Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:13 AM GMT

PDB ID	:	3HMX
Title	:	Crystal structure of ustekinumab FAB/IL-12 complex
Authors	:	Luo, J.
Deposited on	:	2009-05-29
Resolution	:	3.00 Å(reported)

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

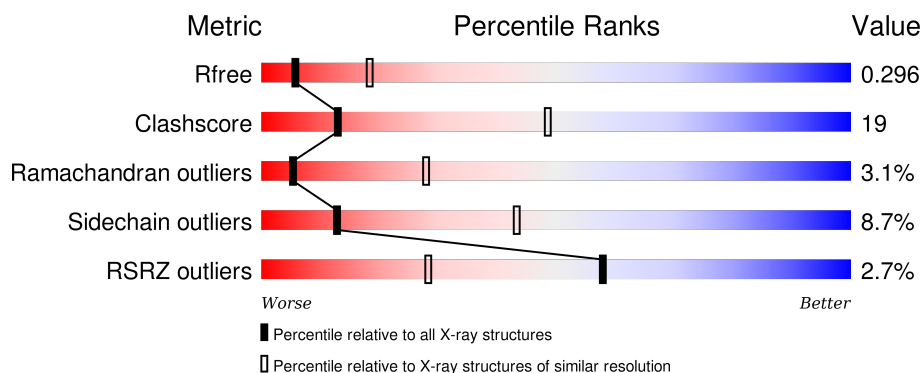|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.296
Clashscore		19
Ramachandran outliers		3.1%
Sidechain outliers		8.7%
RSRZ outliers		2.7%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 <=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	306	5% / 58% 32% 7% •
2	B	197	2% / 56% 28% 5% • 11%
3	L	214	% / 56% 39% 6%
4	H	226	2% / 66% 26% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7078 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-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total 2331	C 1475	N 380	O 464	S 12	0	0	0

- Molecule 2 is a protein called Interleukin-12 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total 1351	C 852	N 229	O 254	S 16	0	0	0

- Molecule 3 is a protein called USTEKINUMAB FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total 1649	C 1034	N 274	O 336	S 5	0	0	0

- Molecule 4 is a protein called USTEKINUMAB FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	217	Total 1642	C 1045	N 273	O 316	S 8	0	0	0

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	15	Total 15	O 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	O 2	0	0
6	L	11	Total 11	O 11	0	0
6	H	16	Total 16	O 16	0	0

3 Residue-property plots (i)

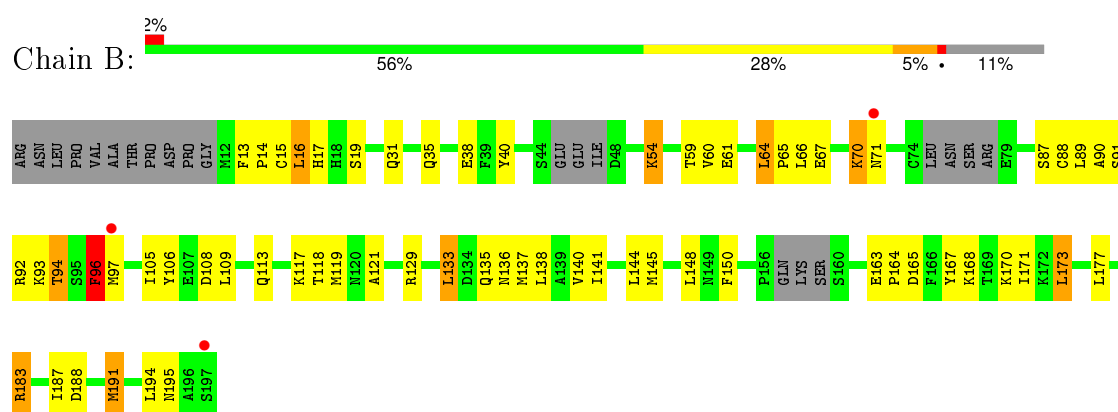These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.
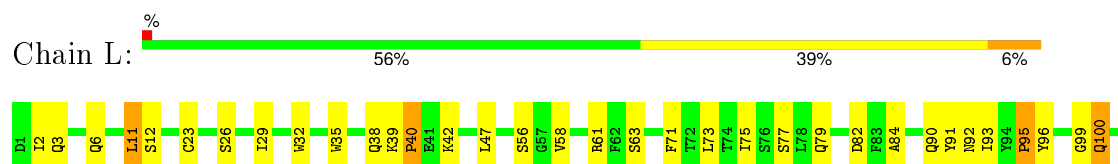
- Molecule 1: Interleukin-12 subunit beta
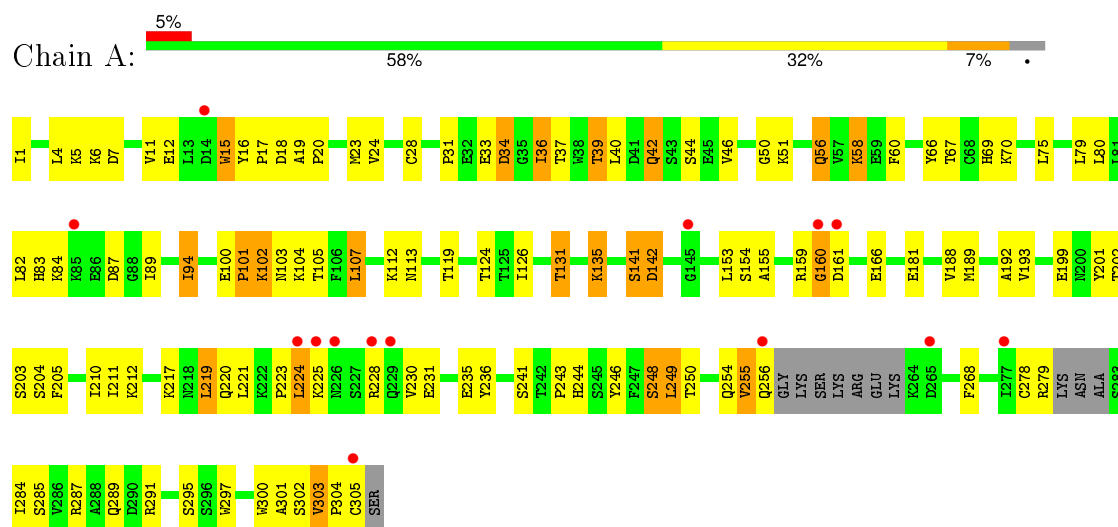
- Molecule 2: Interleukin-12 subunit alpha

- Molecule 3: USTEKINUMAB FAB LIGHT CHAIN

E105 I106 K107 R108 T109 V110 A111 S114 P120 S121 D122 E123 Q124 L125 K126 S127 V132 C134 L135 L136 N137 N138 F139 R142 V146 Q147 W148 K149 V150 D151 N152 A153 L154 Q155 N158 E161 S162 V163 T164 E165 Q166 D167 D170 S171 T172 Y173 S174 L175 S176 S177 T178

L179 T180 L181 S182 K183 Y186 E187 K188 H189 A193 C194 E195 V196 T197 H198 Q199 G200 L201 V205 T206 K207 S208 F209 N210 R211 G212 E213 C214

● Molecule 4: USTEKINUMAB FAB HEAVY CHAIN

Chain H:

E1 V11 W33 L34 R38 Q39 M40 P41 G42 D46 I50 M51 I58 R59 P62 M70 S71 V72 Y80 L81 Q82 A88 T91 C96 R100 P101 D107 F108 V117 S118 K123 G124 P125 P132 S133 S134 K135 S136 THR SER GLY G140

L144 G145 Y151 F152 P153 E154 P155 V156 T157 V158 S159 W160 N161 S162 S167 G168 V169 H170 T171 F172 L184 V187 V188 T189 S194 L195 G196 T197 Q198 T199 Y200 I201 C202 N203 V204 N205 H206 K207 P208 S209 N210 T211 R216 V217 E218 P219 K220 SER CYS ASP LYS THR HIS

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.09Å 116.44Å 182.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.66 – 3.00 26.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.66-3.00) 99.7 (26.66-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.73 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.211 , 0.303 0.204 , 0.296	Depositor DCC
R_{free} test set	1168 reflections (4.83%)	DCC
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 69.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Outliers	0 of 24242 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7078	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.27	0/2388	0.47	0/3249
2	B	0.26	0/1369	0.44	0/1845
3	L	0.29	0/1686	0.49	0/2290
4	H	0.30	0/1685	0.49	0/2294
All	All	0.28	0/7128	0.47	0/9678

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 ⓘ

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	2331	0	2216	97	0
2	B	1351	0	1312	48	0
3	L	1649	0	1593	73	0
4	H	1642	0	1607	56	0
5	A	61	0	52	3	0
6	A	15	0	0	1	0
6	B	2	0	0	0	0
6	H	16	0	0	1	0
6	L	11	0	0	0	0
All	All	7078	0	6780	264	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 19.

All (264) 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)
3:L:187:GLU:HA	3:L:211:ARG:HH22	1.22	1.02
2:B:91:SER:HA	2:B:94:THR:HG23	1.46	0.96
1:A:33:GLU:HG2	1:A:51:LYS:HD2	1.46	0.96
3:L:29:ILE:HA	3:L:92:ASN:HD22	1.31	0.95
4:H:88:ALA:O	4:H:91:THR:HG23	1.65	0.95
2:B:94:THR:HG22	2:B:194:LEU:HD22	1.56	0.87
1:A:15:TRP:CE3	1:A:15:TRP:HA	2.13	0.83
1:A:15:TRP:HA	1:A:15:TRP:HE3	1.46	0.80
3:L:38:GLN:HE22	4:H:39:GLN:HE22	1.30	0.80
1:A:303:VAL:HG22	1:A:304:PRO:HD2	1.64	0.79
1:A:284:ILE:HB	1:A:303:VAL:HG12	1.65	0.78
1:A:1:ILE:HG13	1:A:11:VAL:HG12	1.65	0.78
1:A:255:VAL:HG22	1:A:256:GLN:H	1.48	0.77
1:A:36:ILE:HD11	1:A:50:GLY:C	2.05	0.76
4:H:91:THR:HG22	4:H:117:VAL:HB	1.68	0.75
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.68	0.74
3:L:95:PRO:HG3	4:H:62:PRO:HD2	1.72	0.71
3:L:198:HIS:CD2	3:L:200:GLY:H	2.09	0.70
4:H:153:PRO:O	4:H:206:HIS:HE1	1.73	0.70
3:L:175:LEU:HD12	3:L:176:SER:N	2.07	0.70
3:L:90:GLN:HE21	3:L:93:ILE:H	1.40	0.69
1:A:15:TRP:CD1	1:A:84:LYS:HD3	2.26	0.69
3:L:120:PRO:HB2	3:L:125:LEU:HD11	1.75	0.68
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.28	0.67
2:B:91:SER:C	2:B:93:LYS:H	1.97	0.67
1:A:248:SER:HB2	1:A:291:ARG:HD2	1.76	0.67
2:B:70:LYS:HD2	2:B:71:ASN:N	2.09	0.67
1:A:36:ILE:H	1:A:36:ILE:HD13	1.59	0.66
2:B:59:THR:HG21	2:B:108:ASP:OD2	1.95	0.66
3:L:91:TYR:HA	3:L:96:TYR:CD2	2.30	0.66
3:L:132:VAL:HG13	3:L:179:LEU:HB3	1.77	0.65
3:L:139:PHE:CE2	3:L:174:SER:HA	2.33	0.64
2:B:13:PHE:HE2	2:B:90:ALA:H	1.45	0.64
3:L:90:GLN:NE2	3:L:93:ILE:H	1.96	0.64
3:L:139:PHE:HE2	3:L:174:SER:HA	1.62	0.64
3:L:108:ARG:HG2	3:L:109:THR:N	2.13	0.63
1:A:100:GLU:HB2	1:A:101:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:HA	1:A:228:ARG:HH11	1.63	0.62
2:B:109:LEU:O	2:B:113:GLN:HB2	1.99	0.62
2:B:106:TYR:HE1	2:B:145:MET:HB3	1.64	0.62
4:H:11:VAL:HG11	4:H:153:PRO:HG3	1.82	0.62
3:L:183:LYS:O	3:L:187:GLU:HG2	2.00	0.62
2:B:167:TYR:HA	2:B:170:LYS:HE3	1.81	0.62
3:L:158:ASN:HD21	3:L:181:LEU:HD21	1.65	0.62
2:B:106:TYR:CE1	2:B:145:MET:HB3	2.35	0.61
5:A:504:MAN:O3	5:A:504:MAN:H62	2.00	0.61
4:H:220:LYS:HE3	4:H:220:LYS:N	2.16	0.61
3:L:125:LEU:HD21	3:L:186:TYR:CE2	2.35	0.61
3:L:187:GLU:HA	3:L:211:ARG:NH2	2.05	0.61
2:B:64:LEU:H	2:B:64:LEU:HD12	1.66	0.60
1:A:155:ALA:HB3	1:A:166:GLU:HB3	1.83	0.60
4:H:161:ASN:ND2	4:H:201:ILE:H	1.99	0.60
3:L:61:ARG:HG3	3:L:75:ILE:HG23	1.82	0.60
2:B:137:MET:O	2:B:141:ILE:HG13	2.02	0.59
2:B:109:LEU:HD21	2:B:187:ILE:HD11	1.84	0.59
1:A:36:ILE:HD11	1:A:50:GLY:CA	2.32	0.59
3:L:29:ILE:HA	3:L:92:ASN:ND2	2.12	0.59
4:H:144:LEU:HG	4:H:188:VAL:HG23	1.84	0.58
1:A:107:LEU:HD21	1:A:203:SER:HB2	1.84	0.58
4:H:123:LYS:HG2	4:H:124:GLY:O	2.03	0.58
1:A:284:ILE:O	1:A:302:SER:HA	2.03	0.58
2:B:105:ILE:O	2:B:109:LEU:HD23	2.03	0.58
1:A:248:SER:CB	1:A:291:ARG:HD2	2.33	0.57
3:L:210:ASN:O	3:L:211:ARG:HG3	2.03	0.57
3:L:38:GLN:O	3:L:84:ALA:HB1	2.04	0.57
2:B:165:ASP:OD1	2:B:168:LYS:HB2	2.05	0.57
4:H:91:THR:HG22	4:H:117:VAL:H	1.69	0.57
4:H:132:PRO:HG3	4:H:144:LEU:HB3	1.87	0.57
3:L:124:GLN:O	3:L:127:SER:HB3	2.05	0.57
1:A:223:PRO:HB3	1:A:228:ARG:NH1	2.20	0.57
4:H:33:TRP:HE3	4:H:50:ILE:HG23	1.70	0.56
2:B:144:LEU:O	2:B:148:LEU:HG	2.04	0.56
4:H:162:SER:HA	4:H:203:ASN:ND2	2.21	0.56
1:A:131:THR:HG23	1:A:193:VAL:HB	1.87	0.55
3:L:108:ARG:HH21	3:L:111:ALA:HB2	1.72	0.55
1:A:16:TYR:CE2	1:A:19:ALA:HB2	2.41	0.55
1:A:285:SER:HB2	1:A:300:TRP:CE3	2.42	0.54
2:B:119:MET:HE3	2:B:173:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:HG2	1:A:255:VAL:H	1.72	0.54
3:L:167:ASP:HB3	3:L:170:ASP:OD2	2.07	0.54
4:H:145:GLY:HA2	4:H:160:TRP:CH2	2.43	0.54
4:H:91:THR:CG2	4:H:117:VAL:H	2.21	0.53
3:L:136:LEU:N	3:L:136:LEU:HD12	2.23	0.53
1:A:5:LYS:NZ	6:A:307:HOH:O	2.40	0.53
2:B:91:SER:C	2:B:93:LYS:N	2.62	0.53
1:A:219:LEU:HD12	1:A:219:LEU:H	1.74	0.53
4:H:125:PRO:HB3	4:H:151:TYR:HB3	1.90	0.53
1:A:135:LYS:HG2	1:A:189:MET:HB2	1.90	0.53
2:B:141:ILE:O	2:B:145:MET:HG3	2.08	0.53
1:A:79:LEU:O	1:A:80:LEU:HD23	2.08	0.53
4:H:220:LYS:HE3	4:H:220:LYS:H	1.73	0.53
1:A:36:ILE:H	1:A:36:ILE:CD1	2.22	0.52
1:A:34:ASP:HB2	1:A:70:LYS:NZ	2.24	0.52
4:H:51:MET:SD	4:H:70:MET:HB3	2.49	0.52
1:A:20:PRO:O	1:A:58:LYS:HE3	2.10	0.52
1:A:15:TRP:NE1	1:A:84:LYS:HD3	2.24	0.52
1:A:284:ILE:HD11	1:A:305:CYS:HA	1.92	0.52
4:H:161:ASN:HD21	4:H:201:ILE:H	1.56	0.52
3:L:146:VAL:HG22	3:L:196:VAL:HG22	1.92	0.52
1:A:219:LEU:HD12	1:A:219:LEU:N	2.24	0.52
3:L:63:SER:O	3:L:73:LEU:HD12	2.10	0.52
2:B:16:LEU:HD23	2:B:191:MET:HB3	1.92	0.51
4:H:91:THR:HG22	4:H:117:VAL:CB	2.38	0.51
1:A:220:GLN:O	1:A:221:LEU:HD12	2.10	0.51
3:L:174:SER:O	4:H:172:PHE:HE2	1.92	0.51
1:A:83:HIS:HD2	5:A:501:NAG:O6	1.93	0.51
4:H:107:ASP:HB3	4:H:108:PHE:HD2	1.76	0.51
4:H:118:SER:HB3	4:H:152:PHE:CZ	2.46	0.51
1:A:303:VAL:CG2	1:A:304:PRO:HD2	2.36	0.51
1:A:16:TYR:CZ	1:A:19:ALA:HB2	2.46	0.51
1:A:284:ILE:N	1:A:284:ILE:HD12	2.25	0.50
4:H:58:ILE:HG22	4:H:59:ARG:N	2.26	0.50
4:H:162:SER:H	4:H:203:ASN:HD21	1.58	0.50
1:A:39:THR:CG2	1:A:69:HIS:HE1	2.24	0.50
1:A:94:ILE:HG12	1:A:199:GLU:OE1	2.11	0.50
1:A:285:SER:HB2	1:A:300:TRP:HE3	1.76	0.50
3:L:12:SER:HB3	3:L:105:GLU:OE2	2.11	0.49
1:A:36:ILE:N	1:A:36:ILE:HD13	2.28	0.49
3:L:193:ALA:CB	3:L:208:SER:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HA	1:A:212:LYS:O	2.12	0.49
3:L:165:GLU:O	3:L:166:GLN:C	2.50	0.49
2:B:19:SER:OG	2:B:188:ASP:HA	2.13	0.49
3:L:122:ASP:O	3:L:126:LYS:HG2	2.12	0.49
1:A:224:LEU:HG	1:A:225:LYS:H	1.77	0.49
1:A:23:MET:O	1:A:23:MET:HG2	2.12	0.49
4:H:153:PRO:O	4:H:206:HIS:CE1	2.61	0.48
4:H:201:ILE:HG22	4:H:216:ARG:HB2	1.95	0.48
4:H:161:ASN:HA	4:H:201:ILE:HD11	1.94	0.48
1:A:153:LEU:HD13	1:A:154:SER:N	2.29	0.48
1:A:40:LEU:HD13	1:A:66:TYR:CZ	2.49	0.48
1:A:236:TYR:CD1	1:A:244:HIS:CG	3.02	0.48
1:A:230:VAL:HG23	1:A:278:CYS:HB2	1.96	0.48
1:A:101:PRO:HG2	1:A:105:THR:HG21	1.96	0.47
3:L:137:ASN:ND2	4:H:189:THR:HG21	2.29	0.47
3:L:39:LYS:HB3	3:L:40:PRO:HD2	1.96	0.47
4:H:201:ILE:HG22	4:H:216:ARG:HA	1.95	0.47
3:L:29:ILE:HD11	3:L:71:PHE:CE1	2.49	0.47
3:L:210:ASN:HD22	3:L:210:ASN:N	2.12	0.47
3:L:195:GLU:HG3	3:L:206:THR:HB	1.97	0.47
2:B:173:LEU:HD22	2:B:177:LEU:HG	1.97	0.47
4:H:154:GLU:CB	4:H:155:PRO:HA	2.45	0.47
4:H:33:TRP:CE3	4:H:50:ILE:HG23	2.50	0.47
2:B:15:CYS:HB3	2:B:191:MET:HG3	1.97	0.47
3:L:6:GLN:OE1	3:L:99:GLY:HA3	2.15	0.47
1:A:101:PRO:HB2	1:A:102:LYS:H	1.58	0.47
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.50	0.47
1:A:221:LEU:HA	1:A:231:GLU:O	2.13	0.46
4:H:154:GLU:HB3	4:H:155:PRO:HA	1.97	0.46
3:L:100:GLN:H	3:L:100:GLN:CD	2.16	0.46
1:A:181:GLU:OE1	2:B:183:ARG:NH1	2.48	0.46
1:A:255:VAL:HG22	1:A:256:GLN:N	2.26	0.46
3:L:166:GLN:HG3	3:L:173:TYR:CE2	2.50	0.46
4:H:216:ARG:HD2	4:H:218:GLU:OE2	2.15	0.46
4:H:71:SER:OG	4:H:80:TYR:HB2	2.15	0.46
3:L:108:ARG:HG2	3:L:109:THR:H	1.80	0.46
1:A:94:ILE:HD12	1:A:192:ALA:HB1	1.98	0.46
1:A:141:SER:O	1:A:142:ASP:C	2.53	0.46
3:L:125:LEU:O	3:L:183:LYS:HD2	2.15	0.46
1:A:254:GLN:CG	1:A:255:VAL:H	2.26	0.46
1:A:287:ARG:HD2	1:A:297:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:HB2	3:L:32:TRP:CZ2	2.51	0.46
3:L:154:LEU:HD13	3:L:155:GLN:H	1.81	0.46
4:H:133:SER:OG	4:H:134:SER:N	2.49	0.46
3:L:188:LYS:O	3:L:189:HIS:CG	2.69	0.46
1:A:255:VAL:HG13	1:A:256:GLN:N	2.31	0.45
1:A:107:LEU:H	1:A:107:LEU:CD2	2.28	0.45
5:A:501:NAG:H83	5:A:501:NAG:O3	2.15	0.45
4:H:100:ARG:HA	4:H:101:PRO:HD3	1.71	0.45
3:L:149:LYS:HA	3:L:153:ALA:O	2.15	0.45
1:A:6:LYS:O	1:A:7:ASP:HB2	2.16	0.45
1:A:103:ASN:CG	1:A:104:LYS:H	2.19	0.45
2:B:105:ILE:O	2:B:108:ASP:HB2	2.14	0.45
2:B:173:LEU:CD2	2:B:177:LEU:HG	2.46	0.45
4:H:158:VAL:HG22	4:H:204:VAL:HG22	1.98	0.45
3:L:3:GLN:HB2	3:L:26:SER:HB3	1.97	0.45
1:A:1:ILE:O	1:A:1:ILE:HG23	2.17	0.45
3:L:2:ILE:HD11	3:L:93:ILE:HD12	1.97	0.45
1:A:100:GLU:CB	1:A:101:PRO:HD3	2.44	0.45
2:B:96:PHE:HD2	2:B:97:MET:H	1.64	0.45
3:L:125:LEU:C	3:L:127:SER:H	2.20	0.45
2:B:109:LEU:HD12	2:B:141:ILE:HG23	1.99	0.45
1:A:107:LEU:CD2	1:A:203:SER:HB2	2.46	0.45
3:L:136:LEU:N	3:L:136:LEU:CD1	2.80	0.45
3:L:11:LEU:HD12	3:L:11:LEU:C	2.38	0.45
1:A:28:CYS:SG	1:A:75:LEU:HD23	2.57	0.44
2:B:163:GLU:HA	2:B:164:PRO:HD3	1.71	0.44
1:A:39:THR:HG22	1:A:67:THR:HB	1.98	0.44
1:A:250:THR:HG22	1:A:289:GLN:O	2.18	0.44
4:H:38:ARG:HG2	4:H:46:ASP:HB2	2.00	0.44
2:B:31:GLN:O	2:B:35:GLN:HB2	2.18	0.44
3:L:151:ASP:C	3:L:153:ALA:H	2.21	0.44
1:A:287:ARG:HG3	1:A:300:TRP:CZ3	2.52	0.44
4:H:34:LEU:O	4:H:50:ILE:HD13	2.18	0.44
1:A:201:TYR:N	1:A:201:TYR:CD1	2.84	0.44
2:B:113:GLN:O	2:B:117:LYS:HB2	2.18	0.43
3:L:114:SER:HB2	3:L:137:ASN:HB3	2.00	0.43
1:A:135:LYS:HD3	1:A:189:MET:HB3	2.00	0.43
3:L:201:LEU:HD13	3:L:205:VAL:CG1	2.48	0.43
3:L:210:ASN:O	3:L:211:ARG:CG	2.65	0.43
4:H:161:ASN:HD21	4:H:200:TYR:HA	1.83	0.43
4:H:42:GLY:HA2	6:H:238:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG22	1:A:285:SER:N	2.33	0.43
2:B:137:MET:O	2:B:137:MET:HG2	2.18	0.43
4:H:184:LEU:C	4:H:184:LEU:HD12	2.38	0.43
1:A:37:THR:HB	1:A:46:VAL:HG22	1.99	0.43
4:H:161:ASN:ND2	4:H:201:ILE:HG13	2.33	0.43
1:A:220:GLN:C	1:A:221:LEU:HD12	2.39	0.43
1:A:246:TYR:CZ	2:B:65:PRO:HD3	2.54	0.43
3:L:135:LEU:HD22	4:H:187:VAL:HG21	2.00	0.43
3:L:174:SER:HB2	4:H:170:HIS:HD2	1.84	0.43
1:A:16:TYR:HA	1:A:17:PRO:HD3	1.89	0.43
2:B:183:ARG:HA	2:B:183:ARG:HD3	1.73	0.43
1:A:268:PHE:HE2	1:A:297:TRP:CZ2	2.36	0.43
1:A:285:SER:HA	1:A:301:ALA:O	2.19	0.43
1:A:79:LEU:C	1:A:80:LEU:HD23	2.39	0.43
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.54	0.43
1:A:243:PRO:HG3	2:B:67:GLU:OE1	2.18	0.43
2:B:14:PRO:O	2:B:17:HIS:HB3	2.19	0.42
3:L:149:LYS:HG2	3:L:154:LEU:HD22	2.01	0.42
3:L:106:ILE:HD12	3:L:166:GLN:OE1	2.20	0.42
1:A:205:PHE:CD2	1:A:210:ILE:HG12	2.54	0.42
2:B:38:GLU:HG2	2:B:38:GLU:H	1.61	0.42
2:B:70:LYS:HD2	2:B:71:ASN:H	1.84	0.42
4:H:209:SER:C	4:H:211:THR:H	2.23	0.42
4:H:81:LEU:HD12	4:H:82:GLN:H	1.84	0.42
1:A:112:LYS:O	1:A:113:ASN:HB3	2.20	0.42
4:H:152:PHE:HA	4:H:153:PRO:HA	1.79	0.42
2:B:91:SER:CA	2:B:94:THR:HG23	2.34	0.41
1:A:16:TYR:CD2	1:A:19:ALA:HB2	2.55	0.41
4:H:100:ARG:HB2	4:H:107:ASP:OD1	2.20	0.41
3:L:12:SER:HA	3:L:105:GLU:O	2.19	0.41
1:A:60:PHE:CE2	1:A:82:LEU:HB2	2.55	0.41
3:L:142:ARG:HB3	3:L:173:TYR:CG	2.54	0.41
2:B:137:MET:HA	2:B:140:VAL:HG22	2.03	0.41
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.54	0.41
1:A:107:LEU:H	1:A:107:LEU:HD23	1.85	0.41
2:B:133:LEU:HD12	2:B:138:LEU:HG	2.01	0.41
1:A:188:VAL:O	1:A:202:THR:HA	2.20	0.41
3:L:132:VAL:CG1	3:L:179:LEU:HB3	2.45	0.41
4:H:161:ASN:HD22	4:H:201:ILE:HG13	1.86	0.41
1:A:142:ASP:OD1	1:A:142:ASP:O	2.38	0.41
4:H:207:LYS:O	4:H:209:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LEU:N	2:B:66:LEU:HD12	2.35	0.41
3:L:174:SER:CB	4:H:170:HIS:HD2	2.34	0.41
2:B:16:LEU:HD23	2:B:16:LEU:HA	1.74	0.41
3:L:135:LEU:CD2	4:H:187:VAL:HG21	2.50	0.41
1:A:159:ARG:CG	1:A:160:GLY:N	2.83	0.41
1:A:4:LEU:HB3	1:A:5:LYS:H	1.72	0.41
1:A:236:TYR:HD1	1:A:244:HIS:ND1	2.19	0.41
2:B:118:THR:O	2:B:121:ALA:HB3	2.20	0.41
2:B:60:VAL:HG13	2:B:61:GLU:N	2.35	0.41
3:L:79:GLN:O	3:L:82:ASP:HB2	2.21	0.41
1:A:236:TYR:CZ	1:A:249:LEU:HB2	2.56	0.41
1:A:103:ASN:O	1:A:104:LYS:C	2.60	0.40
1:A:126:ILE:HD12	1:A:126:ILE:H	1.86	0.40
2:B:87:SER:OG	2:B:88:CYS:N	2.53	0.40
2:B:88:CYS:O	2:B:89:LEU:HD23	2.21	0.40
1:A:255:VAL:HG13	1:A:256:GLN:O	2.21	0.40
4:H:169:VAL:HG22	4:H:188:VAL:CG1	2.50	0.40
1:A:42:GLN:HG3	1:A:42:GLN:H	1.73	0.40
3:L:47:LEU:HA	3:L:58:VAL:HG11	2.02	0.40
1:A:254:GLN:HB2	1:A:300:TRP:CH2	2.56	0.40
3:L:108:ARG:NE	3:L:109:THR:O	2.53	0.40
2:B:40:TYR:HD1	2:B:171:ILE:CD1	2.34	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	289/306 (94%)	240 (83%)	36 (12%)	13 (4%)	3	18
2	B	168/197 (85%)	134 (80%)	29 (17%)	5 (3%)	5	29
3	L	212/214 (99%)	181 (85%)	27 (13%)	4 (2%)	10	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	213/226 (94%)	190 (89%)	18 (8%)	5 (2%)	8	36
All	All	882/943 (94%)	745 (84%)	110 (12%)	27 (3%)	5	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	PRO
1	A	217	LYS
1	A	255	VAL
2	B	54	LYS
3	L	138	ASN
3	L	211	ARG
2	B	96	PHE
1	A	87	ASP
1	A	102	LYS
1	A	161	ASP
1	A	295	SER
2	B	92	ARG
2	B	129	ARG
2	B	150	PHE
3	L	40	PRO
4	H	41	PRO
4	H	133	SER
4	H	167	SER
1	A	34	ASP
1	A	141	SER
3	L	166	GLN
4	H	208	PRO
1	A	142	ASP
1	A	224	LEU
4	H	72	VAL
1	A	160	GLY
1	A	31	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	262/277 (95%)	236 (90%)	26 (10%)	10	35
2	B	147/183 (80%)	134 (91%)	13 (9%)	12	42
3	L	187/188 (100%)	168 (90%)	19 (10%)	9	33
4	H	184/195 (94%)	174 (95%)	10 (5%)	27	66
All	All	780/843 (92%)	712 (91%)	68 (9%)	13	43

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	15	TRP
1	A	18	ASP
1	A	24	VAL
1	A	36	ILE
1	A	39	THR
1	A	42	GLN
1	A	44	SER
1	A	56	GLN
1	A	58	LYS
1	A	89	ILE
1	A	94	ILE
1	A	107	LEU
1	A	119	THR
1	A	124	THR
1	A	131	THR
1	A	135	LYS
1	A	204	SER
1	A	211	ILE
1	A	219	LEU
1	A	235	GLU
1	A	241	SER
1	A	248	SER
1	A	249	LEU
1	A	279	ARG
1	A	303	VAL
2	B	16	LEU
2	B	54	LYS
2	B	64	LEU
2	B	70	LYS
2	B	94	THR
2	B	96	PHE
2	B	133	LEU

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Mol	Chain	Res	Type
2	B	135	GLN
2	B	136	ASN
2	B	173	LEU
2	B	183	ARG
2	B	191	MET
2	B	195	ASN
3	L	11	LEU
3	L	42	LYS
3	L	56	SER
3	L	77	SER
3	L	95	PRO
3	L	100	GLN
3	L	105	GLU
3	L	108	ARG
3	L	133	VAL
3	L	150	VAL
3	L	154	LEU
3	L	161	GLU
3	L	163	VAL
3	L	172	THR
3	L	175	LEU
3	L	180	THR
3	L	205	VAL
3	L	206	THR
3	L	213	GLU
4	H	38	ARG
4	H	50	ILE
4	H	91	THR
4	H	96	CYS
4	H	107	ASP
4	H	157	THR
4	H	188	VAL
4	H	189	THR
4	H	198	GLN
4	H	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	56	GLN
1	A	69	HIS

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	98	GLN
1	A	220	GLN
1	A	226	ASN
1	A	256	GLN
2	B	28	ASN
2	B	35	GLN
2	B	71	ASN
2	B	113	GLN
2	B	120	ASN
2	B	130	GLN
2	B	135	GLN
2	B	136	ASN
2	B	146	GLN
3	L	3	GLN
3	L	27	GLN
3	L	90	GLN
3	L	92	ASN
3	L	155	GLN
3	L	158	ASN
3	L	198	HIS
3	L	210	ASN
4	H	39	GLN
4	H	103	GLN
4	H	161	ASN
4	H	198	GLN
4	H	206	HIS

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)

5 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	#$|Z| > 2$
5	NAG	A	501	1,5	14,14,15	0.38	0	15,19,21	1.57	1 (6%)
5	NAG	A	502	5	14,14,15	0.54	0	15,19,21	2.00	3 (20%)
5	BMA	A	503	5	11,11,12	1.34	1 (9%)	14,15,17	2.62	7 (50%)
5	MAN	A	504	5	11,11,12	1.44	2 (18%)	14,15,17	2.63	7 (50%)
5	MAN	A	505	5	11,11,12	0.56	0	14,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	502	5	-	0/6/23/26	0/1/1/1
5	BMA	A	503	5	-	0/2/19/22	0/1/1/1
5	MAN	A	504	5	-	0/2/19/22	0/1/1/1
5	MAN	A	505	5	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	BMA	O5-C1	-3.55	1.37	1.43
5	A	504	MAN	C4-C3	2.01	1.57	1.52
5	A	504	MAN	C6-C5	2.04	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	BMA	C1-O5-C5	-7.00	103.37	112.25
5	A	503	BMA	C2-C3-C4	-3.02	105.91	111.04
5	A	502	NAG	C2-N2-C7	-2.97	119.23	123.04
5	A	504	MAN	C1-C2-C3	-2.16	106.99	109.54
5	A	502	NAG	C6-C5-C4	-2.01	108.05	113.02
5	A	504	MAN	O5-C1-C2	2.04	114.16	110.86
5	A	503	BMA	O5-C5-C6	2.19	112.08	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	BMA	C1-C2-C3	2.42	112.41	109.54
5	A	503	BMA	O4-C4-C5	2.50	115.88	109.24
5	A	503	BMA	O6-C6-C5	2.57	119.82	111.33
5	A	504	MAN	O6-C6-C5	3.15	121.73	111.33
5	A	503	BMA	O2-C2-C3	3.30	116.75	110.12
5	A	504	MAN	O2-C2-C3	3.30	116.75	110.12
5	A	504	MAN	O5-C5-C6	3.55	115.03	107.35
5	A	504	MAN	O4-C4-C3	3.69	118.64	110.34
5	A	501	NAG	C1-O5-C5	5.11	118.74	112.25
5	A	504	MAN	C1-O5-C5	5.80	119.61	112.25
5	A	502	NAG	C1-O5-C5	5.84	119.66	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	MAN	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	NAG	2	0
5	A	504	MAN	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(Å^2)	Q<0.9
1	A	295/306 (96%)	-0.01	14 (4%)	35	14	60, 97, 200, 255	0
2	B	176/197 (89%)	-0.17	3 (1%)	73	45	70, 106, 181, 238	0
3	L	214/214 (100%)	-0.17	3 (1%)	78	51	52, 90, 121, 164	0
4	H	217/226 (96%)	-0.21	4 (1%)	71	43	45, 81, 134, 178	0
All	All	902/943 (95%)	-0.13	24 (2%)	58	28	45, 92, 175, 255	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	LYS	4.6
1	A	224	LEU	4.2
1	A	256	GLN	4.1
3	L	134	CYS	3.4
2	B	71	ASN	3.2
1	A	226	ASN	3.2
3	L	176	SER	3.2
1	A	277	ILE	3.2
2	B	97	MET	3.0
1	A	161	ASP	2.9
1	A	228	ARG	2.9
1	A	265	ASP	2.9
4	H	194	SER	2.7
4	H	195	LEU	2.6
1	A	145	GLY	2.5
1	A	305	CYS	2.5
4	H	196	GLY	2.5
4	H	197	THR	2.3
3	L	177	SER	2.3
1	A	14	ASP	2.3
2	B	197	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	85	LYS	2.2
1	A	160	GLY	2.1
1	A	229	GLN	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. 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(Å^2)	Q<0.9
5	NAG	A	501	14/15	0.96	0.14	-2.30	84,92,105,106	0
5	MAN	A	505	11/12	0.87	0.18	-	119,135,140,144	0
5	MAN	A	504	11/12	0.82	0.32	-	147,154,159,159	0
5	BMA	A	503	11/12	0.95	0.23	-	109,116,129,137	0
5	NAG	A	502	14/15	0.98	0.13	-	80,98,109,111	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.