



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:31 am GMT

PDB ID : 3IU3  
Title : Crystal structure of the Fab fragment of therapeutic antibody Basiliximab in complex with IL-2Ra (CD25) ectodomain  
Authors : Du, J.; Yang, H.; Wang, J.; Ding, J.  
Deposited on : 2009-08-29  
Resolution : 2.90 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

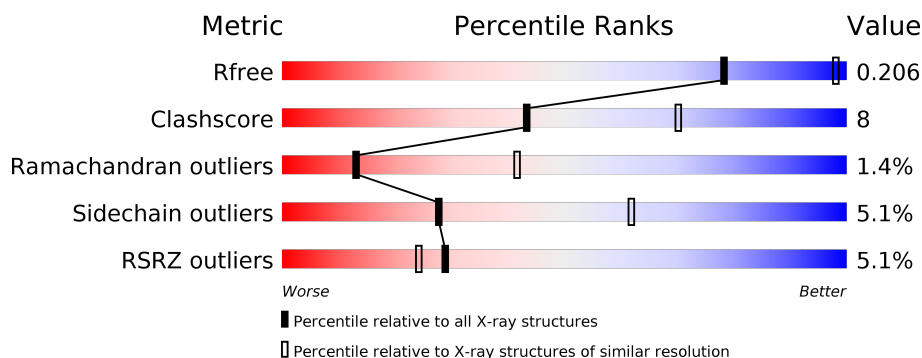
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	215	<div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	C	215	<div> <div>%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
1	H	215	<div> <div>84%</div> <div>15%</div> <div>•</div> </div>
2	B	210	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
2	D	210	<div> <div>86%</div> <div>12%</div> <div>•</div> </div>
2	L	210	<div> <div>83%</div> <div>15%</div> <div>••</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	223	<div><div><div></div><div></div><div></div><div></div></div><div>15%40%10%47%</div></div>
3	J	223	<div><div><div></div><div></div><div></div><div></div></div><div>10%37%11%48%</div></div>
3	K	223	<div><div><div></div><div></div><div></div><div></div></div><div>9%43%5%49%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12566 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 Heavy chain of Fab fragment of Basiliximab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			
1	C	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			
1	H	215	Total	C	N	O	S	0	0	0
			1630	1032	270	321	7			

- Molecule 2 is a protein called Light chain of Fab fragment of Basiliximab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1591	989	269	325	8			
2	D	209	Total	C	N	O	S	0	0	0
			1595	991	270	326	8			
2	L	208	Total	C	N	O	S	0	0	0
			1591	989	269	325	8			

- Molecule 3 is a protein called Interleukin-2 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	119	Total	C	N	O	S	0	0	0
			954	591	174	175	14			
3	J	116	Total	C	N	O	S	0	0	0
			923	570	165	174	14			
3	K	114	Total	C	N	O	S	0	0	0
			905	560	161	170	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	218	HIS	-	EXPRESSION TAG	UNP P01589
I	219	HIS	-	EXPRESSION TAG	UNP P01589

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
I	220	HIS	-	EXPRESSION TAG	UNP P01589
I	221	HIS	-	EXPRESSION TAG	UNP P01589
I	222	HIS	-	EXPRESSION TAG	UNP P01589
I	223	HIS	-	EXPRESSION TAG	UNP P01589
J	218	HIS	-	EXPRESSION TAG	UNP P01589
J	219	HIS	-	EXPRESSION TAG	UNP P01589
J	220	HIS	-	EXPRESSION TAG	UNP P01589
J	221	HIS	-	EXPRESSION TAG	UNP P01589
J	222	HIS	-	EXPRESSION TAG	UNP P01589
J	223	HIS	-	EXPRESSION TAG	UNP P01589
K	218	HIS	-	EXPRESSION TAG	UNP P01589
K	219	HIS	-	EXPRESSION TAG	UNP P01589
K	220	HIS	-	EXPRESSION TAG	UNP P01589
K	221	HIS	-	EXPRESSION TAG	UNP P01589
K	222	HIS	-	EXPRESSION TAG	UNP P01589
K	223	HIS	-	EXPRESSION TAG	UNP P01589

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Heavy chain of Fab fragment of Basiliximab

Chain A: 




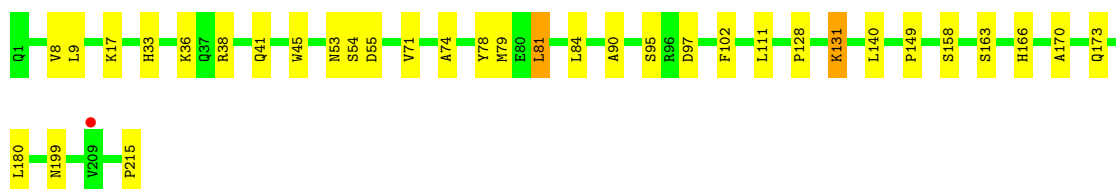
- Molecule 1: Heavy chain of Fab fragment of Basiliximab

Chain C: 




- Molecule 1: Heavy chain of Fab fragment of Basiliximab

Chain H: 




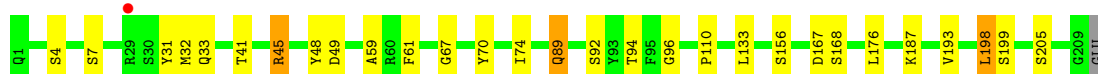
- Molecule 2: Light chain of Fab fragment of Basiliximab

Chain B: 

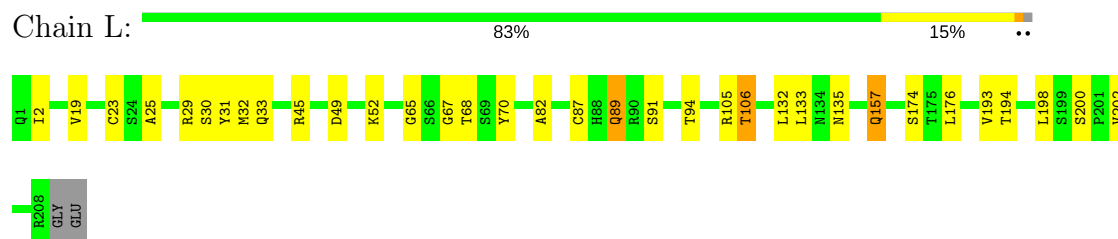


- Molecule 2: Light chain of Fab fragment of Basiliximab

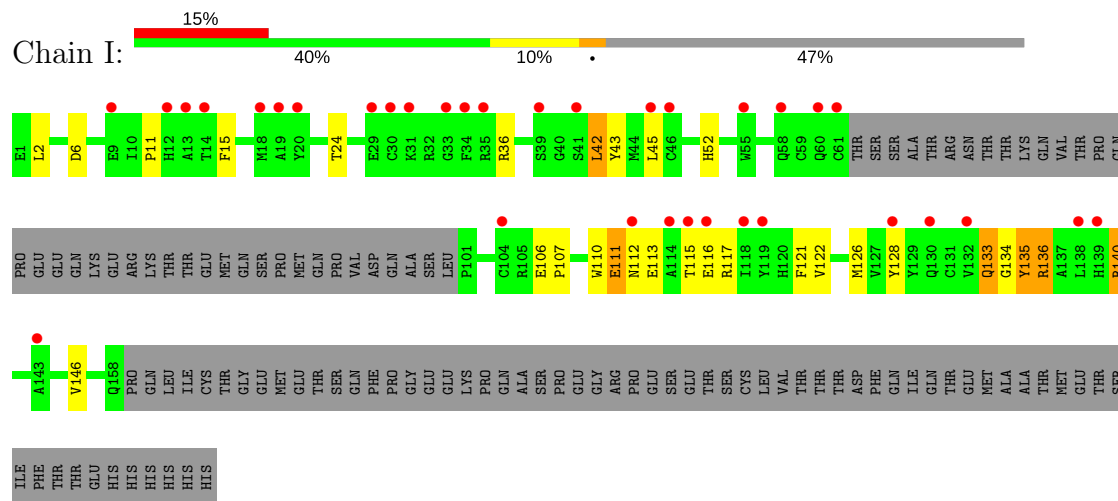
Chain D: 



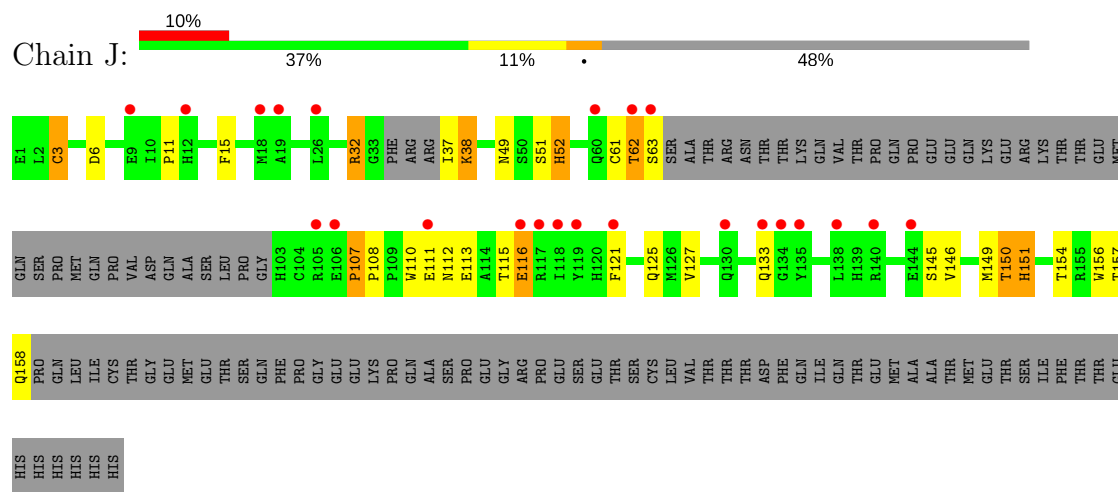
- Molecule 2: Light chain of Fab fragment of Basiliximab



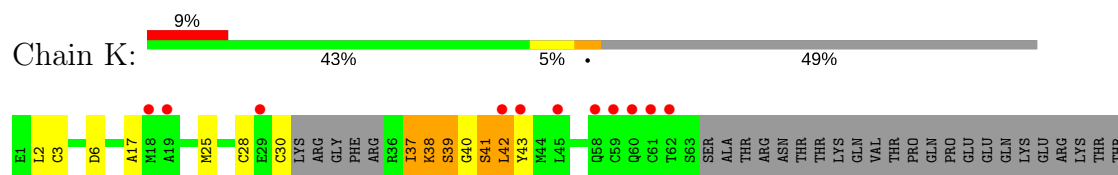
- Molecule 3: Interleukin-2 receptor alpha chain

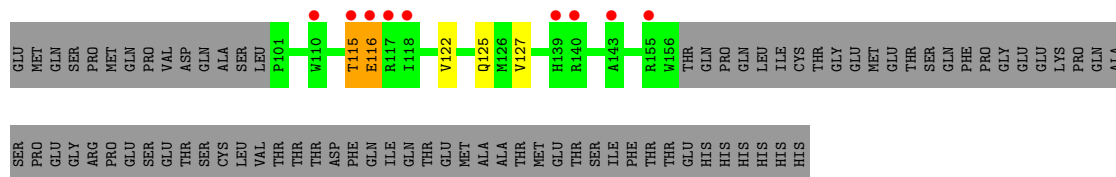


- Molecule 3: Interleukin-2 receptor alpha chain



- Molecule 3: Interleukin-2 receptor alpha chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.05Å 137.05Å 459.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.38 – 2.90 49.84 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (47.38-2.90) 97.9 (49.84-2.90)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.215 , 0.262 0.214 , 0.206	Depositor DCC
$R_{free}$ test set	2872 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.4	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0/1675	0.54	0/2281
1	C	0.34	0/1675	0.54	0/2281
1	H	0.33	0/1675	0.52	0/2281
2	B	0.35	0/1626	0.52	0/2203
2	D	0.36	0/1630	0.50	0/2208
2	L	0.34	0/1626	0.52	0/2203
3	I	0.38	0/981	0.52	0/1323
3	J	0.36	0/947	0.51	0/1278
3	K	0.34	0/930	0.48	0/1256
All	All	0.35	0/12765	0.52	0/17314

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	1630	0	1575	23	0
1	C	1630	0	1575	22	0
1	H	1630	0	1575	19	0
2	B	1591	0	1541	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1595	0	1544	14	0
2	L	1591	0	1541	21	0
3	I	954	0	889	25	0
3	J	923	0	856	34	0
3	K	905	0	834	22	0
4	I	39	0	34	1	0
4	J	39	0	34	2	0
4	K	39	0	34	1	0
All	All	12566	0	12032	189	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 8.

All (189) 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:J:146:VAL:O	3:J:157:THR:HG23	1.56	1.04
1:C:38:ARG:HH11	1:C:38:ARG:HG2	1.23	1.00
1:C:33:HIS:HD2	1:C:45:TRP:HE1	1.09	0.96
3:I:133:GLN:HA	3:I:133:GLN:OE1	1.61	0.95
1:H:33:HIS:HD2	1:H:45:TRP:HE1	1.05	0.95
1:A:31:TRP:CH2	3:K:42:LEU:HD23	2.01	0.94
3:I:135:TYR:HB3	3:I:136:ARG:CD	2.02	0.90
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.35	0.90
1:A:131:LYS:O	1:A:132:SER:HB3	1.71	0.89
3:J:146:VAL:O	3:J:157:THR:CG2	2.23	0.86
1:A:158:SER:H	1:A:199:ASN:HD21	1.22	0.86
3:J:156:TRP:O	3:J:157:THR:HG22	1.76	0.85
3:J:145:SER:HA	3:J:157:THR:OG1	1.78	0.83
2:L:32:MET:HE2	2:L:87:CYS:HB2	1.59	0.83
3:J:156:TRP:O	3:J:157:THR:CG2	2.28	0.81
2:B:33:GLN:HE21	2:B:49:ASP:H	1.28	0.81
1:A:33:HIS:HD2	1:A:45:TRP:HE1	1.26	0.80
1:C:8:VAL:HG11	1:C:16:VAL:HG21	1.62	0.79
3:I:133:GLN:CA	3:I:133:GLN:OE1	2.30	0.79
3:J:151:HIS:ND1	3:J:151:HIS:N	2.30	0.79
1:H:33:HIS:CD2	1:H:45:TRP:HE1	1.97	0.78
3:K:17:ALA:HB2	3:K:127:VAL:HG12	1.65	0.77
3:J:156:TRP:C	3:J:157:THR:HG23	2.04	0.76
4:J:300:NAG:O3	4:J:301:NAG:O5	2.03	0.76
1:C:33:HIS:CD2	1:C:45:TRP:HE1	2.00	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:GLY:O	3:K:41:SER:HB3	1.87	0.75
3:J:156:TRP:C	3:J:157:THR:CG2	2.56	0.74
1:H:33:HIS:HD2	1:H:45:TRP:NE1	1.84	0.73
3:I:135:TYR:HB3	3:I:136:ARG:HD2	1.69	0.72
3:I:110:TRP:CE2	3:I:112:ASN:ND2	2.59	0.70
3:K:38:LYS:HG2	3:K:39:SER:N	2.07	0.70
1:A:31:TRP:CZ2	3:K:42:LEU:HD23	2.27	0.70
3:I:110:TRP:O	3:I:111:GLU:HB2	1.92	0.69
1:H:53:ASN:O	1:H:55:ASP:N	2.25	0.69
1:A:31:TRP:CZ3	3:K:42:LEU:CD2	2.76	0.69
3:J:51:SER:O	3:J:52:HIS:HB2	1.94	0.68
1:A:31:TRP:CH2	3:K:42:LEU:CD2	2.75	0.68
3:I:140:ARG:HG3	3:I:140:ARG:HH11	1.60	0.67
1:A:33:HIS:CD2	1:A:45:TRP:HE1	2.11	0.67
3:K:115:THR:HG22	3:K:116:GLU:H	1.60	0.66
1:H:81:LEU:HB3	1:H:84:LEU:HD21	1.78	0.66
1:C:33:HIS:HD2	1:C:45:TRP:NE1	1.89	0.65
3:K:40:GLY:O	3:K:41:SER:CB	2.44	0.65
3:K:38:LYS:HG2	3:K:39:SER:H	1.61	0.65
3:J:149:MET:O	3:J:150:THR:C	2.36	0.64
3:J:145:SER:HA	3:J:157:THR:HG1	1.62	0.64
1:C:158:SER:H	1:C:199:ASN:HD21	1.46	0.63
3:I:135:TYR:HB3	3:I:136:ARG:HD3	1.80	0.62
2:B:89:GLN:HE21	2:B:91:SER:HB2	1.65	0.62
3:K:38:LYS:O	3:K:39:SER:C	2.38	0.62
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.12	0.62
3:K:38:LYS:O	3:K:40:GLY:N	2.33	0.62
1:C:38:ARG:HG2	1:C:38:ARG:NH1	2.01	0.61
2:B:60:ARG:NH1	2:B:81:ASP:OD1	2.33	0.61
1:C:28:THR:HA	1:C:51:PRO:HB2	1.82	0.61
2:D:89:GLN:HE22	2:D:92:SER:H	1.49	0.61
3:I:135:TYR:CD1	3:I:136:ARG:NH1	2.68	0.61
3:J:150:THR:OG1	3:J:151:HIS:N	2.34	0.61
2:B:89:GLN:HG2	2:B:91:SER:H	1.69	0.58
1:A:53:ASN:HD21	1:A:55:ASP:HB2	1.69	0.58
2:B:33:GLN:NE2	2:B:49:ASP:H	1.99	0.58
1:H:166:HIS:CE1	2:L:135:ASN:HD21	2.22	0.58
3:J:150:THR:HG1	3:J:151:HIS:H	1.50	0.57
2:B:89:GLN:NE2	2:B:92:SER:H	2.02	0.57
1:A:158:SER:N	1:A:199:ASN:HD21	1.98	0.56
3:K:38:LYS:CG	3:K:39:SER:N	2.66	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ARG:HD3	2:B:89:GLN:HG3	1.86	0.56
2:D:33:GLN:HE21	2:D:49:ASP:H	1.53	0.56
2:B:33:GLN:HE21	2:B:49:ASP:N	2.02	0.56
3:I:135:TYR:CB	3:I:136:ARG:HD2	2.35	0.56
3:J:150:THR:HB	3:J:151:HIS:CE1	2.41	0.56
1:A:99:GLY:HA2	3:K:43:TYR:OH	2.06	0.55
2:L:32:MET:CE	2:L:87:CYS:HB2	2.35	0.55
3:J:157:THR:O	3:J:158:GLN:C	2.44	0.55
3:J:149:MET:O	3:J:149:MET:HG3	2.06	0.55
3:I:110:TRP:CZ2	3:I:112:ASN:ND2	2.74	0.55
3:I:140:ARG:HG3	3:I:140:ARG:NH1	2.22	0.55
2:D:59:ALA:HB1	2:L:202:VAL:HG11	1.87	0.55
1:H:166:HIS:HE1	2:L:135:ASN:HD21	1.55	0.54
3:I:115:THR:C	3:I:117:ARG:H	2.11	0.54
2:L:2:ILE:HD12	2:L:2:ILE:H	1.73	0.54
1:A:183:VAL:HG11	2:B:132:LEU:CD2	2.38	0.53
3:J:146:VAL:HB	3:J:157:THR:HG21	1.91	0.53
1:C:8:VAL:HG11	1:C:16:VAL:CG2	2.37	0.53
2:B:187:LYS:HE3	2:B:207:ASN:HD22	1.74	0.53
3:I:135:TYR:C	3:I:136:ARG:HD2	2.30	0.53
1:A:38:ARG:CG	1:A:38:ARG:HH11	2.17	0.52
2:B:33:GLN:HG3	2:B:48:TYR:HA	1.91	0.52
3:J:146:VAL:N	3:J:157:THR:OG1	2.36	0.52
3:J:3:CYS:HA	3:J:154:THR:HG21	1.90	0.52
3:I:126:MET:HG2	3:I:146:VAL:HG22	1.91	0.51
1:H:38:ARG:HG2	1:H:90:ALA:HB2	1.93	0.51
3:J:150:THR:HB	3:J:151:HIS:ND1	2.25	0.51
3:K:37:ILE:HD11	3:K:41:SER:HB3	1.91	0.51
1:C:33:HIS:CE1	1:C:97:ASP:OD2	2.63	0.51
3:K:25:MET:HE2	3:K:43:TYR:CD2	2.46	0.51
1:A:183:VAL:HG11	2:B:132:LEU:HD22	1.93	0.51
3:I:115:THR:O	3:I:117:ARG:N	2.44	0.51
3:I:110:TRP:CD2	3:I:112:ASN:ND2	2.80	0.50
1:C:158:SER:N	1:C:199:ASN:HD21	2.09	0.50
2:L:105:ARG:NH2	2:L:106:THR:HG22	2.26	0.50
2:L:65:GLY:HA3	2:L:70:TYR:HA	1.93	0.50
2:B:142:LYS:HB3	2:B:194:THR:HB	1.94	0.50
1:C:33:HIS:HE1	1:C:97:ASP:OD2	1.95	0.50
2:L:49:ASP:HB2	2:L:52:LYS:HD2	1.94	0.49
2:L:33:GLN:NE2	2:L:49:ASP:H	2.10	0.49
2:L:105:ARG:HG2	2:L:106:THR:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:ALA:O	2:L:68:THR:HG23	2.13	0.49
1:H:158:SER:H	1:H:199:ASN:HD21	1.60	0.49
3:J:149:MET:O	3:J:150:THR:O	2.30	0.49
3:K:25:MET:CE	3:K:43:TYR:CE2	2.96	0.49
2:D:31:TYR:HB3	2:D:49:ASP:HA	1.94	0.49
3:I:115:THR:C	3:I:117:ARG:N	2.66	0.49
3:K:2:LEU:HD23	3:K:122:VAL:HG12	1.95	0.48
2:L:105:ARG:HG2	2:L:106:THR:H	1.78	0.48
3:I:42:LEU:HD12	3:I:43:TYR:CD2	2.48	0.48
1:C:38:ARG:CG	1:C:38:ARG:NH1	2.73	0.47
2:B:6:GLN:HG3	2:B:87:CYS:SG	2.54	0.47
1:H:36:LYS:HE2	1:H:38:ARG:HG3	1.97	0.47
3:K:28:CYS:HB2	3:K:42:LEU:O	2.15	0.47
1:C:121:PRO:HB3	1:C:147:TYR:HB3	1.95	0.47
3:I:52:HIS:CE1	4:I:300:NAG:H4	2.50	0.46
3:J:110:TRP:CE2	3:J:113:GLU:HG2	2.50	0.46
3:J:150:THR:CB	3:J:151:HIS:ND1	2.79	0.46
3:J:37:ILE:HG13	3:J:38:LYS:H	1.81	0.46
3:J:62:THR:HG22	3:J:63:SER:H	1.79	0.46
3:K:25:MET:HE3	3:K:43:TYR:CE2	2.50	0.46
1:A:53:ASN:ND2	1:A:55:ASP:HB2	2.31	0.45
2:L:31:TYR:HB3	2:L:49:ASP:HA	1.99	0.45
2:L:89:GLN:NE2	2:L:91:SER:H	2.14	0.45
3:I:2:LEU:HD12	3:I:122:VAL:HG12	1.99	0.45
3:I:24:THR:HG22	3:I:121:PHE:HA	1.99	0.45
2:L:133:LEU:HD21	2:L:193:VAL:HG13	1.97	0.45
4:J:300:NAG:O3	4:J:300:NAG:O7	2.34	0.45
2:D:167:ASP:O	2:D:168:SER:HB2	2.16	0.45
1:A:28:THR:HG23	1:A:52:GLY:HA2	1.99	0.44
2:D:4:SER:HB2	2:D:96:GLY:HA2	1.99	0.44
4:K:300:NAG:C3	4:K:301:NAG:O5	2.66	0.44
2:B:110:PRO:HD2	2:B:198:LEU:HD13	2.00	0.44
1:A:33:HIS:HD2	1:A:45:TRP:NE1	2.03	0.44
1:H:128:PRO:HD2	1:H:215:PRO:HA	2.00	0.44
2:L:194:THR:HG23	2:L:200:SER:HB3	2.01	0.43
1:C:9:LEU:HD21	1:C:149:PRO:HG3	2.00	0.43
1:H:95:SER:OG	1:H:102:PHE:HB3	2.18	0.43
2:D:61:PHE:CE1	2:D:74:ILE:HG12	2.54	0.43
2:L:157:GLN:HB3	2:L:157:GLN:HE21	1.58	0.43
2:L:2:ILE:O	2:L:94:THR:HG21	2.18	0.43
1:A:16:VAL:HG12	1:A:84:LEU:HD11	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LYS:HB2	1:C:46:ILE:HD11	1.99	0.43
2:B:183:TYR:HA	2:B:189:TYR:OH	2.18	0.43
1:C:36:LYS:HB3	1:C:44:GLU:HB3	1.99	0.43
1:C:131:LYS:HE2	2:D:205:SER:O	2.19	0.43
3:J:61:CYS:HB2	3:J:112:ASN:HB2	2.00	0.43
2:D:133:LEU:HD21	2:D:193:VAL:HG13	2.01	0.43
1:H:173:GLN:HE21	1:H:173:GLN:HB2	1.67	0.43
3:J:150:THR:HG1	3:J:151:HIS:CE1	2.36	0.43
1:C:128:PRO:HG3	1:C:140:LEU:HB3	2.00	0.43
1:C:203:LYS:HB2	1:C:204:PRO:HD3	2.00	0.43
1:A:38:ARG:CG	1:A:38:ARG:NH1	2.80	0.43
3:J:145:SER:CA	3:J:157:THR:OG1	2.57	0.42
1:C:65:LYS:HG2	1:C:81:LEU:HD12	2.00	0.42
2:D:32:MET:HE3	2:D:70:TYR:CD1	2.54	0.42
2:D:33:GLN:HG3	2:D:48:TYR:HA	2.00	0.42
2:L:23:CYS:SG	2:L:32:MET:HE1	2.60	0.42
1:H:33:HIS:HE1	1:H:97:ASP:OD2	2.02	0.42
3:J:107:PRO:HA	3:J:108:PRO:HD3	1.93	0.42
3:J:146:VAL:H	3:J:157:THR:CG2	2.33	0.42
2:L:29:ARG:NE	2:L:30:SER:H	2.17	0.42
2:B:60:ARG:HH11	2:B:81:ASP:CG	2.22	0.42
1:A:8:VAL:HG11	1:A:16:VAL:HG21	2.01	0.42
2:D:45:ARG:HG3	2:D:45:ARG:H	1.59	0.42
1:H:9:LEU:HD21	1:H:149:PRO:HG3	2.02	0.42
1:H:17:LYS:HE2	1:H:78:TYR:CD2	2.55	0.41
2:B:60:ARG:HD2	2:B:76:SER:O	2.20	0.41
2:D:156:SER:HB3	2:D:176:LEU:HD23	2.02	0.41
1:H:128:PRO:HG3	1:H:140:LEU:HB3	2.02	0.41
3:I:106:GLU:HA	3:I:107:PRO:HD3	1.90	0.41
3:K:25:MET:HE2	3:K:43:TYR:CE2	2.56	0.41
1:H:170:ALA:HA	1:H:180:LEU:HB3	2.02	0.41
3:J:115:THR:O	3:J:116:GLU:CB	2.68	0.41
1:C:127:ALA:HA	1:C:128:PRO:HD3	1.99	0.41
1:H:71:VAL:HG12	1:H:74:ALA:H	1.86	0.41
3:I:15:PHE:HA	3:I:128:TYR:O	2.21	0.41
3:J:32:ARG:HD2	3:J:32:ARG:H	1.84	0.41
2:D:110:PRO:HD2	2:D:198:LEU:HD13	2.03	0.41
1:A:31:TRP:CE3	3:K:42:LEU:HD22	2.57	0.40
3:J:15:PHE:HB2	3:J:127:VAL:CG1	2.51	0.40
3:I:135:TYR:CB	3:I:136:ARG:CD	2.87	0.40
3:J:121:PHE:CD2	3:J:125:GLN:HG2	2.56	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	213/215 (99%)	201 (94%)	11 (5%)	1 (0%)	32	68
1	C	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
1	H	213/215 (99%)	198 (93%)	13 (6%)	2 (1%)	20	54
2	B	206/210 (98%)	201 (98%)	5 (2%)	0	100	100
2	D	207/210 (99%)	198 (96%)	8 (4%)	1 (0%)	32	68
2	L	206/210 (98%)	198 (96%)	6 (3%)	2 (1%)	18	51
3	I	115/223 (52%)	100 (87%)	11 (10%)	4 (4%)	4	17
3	J	110/223 (49%)	88 (80%)	14 (13%)	8 (7%)	1	3
3	K	108/223 (48%)	93 (86%)	11 (10%)	4 (4%)	4	16
All	All	1591/1944 (82%)	1483 (93%)	86 (5%)	22 (1%)	13	41

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	54	SER
1	H	131	LYS
3	I	111	GLU
3	J	52	HIS
3	J	150	THR
3	K	39	SER
3	I	134	GLY
3	J	38	LYS
3	J	133	GLN
3	K	41	SER
1	A	132	SER
2	L	67	GLY
3	I	116	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	J	11	PRO
3	J	49	ASN
3	J	111	GLU
3	K	37	ILE
3	K	38	LYS
2	L	82	ALA
2	D	67	GLY
3	I	11	PRO
3	J	107	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	181/181 (100%)	171 (94%)	10 (6%)	25	58
1	C	181/181 (100%)	173 (96%)	8 (4%)	33	67
1	H	181/181 (100%)	174 (96%)	7 (4%)	37	72
2	B	181/182 (100%)	174 (96%)	7 (4%)	37	72
2	D	181/182 (100%)	173 (96%)	8 (4%)	33	67
2	L	181/182 (100%)	172 (95%)	9 (5%)	28	62
3	I	104/200 (52%)	95 (91%)	9 (9%)	12	34
3	J	102/200 (51%)	96 (94%)	6 (6%)	23	55
3	K	100/200 (50%)	93 (93%)	7 (7%)	18	45
All	All	1392/1689 (82%)	1321 (95%)	71 (5%)	28	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	38	ARG
1	A	41	GLN
1	A	107	GLN
1	A	111	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	152	VAL
1	A	195	THR
1	A	201	ASN
1	A	208	LYS
1	A	209	VAL
2	B	20	THR
2	B	45	ARG
2	B	89	GLN
2	B	105	ARG
2	B	126	THR
2	B	139	ARG
2	B	176	LEU
1	C	11	ARG
1	C	38	ARG
1	C	41	GLN
1	C	111	LEU
1	C	131	LYS
1	C	140	LEU
1	C	195	THR
1	C	209	VAL
2	D	7	SER
2	D	41	THR
2	D	45	ARG
2	D	89	GLN
2	D	94	THR
2	D	187	LYS
2	D	198	LEU
2	D	199	SER
1	H	8	VAL
1	H	41	GLN
1	H	79	MET
1	H	81	LEU
1	H	111	LEU
1	H	131	LYS
1	H	163	SER
2	L	19	VAL
2	L	45	ARG
2	L	89	GLN
2	L	106	THR
2	L	132	LEU
2	L	157	GLN
2	L	174	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	176	LEU
2	L	198	LEU
3	I	6	ASP
3	I	36	ARG
3	I	42	LEU
3	I	45	LEU
3	I	113	GLU
3	I	133	GLN
3	I	135	TYR
3	I	136	ARG
3	I	140	ARG
3	J	3	CYS
3	J	6	ASP
3	J	32	ARG
3	J	62	THR
3	J	116	GLU
3	J	151	HIS
3	K	3	CYS
3	K	6	ASP
3	K	30	CYS
3	K	42	LEU
3	K	115	THR
3	K	116	GLU
3	K	125	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	41	GLN
1	A	199	ASN
1	A	201	ASN
2	B	33	GLN
2	B	89	GLN
2	B	196	GLN
2	B	207	ASN
1	C	33	HIS
1	C	199	ASN
2	D	33	GLN
2	D	89	GLN
2	D	144	GLN
1	H	33	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	41	GLN
1	H	166	HIS
1	H	173	GLN
1	H	199	ASN
1	H	201	ASN
2	L	33	GLN
2	L	157	GLN
3	I	125	GLN
3	K	57	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	I	300	3,4	14,14,15	0.71	0	15,19,21	1.77	3 (20%)
4	NAG	I	301	4	14,14,15	0.51	0	15,19,21	1.46	1 (6%)
4	BMA	I	302	4	11,11,12	0.91	1 (9%)	13,15,17	1.49	2 (15%)
4	NAG	J	300	3,4	14,14,15	0.56	0	15,19,21	0.62	0
4	NAG	J	301	4	14,14,15	0.64	0	15,19,21	0.94	1 (6%)
4	BMA	J	302	4	11,11,12	0.73	0	13,15,17	0.65	0
4	NAG	K	300	3,4	14,14,15	0.77	1 (7%)	15,19,21	2.48	8 (53%)
4	NAG	K	301	4	14,14,15	0.52	0	15,19,21	1.93	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	K	302	4	11,11,12	0.78	0	13,15,17	1.33	2 (15%)

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	I	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	I	301	4	-	0/6/23/26	0/1/1/1
4	BMA	I	302	4	-	0/2/19/22	0/1/1/1
4	NAG	J	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	301	4	-	0/6/23/26	0/1/1/1
4	BMA	J	302	4	-	0/2/19/22	0/1/1/1
4	NAG	K	300	3,4	-	0/6/23/26	0/1/1/1
4	NAG	K	301	4	-	0/6/23/26	0/1/1/1
4	BMA	K	302	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	300	NAG	C1-C2	2.17	1.55	1.52
4	I	302	BMA	C2-C3	2.21	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	301	NAG	C6-C5-C4	-2.27	107.69	113.00
4	K	300	NAG	C3-C4-C5	-2.19	106.35	110.22
4	I	300	NAG	O4-C4-C5	-2.12	103.94	109.28
4	K	300	NAG	O7-C7-N2	2.01	125.78	121.92
4	K	300	NAG	C4-C3-C2	2.04	114.01	111.02
4	J	301	NAG	C4-C3-C2	2.22	114.27	111.02
4	K	302	BMA	C1-O5-C5	2.26	115.28	112.17
4	I	300	NAG	C2-N2-C7	2.45	126.52	122.94
4	K	300	NAG	C1-O5-C5	2.62	115.78	112.17
4	K	301	NAG	C1-O5-C5	2.63	115.78	112.17
4	K	300	NAG	C6-C5-C4	2.92	119.84	113.00
4	I	302	BMA	C2-C3-C4	3.05	116.19	110.88
4	K	300	NAG	O4-C4-C3	3.47	117.90	110.36
4	K	302	BMA	C1-C2-C3	3.54	114.14	109.65
4	I	301	NAG	C4-C3-C2	3.72	116.47	111.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	302	BMA	C1-C2-C3	3.79	114.46	109.65
4	K	301	NAG	C3-C4-C5	3.81	116.93	110.22
4	K	300	NAG	O5-C1-C2	4.08	117.14	111.47
4	K	301	NAG	C4-C3-C2	4.42	117.50	111.02
4	K	300	NAG	C2-N2-C7	4.86	130.04	122.94
4	I	300	NAG	C4-C3-C2	5.14	118.54	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	300	NAG	1	0
4	J	300	NAG	2	0
4	J	301	NAG	1	0
4	K	300	NAG	1	0
4	K	301	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

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	215/215 (100%)	-0.01	0 <span>100</span> <span>100</span>	49, 71, 101, 122	0
1	C	215/215 (100%)	-0.00	2 (0%) <span>84</span> <span>83</span>	46, 74, 104, 136	0
1	H	215/215 (100%)	0.01	1 (0%) <span>90</span> <span>90</span>	53, 78, 113, 154	0
2	B	208/210 (99%)	-0.11	1 (0%) <span>90</span> <span>90</span>	43, 64, 102, 121	0
2	D	209/210 (99%)	-0.06	1 (0%) <span>90</span> <span>90</span>	42, 65, 111, 126	0
2	L	208/210 (99%)	-0.14	0 <span>100</span> <span>100</span>	52, 71, 111, 136	0
3	I	119/223 (53%)	1.29	34 (28%) <span>1</span> <span>0</span>	79, 130, 186, 224	0
3	J	116/223 (52%)	1.05	23 (19%) <span>1</span> <span>1</span>	65, 132, 175, 191	0
3	K	114/223 (51%)	0.96	20 (17%) <span>2</span> <span>1</span>	71, 131, 179, 202	0
All	All	1619/1944 (83%)	0.20	82 (5%) <span>29</span> <span>24</span>	42, 77, 159, 224	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	115	THR	6.8
3	I	116	GLU	6.5
3	I	114	ALA	6.1
3	K	18	MET	6.0
3	I	35	ARG	5.5
3	J	116	GLU	5.4
3	J	130	GLN	5.0
3	I	138	LEU	4.4
3	K	19	ALA	4.1
3	I	34	PHE	3.9
3	K	139	HIS	3.9
3	J	19	ALA	3.9
3	K	143	ALA	3.9
3	K	116	GLU	3.8
3	K	60	GLN	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	I	143	ALA	3.7
3	K	140	ARG	3.6
3	I	118	ILE	3.6
3	I	20	TYR	3.5
3	I	19	ALA	3.5
3	I	29	GLU	3.5
3	K	42	LEU	3.4
3	I	12	HIS	3.3
3	I	132	VAL	3.2
3	I	33	GLY	3.2
3	I	39	SER	3.2
3	J	140	ARG	3.1
3	I	13	ALA	3.1
3	I	104	CYS	3.1
3	I	9	GLU	3.1
3	K	59	CYS	3.1
3	K	43	TYR	3.0
3	K	62	THR	3.0
3	J	144	GLU	3.0
3	K	29	GLU	2.9
3	K	155	ARG	2.9
3	J	18	MET	2.9
3	K	115	THR	2.9
3	J	111	GLU	2.8
3	J	60	GLN	2.8
3	J	133	GLN	2.8
3	I	61	CYS	2.8
3	J	138	LEU	2.8
3	I	14	THR	2.8
3	J	9	GLU	2.6
3	I	130	GLN	2.6
3	I	119	TYR	2.5
3	I	60	GLN	2.5
3	I	128	TYR	2.5
3	K	58	GLN	2.5
3	I	45	LEU	2.5
3	J	105	ARG	2.5
3	J	106	GLU	2.5
3	J	12	HIS	2.4
3	I	18	MET	2.4
2	D	29	ARG	2.4
3	K	61	CYS	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	J	135	TYR	2.4
3	J	119	TYR	2.4
3	I	139	HIS	2.3
3	K	110	TRP	2.3
2	B	29	ARG	2.3
1	C	1	GLN	2.3
3	I	112	ASN	2.2
3	J	63	SER	2.2
1	H	209	VAL	2.2
3	I	30	CYS	2.2
3	I	41	SER	2.2
3	J	62	THR	2.2
3	I	31	LYS	2.2
3	J	118	ILE	2.2
3	J	117	ARG	2.1
3	K	118	ILE	2.1
1	C	29	ARG	2.0
3	I	46	CYS	2.0
3	J	134	GLY	2.0
3	J	121	PHE	2.0
3	I	58	GLN	2.0
3	I	55	TRP	2.0
3	J	26	LEU	2.0
3	K	117	ARG	2.0
3	K	45	LEU	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	I	301	14/15	0.89	0.12	-	101,129,148,153	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	K	301	14/15	0.79	0.18	-	125,138,154,157	0
4	NAG	K	300	14/15	0.73	0.21	-	71,101,135,138	0
4	BMA	K	302	11/12	0.83	0.14	-	126,148,157,160	0
4	NAG	I	300	14/15	0.76	0.15	-	66,115,130,135	0
4	BMA	I	302	11/12	0.79	0.18	-	141,157,168,168	0
4	BMA	J	302	11/12	0.70	0.18	-	137,155,169,172	0
4	NAG	J	300	14/15	0.66	0.22	-	66,113,133,134	0
4	NAG	J	301	14/15	0.72	0.21	-	125,141,168,169	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.