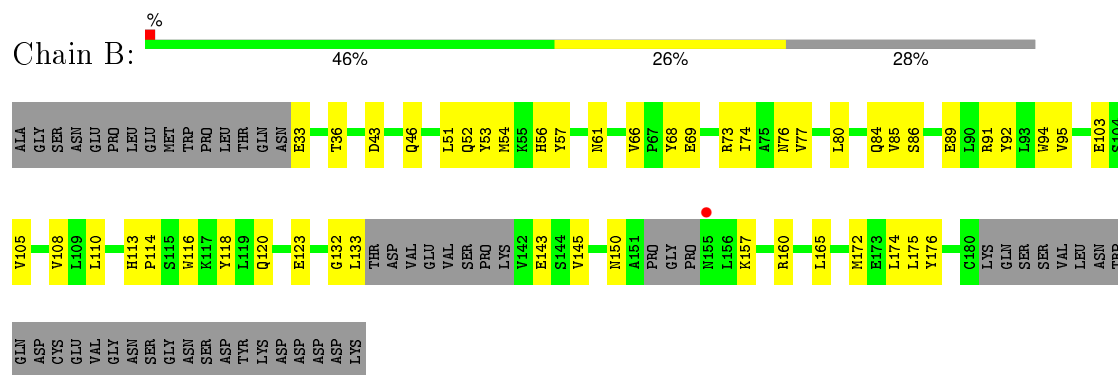
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

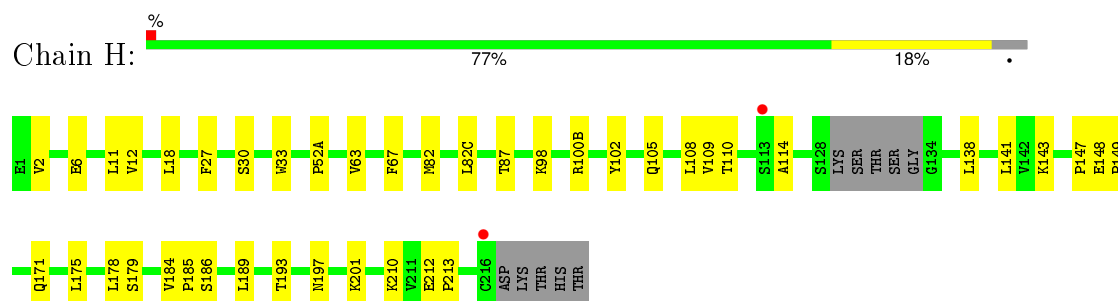
- Molecule 1: Interleukin-34



- Molecule 1: Interleukin-34

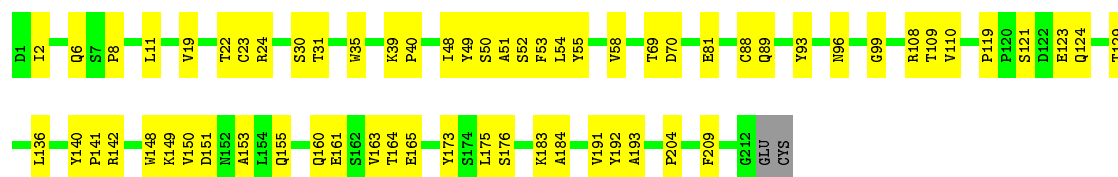


- Molecule 2: FAb1.1 Heavy Chain



- Molecule 2: FAb1.1 Heavy Chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.55Å 122.47Å 149.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.91 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-3.00) 97.5 (49.91-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.231 , 0.265 0.229 , 0.263	Depositor DCC
R_{free} test set	1954 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	3 of 38782 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9109	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.33	0/1303	0.42	0/1766
1	B	0.34	0/1145	0.44	0/1548
2	H	0.33	0/1686	0.47	0/2295
2	I	0.36	0/1664	0.50	0/2266
3	L	0.36	0/1682	0.49	0/2284
3	M	0.35	0/1667	0.48	0/2264
All	All	0.35	0/9147	0.47	0/12423

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	1279	0	1294	40	0
1	B	1126	0	1147	41	0
2	H	1645	0	1609	27	0
2	I	1623	0	1592	58	0
3	L	1645	0	1589	45	0
3	M	1630	0	1579	46	0
4	A	61	0	52	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	50	0	43	3	0
6	A	10	0	0	1	0
6	B	9	0	0	0	0
6	H	9	0	0	1	0
6	I	7	0	0	1	0
6	L	6	0	0	0	0
6	M	9	0	0	0	0
All	All	9109	0	8905	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (253) 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:24:ALA:CB	2:I:29:PHE:CE1	2.09	1.36
2:I:24:ALA:HB2	2:I:29:PHE:CE1	1.67	1.26
2:I:24:ALA:HB3	2:I:29:PHE:CE1	1.78	1.15
2:I:24:ALA:CB	2:I:29:PHE:HE1	1.52	1.14
1:A:69:GLU:OE2	4:A:302:NAG:O6	1.62	1.14
3:L:187:GLU:HA	3:L:211:ARG:HH22	0.94	1.05
2:I:29:PHE:HD2	2:I:34:ILE:HD11	1.18	1.04
2:I:100:SER:O	2:I:100(A):LYS:HB2	1.60	0.99
3:L:187:GLU:HA	3:L:211:ARG:NH2	1.79	0.98
2:I:24:ALA:HB2	2:I:29:PHE:CZ	2.03	0.94
1:A:120:GLN:HE21	3:L:31:THR:HG22	1.34	0.92
1:A:41:LEU:HD21	1:A:125:LEU:HB3	1.53	0.89
2:I:29:PHE:CD2	2:I:34:ILE:HD11	2.08	0.88
3:L:187:GLU:CA	3:L:211:ARG:HH22	1.84	0.88
3:L:187:GLU:OE2	3:L:211:ARG:NH2	2.06	0.88
1:A:139:SER:HB2	1:A:140:PRO:HD2	1.57	0.87
2:I:29:PHE:HD2	2:I:34:ILE:CD1	1.87	0.86
2:I:123:PRO:HD2	3:M:121:SER:OG	1.76	0.86
2:I:24:ALA:HB3	2:I:29:PHE:HE1	1.19	0.85
2:I:184:VAL:CG2	2:I:185:PRO:HD2	2.07	0.83
4:A:302:NAG:O3	4:A:303:MAN:O2	1.98	0.82
1:A:34:GLU:HG2	1:A:35:CYS:H	1.45	0.82
1:B:103:GLU:OE2	2:I:100(A):LYS:NZ	2.13	0.81
2:I:184:VAL:HG22	2:I:185:PRO:HD2	1.61	0.81
2:I:29:PHE:CD2	2:I:34:ILE:CD1	2.63	0.80
1:A:41:LEU:CD2	1:A:125:LEU:HB3	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:192:TYR:HB2	3:M:209:PHE:CE2	2.18	0.79
3:M:6:GLN:HG2	3:M:23:CYS:SG	2.23	0.78
1:B:69:GLU:HG2	1:B:145:VAL:HG23	1.66	0.76
4:A:302:NAG:O3	4:A:303:MAN:C2	2.33	0.76
1:A:68:TYR:CD2	4:A:302:NAG:H82	2.20	0.76
2:H:171:GLN:HG2	2:H:175:LEU:O	1.86	0.76
1:A:157:LYS:NZ	4:A:302:NAG:H81	2.01	0.75
1:B:33:GLU:O	1:B:36:THR:HG22	1.86	0.74
1:A:68:TYR:HD2	4:A:302:NAG:H82	1.52	0.73
3:L:28:ASP:OD1	3:L:68:GLY:HA2	1.87	0.73
3:M:30:SER:OG	3:M:31:THR:N	2.23	0.71
2:H:186:SER:O	2:H:189:LEU:HD23	1.89	0.71
1:A:34:GLU:HG2	1:A:35:CYS:N	2.05	0.71
3:L:155:GLN:HG2	3:L:158:ASN:HD21	1.56	0.70
1:B:66:VAL:O	1:B:157:LYS:HB3	1.93	0.69
2:I:195:ILE:HD11	2:I:208:ASP:HB3	1.74	0.68
1:A:69:GLU:O	4:A:301:NAG:H83	1.96	0.66
3:M:151:ASP:HA	3:M:191:VAL:CG1	2.25	0.66
3:M:119:PRO:HB3	3:M:209:PHE:CE1	2.31	0.66
3:L:122:ASP:HA	3:L:125:LEU:HD12	1.78	0.66
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.29	0.65
3:L:183:LYS:O	3:L:187:GLU:HG2	1.96	0.65
3:L:147:GLN:HB3	3:L:195:GLU:HB3	1.79	0.65
3:L:150:VAL:HG23	3:L:155:GLN:OE1	1.97	0.65
1:B:51:LEU:HG	1:B:56:HIS:NE2	2.10	0.64
2:H:184:VAL:HB	2:H:185:PRO:HD2	1.80	0.64
1:B:68:TYR:HD1	5:B:302:NAG:H82	1.62	0.64
2:I:24:ALA:HB3	2:I:29:PHE:CD1	2.32	0.63
2:I:148:GLU:HB3	2:I:149:PRO:HA	1.79	0.63
1:A:53:TYR:HA	1:A:57:TYR:CD2	2.34	0.63
2:H:87:THR:HG23	2:H:110:THR:HA	1.81	0.63
1:B:76:ASN:O	1:B:80:LEU:HG	1.99	0.62
1:B:91:ARG:HD3	1:B:176:TYR:CZ	2.35	0.62
4:A:302:NAG:HO3	4:A:303:MAN:C2	2.08	0.62
1:A:157:LYS:HZ1	4:A:302:NAG:H81	1.64	0.62
2:I:144:ASP:HB3	2:I:175:LEU:HD23	1.82	0.62
2:H:141:LEU:HD22	2:H:143:LYS:HB2	1.83	0.61
2:I:27:PHE:CE1	2:I:94:ARG:HD2	2.35	0.61
4:A:302:NAG:O3	4:A:303:MAN:H2	1.99	0.61
3:L:108:ARG:HG2	3:L:109:THR:N	2.16	0.61
3:M:149:LYS:HA	3:M:153:ALA:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:CD1	5:B:302:NAG:H82	2.37	0.60
1:A:120:GLN:NE2	3:L:31:THR:HG22	2.11	0.60
3:M:11:LEU:C	3:M:11:LEU:HD12	2.23	0.59
3:M:175:LEU:HD23	3:M:175:LEU:C	2.23	0.59
2:H:141:LEU:CD2	2:H:143:LYS:HB2	2.33	0.59
1:A:132:GLY:C	1:A:133:LEU:HD12	2.22	0.59
3:L:50:SER:HB2	3:L:53:PHE:HD1	1.67	0.58
1:B:86:SER:HB3	1:B:89:GLU:HB2	1.86	0.58
2:H:178:LEU:HD12	2:H:179:SER:N	2.18	0.58
1:B:113:HIS:O	1:B:116:TRP:HB3	2.05	0.57
2:H:11:LEU:HD23	2:H:12:VAL:N	2.19	0.57
3:M:151:ASP:HA	3:M:191:VAL:HG12	1.86	0.57
3:L:210:ASN:O	3:L:212:GLY:N	2.38	0.57
2:I:72:ASP:OD2	2:I:75:LYS:HG3	2.05	0.57
3:M:108:ARG:HG2	3:M:109:THR:N	2.20	0.56
1:B:74:ILE:O	1:B:77:VAL:HG12	2.05	0.56
3:M:136:LEU:HD13	3:M:175:LEU:HD22	1.88	0.56
1:A:50:ARG:O	1:A:54:MET:HB2	2.05	0.56
3:L:150:VAL:HB	3:L:155:GLN:HE22	1.71	0.56
4:A:302:NAG:HO3	4:A:303:MAN:HO2	1.48	0.55
1:A:114:PRO:HD3	1:B:57:TYR:CD1	2.41	0.55
3:M:124:GLN:HG2	3:M:129:THR:O	2.05	0.55
2:H:178:LEU:C	2:H:178:LEU:HD12	2.27	0.55
2:H:12:VAL:CG2	2:H:18:LEU:HD22	2.37	0.55
3:M:161:GLU:HA	3:M:176:SER:O	2.07	0.55
2:I:4:LEU:HD23	2:I:22:CYS:SG	2.47	0.54
2:I:141:LEU:HD22	2:I:143:LYS:HB2	1.88	0.54
2:I:184:VAL:HG23	2:I:185:PRO:HD2	1.85	0.54
2:I:184:VAL:HG22	2:I:185:PRO:CD	2.36	0.53
3:M:24:ARG:HG2	3:M:70:ASP:OD2	2.08	0.53
2:I:6:GLU:OE2	2:I:104:GLY:HA3	2.08	0.53
3:M:2:ILE:HG12	3:M:93:TYR:CD2	2.44	0.53
2:I:195:ILE:HG13	2:I:209:LYS:O	2.09	0.53
3:M:24:ARG:HA	3:M:69:THR:O	2.09	0.53
3:L:34:ALA:HA	3:L:48:ILE:O	2.09	0.53
1:B:94:TRP:CZ2	1:B:172:MET:HB2	2.44	0.53
2:I:178:LEU:HD12	2:I:179:SER:N	2.23	0.52
3:M:11:LEU:HD21	3:M:19:VAL:HG13	1.91	0.52
3:M:183:LYS:HG3	3:M:184:ALA:N	2.24	0.52
3:L:39:LYS:HB3	3:L:40:PRO:HD2	1.90	0.52
3:M:55:TYR:O	3:M:58:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:189:LEU:H	2:H:189:LEU:HD22	1.74	0.52
1:B:132:GLY:O	1:B:133:LEU:HG	2.10	0.52
2:I:156:SER:N	2:I:197:ASN:OD1	2.42	0.52
1:B:61:ASN:OD1	1:B:160:ARG:NH2	2.23	0.52
3:L:166:GLN:HE21	3:L:171:SER:HB3	1.75	0.52
5:B:301:NAG:O4	5:B:302:NAG:H83	2.10	0.51
2:H:30:SER:O	2:H:52(A):PRO:HG2	2.09	0.51
3:L:150:VAL:HG13	3:L:192:TYR:CE2	2.46	0.51
3:L:108:ARG:HH11	3:L:108:ARG:HG2	1.74	0.51
3:L:193:ALA:CB	3:L:208:SER:OG	2.59	0.51
1:A:37:VAL:HG12	1:A:129:VAL:HG22	1.92	0.51
3:M:50:SER:HB2	3:M:53:PHE:HD1	1.75	0.51
2:I:29:PHE:CD2	2:I:34:ILE:HD13	2.46	0.51
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.92	0.51
1:B:74:ILE:HA	1:B:77:VAL:HG12	1.92	0.51
3:M:39:LYS:HE2	3:M:81:GLU:O	2.10	0.51
2:H:12:VAL:HG21	2:H:18:LEU:HD22	1.93	0.50
3:M:150:VAL:HG13	3:M:192:TYR:CE2	2.46	0.50
2:I:98:LYS:O	2:I:100:SER:O	2.30	0.50
2:H:33:TRP:CE2	2:H:100(B):ARG:HD2	2.47	0.49
2:I:100(C):GLY:HA3	3:M:96:ASN:HD21	1.77	0.49
1:B:143:GLU:HG2	1:B:143:GLU:O	2.11	0.49
2:I:135:THR:N	6:I:304:HOH:O	2.45	0.49
3:M:6:GLN:HA	3:M:22:THR:O	2.12	0.49
1:B:143:GLU:CG	1:B:143:GLU:O	2.61	0.49
2:I:100:SER:O	2:I:100(A):LYS:CB	2.42	0.49
1:A:53:TYR:HA	1:A:57:TYR:HD2	1.77	0.49
1:B:77:VAL:HG21	1:B:175:LEU:HD21	1.95	0.49
3:L:49:TYR:O	3:L:50:SER:HB2	2.13	0.48
3:M:89:GLN:HE21	3:M:96:ASN:HB3	1.77	0.48
1:A:107:ASP:HB2	2:H:98:LYS:HB3	1.95	0.48
1:A:53:TYR:CD1	1:A:57:TYR:HE2	2.31	0.48
3:L:50:SER:O	3:L:51:ALA:HB3	2.12	0.48
2:I:87:THR:O	2:I:88:ALA:HB2	2.13	0.48
2:I:173:SER:HB2	2:I:175:LEU:HB2	1.96	0.48
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.96	0.48
3:M:54:LEU:HD11	3:M:58:VAL:HB	1.95	0.48
1:B:92:TYR:O	1:B:95:VAL:HG12	2.13	0.48
1:A:56:HIS:ND1	1:B:110:LEU:HB3	2.28	0.48
2:I:148:GLU:CB	2:I:149:PRO:HA	2.43	0.48
3:M:123:GLU:N	3:M:123:GLU:OE1	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:O	1:A:79:ARG:HG3	2.14	0.47
2:I:153:SER:OG	2:I:197:ASN:HB2	2.14	0.47
1:B:54:MET:CG	1:B:165:LEU:HD12	2.44	0.47
3:M:6:GLN:HG3	3:M:99:GLY:HA3	1.97	0.47
2:I:50:ARG:HG2	2:I:58:ASP:HB2	1.97	0.47
1:A:41:LEU:HD22	1:A:125:LEU:HB3	1.93	0.46
1:A:139:SER:HB2	1:A:140:PRO:CD	2.38	0.46
1:B:73:ARG:HH11	1:B:73:ARG:HB3	1.79	0.46
2:H:108:LEU:HD12	2:H:109:VAL:N	2.30	0.46
1:B:73:ARG:HH11	1:B:73:ARG:CB	2.28	0.46
2:I:63:VAL:HG13	2:I:67:PHE:HB2	1.96	0.46
3:M:24:ARG:CG	3:M:70:ASP:OD2	2.63	0.46
3:L:143:GLU:CD	3:L:143:GLU:H	2.19	0.46
2:I:138:LEU:HD12	2:I:138:LEU:C	2.35	0.46
2:I:203:SER:OG	2:I:205:THR:OG1	2.28	0.46
1:B:51:LEU:HG	1:B:56:HIS:CD2	2.50	0.46
3:L:154:LEU:H	3:L:154:LEU:CD2	2.29	0.46
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.97	0.46
3:M:50:SER:O	3:M:51:ALA:HB3	2.16	0.46
1:B:53:TYR:CD2	1:B:118:TYR:CD1	3.04	0.46
3:M:142:ARG:HD2	3:M:173:TYR:CE2	2.51	0.46
3:M:11:LEU:O	3:M:11:LEU:HD12	2.16	0.45
2:I:27:PHE:CZ	2:I:94:ARG:HD2	2.51	0.45
4:A:303:MAN:H3	4:A:305:MAN:H2	1.48	0.45
3:M:149:LYS:HB2	3:M:193:ALA:HB3	1.98	0.45
1:B:54:MET:HG3	1:B:165:LEU:HD12	1.97	0.45
1:A:58:PHE:CE2	1:A:109:LEU:HD21	2.51	0.45
2:H:2:VAL:HB	2:H:102:TYR:CE2	2.52	0.45
3:L:151:ASP:OD2	3:L:189:HIS:HB3	2.17	0.45
2:I:11:LEU:HB2	2:I:147:PRO:HG3	1.99	0.45
1:A:53:TYR:CD1	1:A:57:TYR:CE2	3.05	0.45
2:I:205:THR:HG22	2:I:207:VAL:HG23	2.00	0.45
1:B:43:ASP:O	1:B:46:GLN:HG2	2.18	0.44
3:L:85:THR:OG1	3:L:103:LYS:HD3	2.17	0.44
3:L:140:TYR:CG	3:L:141:PRO:HA	2.52	0.44
2:I:194:TYR:O	2:I:211:VAL:HG22	2.18	0.44
3:M:151:ASP:HA	3:M:191:VAL:HG13	1.99	0.44
2:I:200:HIS:CD2	2:I:202:PRO:HD2	2.53	0.44
3:L:175:LEU:HD23	3:L:176:SER:N	2.33	0.44
3:M:8:PRO:HG2	3:M:11:LEU:HB3	1.99	0.43
1:B:73:ARG:NH1	1:B:73:ARG:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:VAL:HB	2:H:67:PHE:CG	2.53	0.43
1:B:105:VAL:O	1:B:108:VAL:HG22	2.18	0.43
2:I:210:LYS:HE2	2:I:212:GLU:OE2	2.17	0.43
3:L:193:ALA:HB2	3:L:208:SER:OG	2.19	0.43
1:A:34:GLU:CG	1:A:35:CYS:H	2.14	0.43
1:A:93:LEU:O	1:A:97:VAL:HG12	2.19	0.43
2:I:117:LYS:HD3	2:I:175:LEU:HD21	1.99	0.43
2:I:94:ARG:HH11	2:I:102:TYR:HD2	1.67	0.43
2:I:145:TYR:CD2	2:I:145:TYR:C	2.91	0.43
3:L:211:ARG:O	3:L:211:ARG:HG2	2.19	0.43
1:A:159:VAL:HG21	1:A:164:LEU:HD21	2.00	0.43
2:I:6:GLU:HA	2:I:21:SER:O	2.19	0.42
3:M:140:TYR:CG	3:M:141:PRO:HA	2.54	0.42
2:H:148:GLU:HB3	2:H:149:PRO:HA	2.01	0.42
3:L:83:PHE:O	3:L:84:ALA:HB2	2.19	0.42
2:I:116:THR:HG22	2:I:117:LYS:N	2.34	0.42
2:H:201:LYS:NZ	6:H:306:HOH:O	2.52	0.42
1:A:181:LYS:HE3	1:A:189:GLN:O	2.19	0.42
2:H:6:GLU:H	2:H:105:GLN:HE22	1.67	0.42
1:A:57:TYR:HD1	1:B:114:PRO:HD3	1.85	0.42
2:H:11:LEU:C	2:H:11:LEU:HD23	2.40	0.42
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.54	0.42
1:B:143:GLU:HB2	1:B:145:VAL:HG12	2.01	0.42
1:A:129:VAL:O	1:A:133:LEU:HD13	2.19	0.42
1:A:180:CYS:O	1:A:182:GLN:N	2.52	0.42
2:I:171:GLN:HA	3:M:160:GLN:HE22	1.84	0.42
1:A:162:LYS:NZ	1:A:166:ASP:OD2	2.53	0.42
1:A:157:LYS:HZ2	4:A:302:NAG:H81	1.81	0.41
3:L:183:LYS:HD3	3:L:187:GLU:HG3	2.01	0.41
2:I:184:VAL:CG2	2:I:185:PRO:CD	2.89	0.41
3:M:151:ASP:OD1	3:M:191:VAL:HG12	2.20	0.41
3:L:210:ASN:C	3:L:212:GLY:H	2.23	0.41
1:A:105:VAL:O	1:A:108:VAL:HG22	2.20	0.41
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.55	0.41
2:H:212:GLU:HB2	2:H:213:PRO:HD2	2.01	0.41
3:L:185:ASP:N	3:L:185:ASP:OD1	2.53	0.41
3:M:163:VAL:HG12	3:M:164:THR:O	2.20	0.41
1:A:160:ARG:NH2	6:A:404:HOH:O	2.53	0.41
3:M:148:TRP:HB2	3:M:155:GLN:HB2	2.02	0.41
3:M:40:PRO:CB	3:M:165:GLU:HG3	2.50	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:O	1:B:85:VAL:HG23	2.21	0.41
1:B:77:VAL:HG11	1:B:174:LEU:HD23	2.02	0.41
3:L:136:LEU:CD2	3:L:196:VAL:HG21	2.51	0.41
1:B:33:GLU:O	1:B:36:THR:CG2	2.64	0.41
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.23	0.41
1:B:52:GLN:HA	1:B:56:HIS:HD2	1.85	0.41
1:A:114:PRO:HD3	1:B:57:TYR:HD1	1.82	0.41
1:B:73:ARG:NH1	1:B:73:ARG:HB2	2.35	0.41
1:A:117:LYS:O	1:A:121:GLU:HG3	2.21	0.41
2:I:99:GLY:O	2:I:100(B):ARG:HG2	2.20	0.41
1:B:120:GLN:O	1:B:123:GLU:HB3	2.21	0.41
2:I:12:VAL:HG11	2:I:82(C):LEU:CD1	2.51	0.41
3:L:150:VAL:HG23	3:L:155:GLN:CD	2.41	0.41
1:B:91:ARG:HD3	1:B:176:TYR:CE1	2.56	0.41
2:I:67:PHE:N	2:I:67:PHE:CD2	2.89	0.41
3:L:155:GLN:HG2	3:L:158:ASN:ND2	2.32	0.40
3:M:109:THR:HG22	3:M:110:VAL:O	2.21	0.40
3:M:6:GLN:HB3	3:M:6:GLN:HE21	1.69	0.40
3:L:136:LEU:HD11	3:L:146:VAL:HG22	2.03	0.40
3:L:50:SER:HB2	3:L:53:PHE:CD1	2.52	0.40
3:M:49:TYR:O	3:M:50:SER:HB2	2.22	0.40
3:L:89:GLN:HE21	3:L:96:ASN:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	153/190 (80%)	140 (92%)	12 (8%)	1 (1%)	26	70
1	B	131/190 (69%)	126 (96%)	4 (3%)	1 (1%)	24	66
2	H	216/230 (94%)	206 (95%)	9 (4%)	1 (0%)	34	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	212/230 (92%)	205 (97%)	7 (3%)	0	100	100
3	L	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	34	76
3	M	210/214 (98%)	203 (97%)	6 (3%)	1 (0%)	34	76
All	All	1134/1268 (89%)	1079 (95%)	50 (4%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	211	ARG
1	A	181	LYS
1	B	84	GLN
2	H	114	ALA
3	M	204	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	147/176 (84%)	147 (100%)	0	100	100
1	B	128/176 (73%)	127 (99%)	1 (1%)	86	96
2	H	181/190 (95%)	179 (99%)	2 (1%)	80	94
2	I	178/190 (94%)	172 (97%)	6 (3%)	44	81
3	L	188/188 (100%)	184 (98%)	4 (2%)	61	89
3	M	186/188 (99%)	184 (99%)	2 (1%)	80	94
All	All	1008/1108 (91%)	993 (98%)	15 (2%)	72	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	ASN
2	H	138	LEU
2	H	197	ASN

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Mol	Chain	Res	Type
3	L	31	THR
3	L	154	LEU
3	L	177	SER
3	L	185	ASP
2	I	25	SER
2	I	63	VAL
2	I	96	LEU
2	I	170	LEU
2	I	173	SER
2	I	208	ASP
3	M	48	ILE
3	M	52	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	120	GLN
3	M	3	GLN
3	M	96	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	14,14,15	0.54	0	15,19,21	0.70	0
4	NAG	A	302	4	14,14,15	0.51	0	15,19,21	0.87	0
4	MAN	A	303	4	11,11,12	0.28	0	14,15,17	1.23	1 (7%)
4	BMA	A	304	4	11,11,12	0.58	0	14,15,17	1.10	1 (7%)
4	MAN	A	305	4	11,11,12	0.67	0	14,15,17	1.88	3 (21%)
5	NAG	B	301	1,5	14,14,15	0.49	0	15,19,21	0.82	0
5	NAG	B	302	5	14,14,15	0.56	0	15,19,21	0.92	0
5	MAN	B	303	5	11,11,12	0.26	0	14,15,17	0.98	1 (7%)
5	BMA	B	304	5	11,11,12	0.59	0	14,15,17	0.93	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	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	1/1/1/1
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
5	NAG	B	301	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	302	5	-	0/6/23/26	0/1/1/1
5	MAN	B	303	5	-	0/2/19/22	1/1/1/1
5	BMA	B	304	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	MAN	C2-C3-C4	-3.23	105.56	111.04
5	B	303	MAN	C2-C3-C4	-2.00	107.64	111.04
4	A	305	MAN	C3-C4-C5	2.61	114.74	110.20
5	B	304	BMA	C1-C2-C3	2.78	112.83	109.54
4	A	305	MAN	C2-C3-C4	3.02	116.17	111.04
4	A	304	BMA	C1-C2-C3	3.21	113.34	109.54
4	A	305	MAN	C1-C2-C3	5.34	115.86	109.54

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	303	MAN	C1-C2-C3-C4-C5-O5
4	A	303	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	NAG	1	0
4	A	302	NAG	11	0
4	A	303	MAN	6	0
4	A	305	MAN	1	0
5	B	301	NAG	1	0
5	B	302	NAG	3	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(Å ²)	Q<0.9
1	A	157/190 (82%)	-0.18	0 100 100	50, 78, 114, 116	0
1	B	137/190 (72%)	-0.11	1 (0%) 89 70	54, 77, 127, 129	0
2	H	220/230 (95%)	-0.29	2 (0%) 85 64	42, 61, 90, 113	0
2	I	216/230 (93%)	-0.31	1 (0%) 91 76	40, 56, 90, 99	0
3	L	214/214 (100%)	-0.21	2 (0%) 85 64	37, 56, 94, 115	0
3	M	212/214 (99%)	-0.36	0 100 100	38, 58, 90, 101	0
All	All	1156/1268 (91%)	-0.26	6 (0%) 91 76	37, 63, 103, 129	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	214	CYS	2.7
1	B	155	ASN	2.4
2	I	1	GLU	2.3
3	L	190	LYS	2.3
2	H	216	CYS	2.1
2	H	113	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	301	14/15	0.95	0.19	-1.25	83,85,87,91	0
4	NAG	A	301	14/15	0.97	0.15	-1.60	69,76,81,87	0
5	NAG	B	302	14/15	0.92	0.16	-	82,93,101,107	0
4	NAG	A	302	14/15	0.93	0.14	-	82,84,92,95	0
4	MAN	A	305	11/12	0.84	0.18	-	115,122,125,126	0
4	BMA	A	304	11/12	0.69	0.21	-	104,112,116,116	0
5	MAN	B	303	11/12	0.87	0.12	-	109,111,117,122	0
4	MAN	A	303	11/12	0.86	0.16	-	99,103,112,113	0
5	BMA	B	304	11/12	0.73	0.18	-	119,128,130,130	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.