Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:34 AM GMT

PDB ID	:	2ARJ
Title	:	CD8alpha-alpha in complex with YTS 105.18 Fab
Authors	:	Shore, D.A.; Teyton, L.; Dwek, R.A.; Rudd, P.M.; Wilson, I.A.
Deposited on	:	2005-08-19
Resolution	:	2.88 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

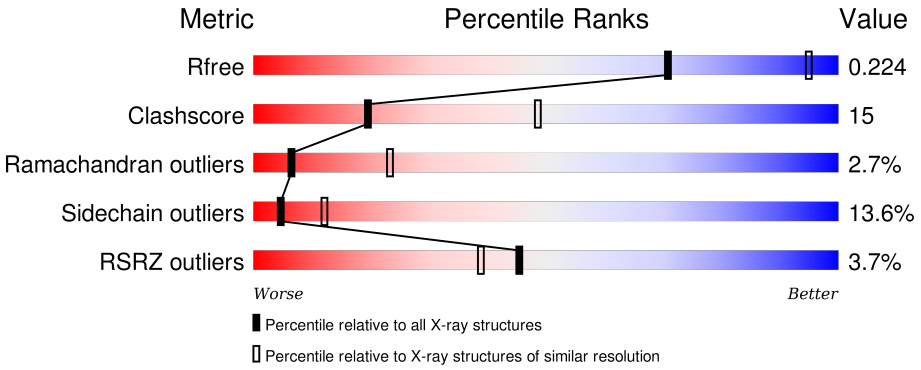
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	211	% 65% 29% 6%
1	L	211	% 72% 22% 5% •
2	B	215	63% 28% 5% • •
2	H	215	5% 70% 20% 6% • •
3	Q	123	11% 59% 23% 10% • 7%

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Mol	Chain	Length	Quality of chain
3	R	123	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8334 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 YTS 105.18 antigen binding region Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1647	1034	277	329	7			
1	A	211	Total	C	N	O	S	0	0	0
			1647	1034	277	329	7			

- Molecule 2 is a protein called YTS 105.18 antigen binding region Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1593	1008	262	315	8			
2	B	212	Total	C	N	O	S	0	0	0
			1593	1008	262	315	8			

- Molecule 3 is a protein called T-cell surface glycoprotein CD8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	116	Total	C	N	O	S	0	0	0
			925	595	150	173	7			
3	Q	115	Total	C	N	O	S	0	0	0
			917	591	148	171	7			

- Molecule 4 is water.

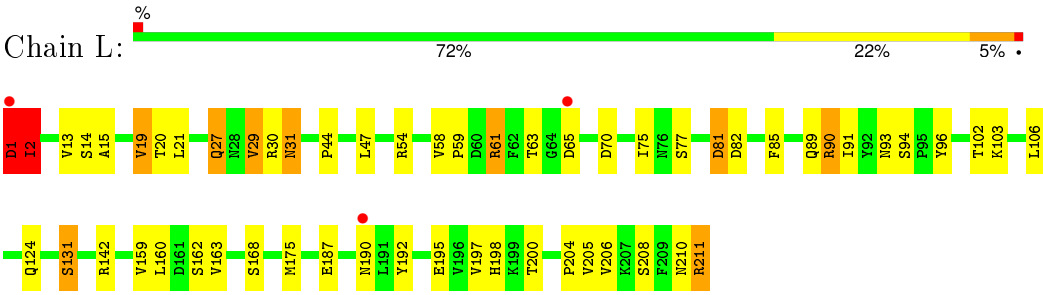
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	2	Total	O	0	0
			2	2		
4	H	1	Total	O	0	0
			1	1		
4	L	6	Total	O	0	0
			6	6		

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.

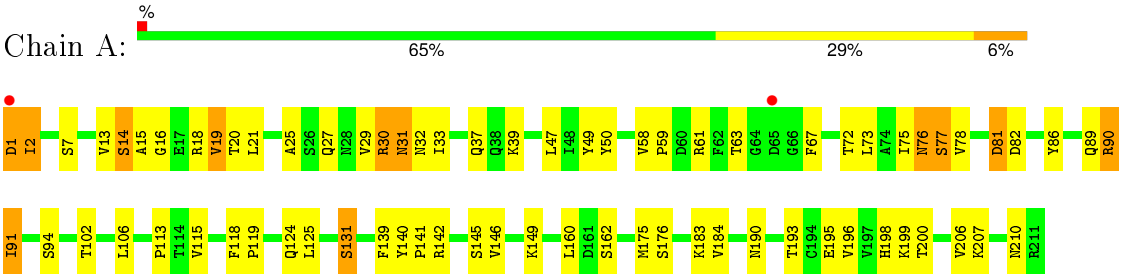
- Molecule 1: YTS 105.18 antigen binding region Light chain

Chain L:



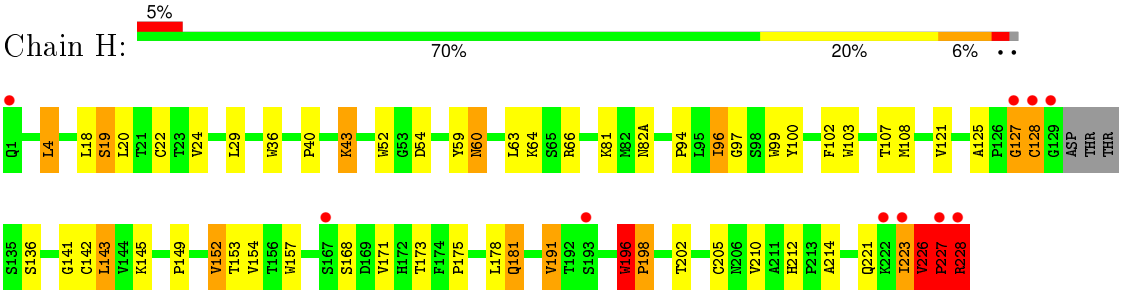
- Molecule 1: YTS 105.18 antigen binding region Light chain

Chain A:



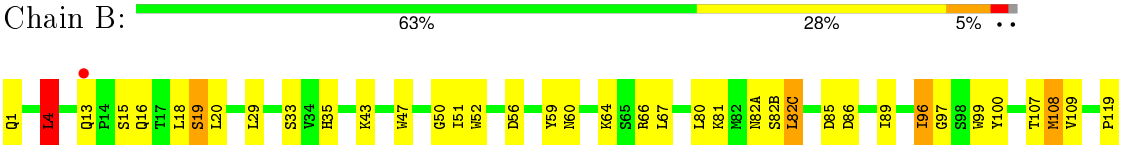
- Molecule 2: YTS 105.18 antigen binding region Heavy chain

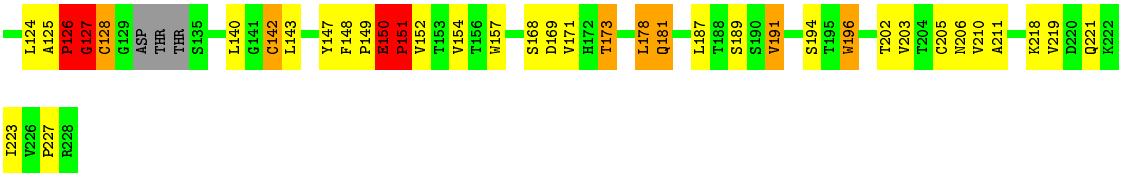
Chain H:



- Molecule 2: YTS 105.18 antigen binding region Heavy chain

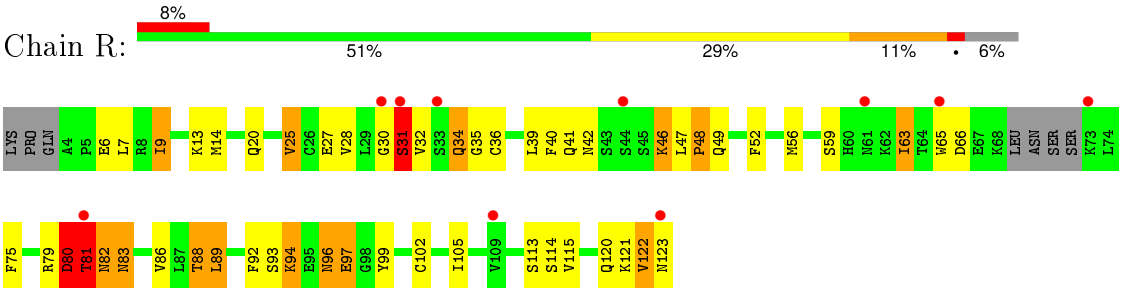
Chain B:





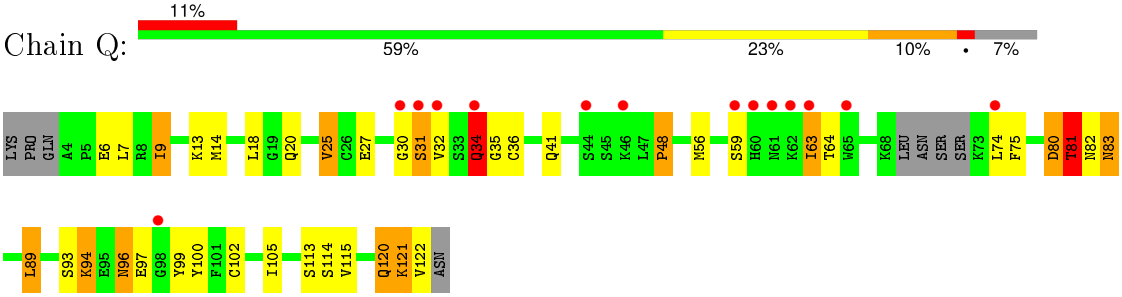
• Molecule 3: T-cell surface glycoprotein CD8 alpha chain

Chain R:



• Molecule 3: T-cell surface glycoprotein CD8 alpha chain

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.34Å 107.14Å 131.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.88 49.61 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.00-2.88) 98.4 (49.61-2.88)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.277 0.222 , 0.224	Depositor DCC
R_{free} test set	1332 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 26749 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8334	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.75	3/1684 (0.2%)	0.67	0/2288
1	L	0.69	1/1684 (0.1%)	0.71	1/2288 (0.0%)
2	B	0.95	9/1636 (0.6%)	0.92	13/2240 (0.6%)
2	H	1.09	9/1636 (0.6%)	0.89	9/2240 (0.4%)
3	Q	0.77	1/937 (0.1%)	0.75	1/1264 (0.1%)
3	R	0.68	2/945 (0.2%)	0.74	0/1275
All	All	0.85	25/8522 (0.3%)	0.79	24/11595 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
2	B	0	4
2	H	0	1
All	All	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	127	GLY	CA-C	28.73	1.97	1.51
1	A	1	ASP	N-CA	18.51	1.83	1.46
1	L	1	ASP	N-CA	16.25	1.78	1.46
2	B	128	CYS	CB-SG	-14.32	1.57	1.82
2	B	126	PRO	N-CD	13.28	1.66	1.47
3	Q	81	THR	C-O	13.02	1.48	1.23
2	B	127	GLY	CA-C	11.36	1.70	1.51
2	H	127	GLY	C-O	-10.41	1.06	1.23
2	B	127	GLY	C-O	-10.14	1.07	1.23
2	B	227	PRO	N-CD	9.47	1.61	1.47
1	A	1	ASP	C-O	7.68	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	226	VAL	CA-C	7.62	1.72	1.52
3	R	81	THR	C-O	7.25	1.37	1.23
2	H	228	ARG	C-OXT	7.20	1.37	1.23
2	B	128	CYS	CA-CB	6.70	1.68	1.53
2	H	226	VAL	CB-CG1	6.39	1.66	1.52
3	R	31	SER	CB-OG	6.34	1.50	1.42
2	H	223	ILE	C-N	-6.25	1.19	1.34
2	H	228	ARG	N-CA	-6.19	1.33	1.46
2	H	227	PRO	C-N	6.15	1.48	1.34
2	H	128	CYS	CB-SG	6.05	1.92	1.82
1	A	1	ASP	CG-OD1	6.02	1.39	1.25
2	B	227	PRO	C-O	-5.97	1.11	1.23
2	B	227	PRO	C-N	5.36	1.46	1.34
2	B	151	PRO	CG-CD	5.07	1.67	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	226	VAL	CG1-CB-CG2	11.11	128.67	110.90
2	B	127	GLY	O-C-N	-9.75	107.10	122.70
2	H	227	PRO	CA-C-N	-9.47	96.36	117.20
2	H	226	VAL	CA-CB-CG1	-8.97	97.45	110.90
2	B	148	PHE	C-N-CD	-8.55	101.80	120.60
2	B	127	GLY	C-N-CA	-7.17	103.77	121.70
2	B	196	TRP	C-N-CD	-6.96	105.28	120.60
2	B	127	GLY	CA-C-O	6.89	133.00	120.60
2	B	227	PRO	O-C-N	6.88	133.71	122.70
2	H	227	PRO	CA-C-O	6.54	135.89	120.20
1	L	90	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	H	4	LEU	CA-CB-CG	6.46	130.15	115.30
2	H	227	PRO	C-N-CA	-6.40	105.69	121.70
2	H	226	VAL	CA-C-O	6.37	133.48	120.10
2	B	126	PRO	C-N-CA	-6.36	108.95	122.30
2	B	148	PHE	C-N-CA	6.21	148.10	122.00
2	B	4	LEU	CA-CB-CG	6.18	129.53	115.30
3	Q	81	THR	C-N-CA	-6.11	106.44	121.70
2	B	142	CYS	CA-CB-SG	-5.92	103.34	114.00
2	H	227	PRO	N-CD-CG	-5.58	94.83	103.20
2	B	196	TRP	C-N-CA	5.26	144.11	122.00
2	H	127	GLY	C-N-CA	5.20	134.71	121.70
2	B	126	PRO	CA-N-CD	-5.20	104.22	111.50
2	B	227	PRO	N-CD-CG	-5.20	95.40	103.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	127	GLY	Mainchain
2	B	128	CYS	Mainchain
2	B	150	GLU	Peptide
2	B	196	TRP	Peptide
2	H	196	TRP	Peptide
1	L	1	ASP	Peptide

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	1647	0	1586	51	0
1	L	1647	0	1586	42	0
2	B	1593	0	1549	50	0
2	H	1593	0	1549	45	0
3	Q	917	0	915	31	0
3	R	925	0	921	42	0
4	A	3	0	0	0	0
4	B	2	0	0	2	0
4	H	1	0	0	0	0
4	L	6	0	0	0	0
All	All	8334	0	8106	246	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 15.

All (246) 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)
1:L:1:ASP:CA	1:L:1:ASP:N	1.78	1.44
1:A:1:ASP:N	1:A:1:ASP:CA	1.83	1.40
2:H:127:GLY:CA	2:H:127:GLY:C	1.97	1.32
2:H:226:VAL:HG12	2:H:227:PRO:CD	1.88	1.04
1:A:90:ARG:CG	1:A:90:ARG:HH11	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:196:TRP:CD2	2:H:198:PRO:HD3	1.98	0.96
1:A:90:ARG:HG3	1:A:90:ARG:NH1	1.59	0.96
2:H:226:VAL:HG12	2:H:227:PRO:HD3	1.46	0.96
3:R:46:LYS:HD2	3:R:46:LYS:H	1.32	0.94
3:Q:9:ILE:HD11	3:Q:114:SER:HB2	1.52	0.90
1:A:90:ARG:HG3	1:A:90:ARG:HH11	0.79	0.90
3:R:81:THR:HG22	3:R:82:ASN:H	1.34	0.88
2:H:196:TRP:CE3	2:H:198:PRO:HD3	2.08	0.88
3:R:9:ILE:HG13	3:R:113:SER:HB2	1.57	0.87
1:A:124:GLN:HE22	1:A:131:SER:HB2	1.39	0.87
1:A:2:ILE:HD13	1:A:27:GLN:HG3	1.57	0.85
1:L:2:ILE:HG22	1:L:27:GLN:HG3	1.58	0.84
1:L:29:VAL:HG11	1:L:90:ARG:HE	1.40	0.84
1:A:2:ILE:HD13	1:A:27:GLN:CG	2.08	0.84
2:H:226:VAL:HG12	2:H:227:PRO:HD2	1.58	0.84
1:L:91:ILE:HD11	2:H:100:TYR:HB3	1.60	0.83
1:A:160:LEU:HD11	2:B:181:GLN:HG3	1.61	0.82
2:B:1:GLN:HA	4:B:229:HOH:O	1.78	0.82
3:Q:75:PHE:HE1	3:Q:89:LEU:HD22	1.44	0.81
1:L:29:VAL:HG11	1:L:90:ARG:NE	1.95	0.80
2:B:203:VAL:O	2:B:223:ILE:HG22	1.82	0.80
1:A:21:LEU:HD22	1:A:102:THR:HG21	1.63	0.79
3:Q:121:LYS:O	3:Q:122:VAL:HB	1.80	0.79
2:H:226:VAL:CG1	2:H:227:PRO:HD2	2.12	0.78
1:L:13:VAL:HG21	1:L:19:VAL:HG13	1.66	0.76
3:R:80:ASP:O	3:R:81:THR:O	2.02	0.76
1:L:90:ARG:NH2	1:L:93:ASN:HB2	2.01	0.76
2:H:226:VAL:CG1	2:H:227:PRO:CD	2.64	0.76
2:H:226:VAL:O	2:H:227:PRO:O	2.05	0.75
3:Q:75:PHE:CE1	3:Q:89:LEU:HD22	2.21	0.74
2:B:1:GLN:CA	4:B:229:HOH:O	2.36	0.73
3:R:9:ILE:HD11	3:R:114:SER:HB2	1.69	0.73
3:R:7:LEU:HD22	3:R:28:VAL:HG22	1.69	0.72
1:L:31:ASN:HD22	1:L:31:ASN:H	1.37	0.70
3:R:75:PHE:CE1	3:R:89:LEU:HD22	2.26	0.70
3:R:93:SER:H	3:R:96:ASN:HD21	1.40	0.69
1:A:19:VAL:HG23	1:A:75:ILE:HB	1.74	0.69
1:L:19:VAL:HG23	1:L:75:ILE:HB	1.76	0.68
2:B:125:ALA:HB2	2:B:223:ILE:HD11	1.76	0.68
3:R:81:THR:HG22	3:R:82:ASN:N	2.08	0.67
2:H:226:VAL:CB	2:H:227:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:227:PRO:C	2:H:228:ARG:HG2	2.15	0.67
3:R:9:ILE:HD12	3:R:9:ILE:H	1.60	0.66
1:L:91:ILE:HG12	2:H:99:TRP:O	1.94	0.66
3:R:75:PHE:HE1	3:R:89:LEU:HD22	1.61	0.66
1:L:160:LEU:HD11	2:H:181:GLN:HG3	1.79	0.65
3:R:46:LYS:N	3:R:46:LYS:HD2	2.09	0.65
3:Q:80:ASP:O	3:Q:81:THR:O	2.15	0.64
2:H:196:TRP:CD2	2:H:198:PRO:CD	2.79	0.64
2:H:125:ALA:HB2	2:H:223:ILE:CG2	2.28	0.64
2:B:171:VAL:HG22	2:B:191:VAL:HG13	1.78	0.63
3:Q:82:ASN:O	3:Q:83:ASN:CB	2.45	0.62
1:L:2:ILE:HD13	1:L:90:ARG:HD3	1.82	0.62
2:H:18:LEU:HD11	2:H:20:LEU:HG	1.82	0.61
1:A:2:ILE:HD11	1:A:25:ALA:HB1	1.82	0.61
3:Q:35:GLY:HA3	3:Q:56:MET:O	2.00	0.61
2:H:196:TRP:CE3	2:H:198:PRO:CD	2.83	0.61
1:A:1:ASP:N	1:A:1:ASP:OD1	2.34	0.61
1:A:76:ASN:HD22	1:A:76:ASN:N	1.98	0.60
1:A:32:ASN:HB3	1:A:91:ILE:HG22	1.84	0.60
2:B:173:THR:HB	2:B:189:SER:OG	2.01	0.60
2:B:223:ILE:HG23	2:B:223:ILE:O	2.01	0.60
1:A:91:ILE:HG12	2:B:99:TRP:O	2.01	0.59
2:B:96:ILE:O	2:B:96:ILE:HG13	2.01	0.59
3:Q:30:GLY:O	3:Q:31:SER:HB3	2.02	0.59
3:Q:9:ILE:HG13	3:Q:113:SER:HB2	1.85	0.59
3:Q:9:ILE:CD1	3:Q:114:SER:HB2	2.28	0.59
3:Q:82:ASN:O	3:Q:83:ASN:HB2	2.01	0.59
1:A:195:GLU:HG3	1:A:206:VAL:HG22	1.84	0.58
3:Q:34:GLN:HE21	3:Q:34:GLN:HA	1.68	0.58
1:L:2:ILE:CD1	1:L:90:ARG:HD3	2.34	0.58
2:H:40:PRO:HB2	2:H:43:LYS:HG3	1.85	0.58
2:H:227:PRO:O	2:H:228:ARG:HG2	2.04	0.57
2:B:157:TRP:CH2	2:B:205:CYS:HB3	2.38	0.57
2:B:150:GLU:HB3	2:B:151:PRO:CD	2.34	0.57
2:H:226:VAL:CB	2:H:227:PRO:CD	2.82	0.57
2:B:125:ALA:HB2	2:B:223:ILE:CD1	2.34	0.57
1:A:21:LEU:HD12	1:A:73:LEU:HD23	1.85	0.57
3:R:35:GLY:HA3	3:R:56:MET:O	2.05	0.57
2:B:67:LEU:HD11	2:B:80:LEU:HD11	1.86	0.56
3:R:102:CYS:SG	3:R:113:SER:HB3	2.45	0.56
2:H:143:LEU:HD22	2:H:145:LYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:99:TYR:HB3	3:Q:115:VAL:HG13	1.87	0.56
2:H:96:ILE:O	2:H:96:ILE:HG13	2.05	0.55
1:L:195:GLU:HG3	1:L:206:VAL:HG22	1.87	0.55
3:R:46:LYS:CD	3:R:46:LYS:H	2.12	0.55
1:A:81:ASP:N	1:A:81:ASP:OD1	2.37	0.55
1:A:20:THR:HG23	1:A:72:THR:HG23	1.87	0.55
1:A:2:ILE:HD13	1:A:27:GLN:HG2	1.86	0.55
2:B:203:VAL:HG22	2:B:223:ILE:HG21	1.88	0.54
3:R:56:MET:HG2	3:R:63:ILE:HG22	1.89	0.54
1:A:118:PHE:HE2	2:B:126:PRO:HD3	1.71	0.54
2:B:124:LEU:C	2:B:223:ILE:HD11	2.29	0.54
3:Q:14:MET:CE	3:Q:20:GLN:HE22	2.22	0.53
2:B:89:ILE:HG13	2:B:108:MET:HG2	1.91	0.53
2:H:157:TRP:CZ3	2:H:205:CYS:HB3	2.44	0.53
1:L:197:VAL:HG22	1:L:204:PRO:HB3	1.91	0.53
2:H:226:VAL:O	2:H:227:PRO:C	2.44	0.53
3:R:121:LYS:O	3:R:123:ASN:N	2.41	0.53
3:Q:93:SER:HB2	3:Q:94:LYS:HE3	1.90	0.53
3:Q:41:GLN:NE2	3:Q:48:PRO:HA	2.23	0.53
1:A:198:HIS:HD2	1:A:200:THR:H	1.55	0.53
2:B:157:TRP:CZ3	2:B:205:CYS:HB3	2.45	0.52
3:Q:96:ASN:HB2	3:Q:100:TYR:OH	2.09	0.52
1:L:124:GLN:HE22	1:L:131:SER:HB2	1.74	0.52
3:Q:93:SER:H	3:Q:96:ASN:HD21	1.58	0.52
1:L:31:ASN:HD22	1:L:31:ASN:N	2.02	0.52
2:H:54:ASP:HB3	3:Q:14:MET:HE3	1.92	0.52
3:Q:14:MET:HE2	3:Q:20:GLN:HE22	1.75	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.93	0.51
1:L:47:LEU:HA	1:L:58:VAL:HG21	1.93	0.51
3:R:79:ARG:C	3:R:80:ASP:O	2.48	0.51
3:R:99:TYR:HB3	3:R:115:VAL:HG13	1.92	0.51
1:A:2:ILE:O	1:A:2:ILE:HG23	2.11	0.51
1:A:13:VAL:HG21	1:A:19:VAL:HG13	1.92	0.51
1:L:198:HIS:CD2	1:L:200:THR:HG23	2.46	0.51
1:L:163:VAL:HG22	1:L:175:MET:HB3	1.93	0.50
1:A:146:VAL:HG22	1:A:196:VAL:HG22	1.92	0.50
3:R:39:LEU:HD23	3:R:52:PHE:HA	1.92	0.50
1:L:90:ARG:HH22	1:L:93:ASN:HB2	1.76	0.50
3:Q:121:LYS:O	3:Q:122:VAL:CB	2.55	0.50
2:H:59:TYR:HB2	2:H:64:LYS:HD2	1.94	0.50
3:R:34:GLN:HA	3:R:34:GLN:HE21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HD12	2:H:19:SER:N	2.27	0.50
1:L:187:GLU:HA	1:L:211:ARG:NE	2.27	0.49
2:B:171:VAL:HG22	2:B:191:VAL:CG1	2.42	0.49
3:R:63:ILE:HG13	3:R:65:TRP:NE1	2.27	0.49
3:R:94:LYS:H	3:R:94:LYS:CD	2.25	0.49
2:H:97:GLY:HA2	3:Q:25:VAL:HG11	1.94	0.49
3:R:9:ILE:HD12	3:R:9:ILE:N	2.25	0.49
3:R:30:GLY:O	3:R:31:SER:HB3	2.12	0.49
2:H:121:VAL:HG12	2:H:221:GLN:HG3	1.94	0.49
3:R:9:ILE:CD1	3:R:9:ILE:H	2.20	0.49
3:Q:56:MET:HG2	3:Q:63:ILE:HG22	1.94	0.49
2:B:35:HIS:HD1	2:B:47:TRP:HE1	1.61	0.49
1:L:198:HIS:HD2	1:L:200:THR:H	1.61	0.49
2:H:171:VAL:HG22	2:H:191:VAL:CG1	2.43	0.48
2:B:66:ARG:NH1	2:B:82(A):ASN:O	2.43	0.48
2:B:15:SER:HA	2:B:82(B):SER:HA	1.94	0.48
2:B:125:ALA:N	2:B:223:ILE:HD11	2.28	0.48
1:A:90:ARG:CG	1:A:90:ARG:NH1	2.46	0.48
1:L:61:ARG:HG3	1:L:75:ILE:HG23	1.94	0.48
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.48	0.48
2:B:140:LEU:HD13	2:B:223:ILE:HG21	1.94	0.48
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.47	0.48
1:A:21:LEU:HD22	1:A:102:THR:CG2	2.40	0.48
3:R:41:GLN:NE2	3:R:48:PRO:HA	2.30	0.47
3:Q:99:TYR:HB3	3:Q:115:VAL:CG1	2.44	0.47
2:H:97:GLY:HA2	3:Q:25:VAL:CG1	2.45	0.47
2:B:52:TRP:HH2	2:B:99:TRP:CZ3	2.32	0.47
2:B:97:GLY:HA2	3:R:25:VAL:CG1	2.44	0.47
2:B:35:HIS:ND1	2:B:50:GLY:HA3	2.29	0.47
2:H:141:GLY:O	2:H:223:ILE:HD11	2.15	0.47
1:L:31:ASN:H	1:L:31:ASN:ND2	2.09	0.47
3:R:92:PHE:HZ	3:R:97:GLU:HG2	1.80	0.46
2:B:82(C):LEU:HD13	2:B:86:ASP:HB3	1.96	0.46
1:A:91:ILE:HD11	2:B:100:TYR:HB3	1.97	0.46
3:R:86:VAL:HG12	3:R:88:THR:HG22	1.97	0.46
1:L:117:ILE:HD13	1:L:208:SER:HA	1.97	0.46
3:R:122:VAL:O	3:R:123:ASN:HB2	2.15	0.46
3:R:46:LYS:N	3:R:46:LYS:CD	2.74	0.45
2:H:152:VAL:HG23	2:H:212:HIS:CD2	2.51	0.45
1:A:16:GLY:HA2	1:A:77:SER:HB2	1.97	0.45
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG13	1:A:78:VAL:HG11	1.97	0.45
1:L:21:LEU:HG	1:L:102:THR:HG21	1.99	0.45
2:B:125:ALA:CB	2:B:223:ILE:HD11	2.44	0.45
2:B:178:LEU:HD22	2:B:181:GLN:H	1.82	0.45
3:Q:18:LEU:HD21	3:Q:120:GLN:HE21	1.82	0.45
1:A:89:GLN:HG2	1:A:90:ARG:O	2.16	0.45
1:L:198:HIS:HD2	1:L:200:THR:HG23	1.82	0.45
3:R:27:GLU:HA	3:R:83:ASN:O	2.17	0.44
3:R:40:PHE:CZ	3:R:42:ASN:HA	2.52	0.44
1:L:190:ASN:HB3	1:L:210:ASN:ND2	2.32	0.44
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.99	0.44
2:B:18:LEU:HD12	2:B:19:SER:N	2.33	0.44
2:H:52:TRP:HH2	2:H:99:TRP:CZ3	2.35	0.44
2:B:18:LEU:HD13	2:B:109:VAL:HG11	1.99	0.44
2:B:18:LEU:HD11	2:B:20:LEU:HG	1.99	0.44
1:A:190:ASN:HB3	1:A:210:ASN:ND2	2.32	0.44
1:A:18:ARG:HA	1:A:75:ILE:O	2.18	0.44
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.53	0.44
3:R:82:ASN:HB3	3:R:83:ASN:H	1.51	0.44
1:A:124:GLN:NE2	1:A:131:SER:HB2	2.20	0.44
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.86	0.44
2:B:52:TRP:CH2	2:B:99:TRP:CZ3	3.05	0.44
2:B:82(C):LEU:HD13	2:B:86:ASP:CB	2.48	0.44
1:L:89:GLN:NE2	1:L:96:TYR:HB3	2.33	0.44
2:H:66:ARG:HA	2:H:82(A):ASN:HD22	1.83	0.44
2:B:211:ALA:HB2	2:B:218:LYS:HD3	1.99	0.44
2:H:125:ALA:HB2	2:H:223:ILE:HG22	2.00	0.44
1:A:149:LYS:HB2	1:A:193:THR:HB	1.99	0.43
1:L:90:ARG:HG3	1:L:91:ILE:N	2.32	0.43
2:H:149:PRO:HD2	2:H:214:ALA:CB	2.48	0.43
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.00	0.43
1:L:192:TYR:O	1:L:208:SER:HB2	2.19	0.43
2:B:35:HIS:CE1	2:B:50:GLY:HA3	2.54	0.43
1:L:1:ASP:CB	1:L:1:ASP:N	2.71	0.43
2:B:97:GLY:HA2	3:R:25:VAL:HG11	2.00	0.43
2:B:13:GLN:CG	2:B:16:GLN:HG3	2.49	0.43
1:A:49:TYR:HD2	1:A:50:TYR:CD2	2.37	0.43
2:B:66:ARG:HA	2:B:82(A):ASN:HD22	1.83	0.43
1:L:85:PHE:CZ	1:L:103:LYS:HG3	2.54	0.43
1:A:31:ASN:H	1:A:31:ASN:HD22	1.67	0.43
2:B:59:TYR:HB2	2:B:64:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:ASN:HD21	2:H:63:LEU:HD12	1.83	0.42
1:L:14:SER:O	1:L:15:ALA:C	2.56	0.42
1:L:81:ASP:N	1:L:81:ASP:OD1	2.52	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.89	0.42
3:Q:89:LEU:HD13	3:Q:96:ASN:HB2	2.01	0.42
2:H:52:TRP:CH2	2:H:99:TRP:CZ3	3.08	0.42
1:A:119:PRO:CG	2:B:127:GLY:HA3	2.49	0.42
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.53	0.42
1:A:30:ARG:HB3	1:A:67:PHE:CZ	2.55	0.42
1:A:29:VAL:HG12	1:A:90:ARG:NH2	2.34	0.42
1:A:2:ILE:HD12	1:A:2:ILE:HA	1.92	0.42
1:A:21:LEU:CD2	1:A:102:THR:HG21	2.43	0.42
2:B:33:SER:HB2	2:B:51:ILE:O	2.19	0.41
3:R:47:LEU:O	3:R:49:GLN:N	2.52	0.41
2:H:94:PRO:HD2	2:H:102:PHE:O	2.20	0.41
2:B:219:VAL:CG2	2:B:221:GLN:HE21	2.33	0.41
1:A:140:TYR:CG	1:A:141:PRO:HA	2.55	0.41
1:L:162:SER:OG	2:H:175:PRO:O	2.27	0.41
1:L:115:VAL:HG13	1:L:205:VAL:HG11	2.03	0.41
3:R:81:THR:CG2	3:R:82:ASN:N	2.79	0.41
2:B:89:ILE:CG1	2:B:108:MET:HG2	2.51	0.41
2:B:4:LEU:HD22	2:B:4:LEU:N	2.36	0.41
2:B:125:ALA:CA	2:B:223:ILE:HD11	2.51	0.41
3:R:92:PHE:HZ	3:R:97:GLU:CG	2.34	0.41
3:Q:80:ASP:O	3:Q:81:THR:C	2.57	0.41
3:Q:27:GLU:HA	3:Q:83:ASN:O	2.21	0.41
1:A:162:SER:O	1:A:175:MET:HB2	2.21	0.41
1:A:125:LEU:HD22	1:A:183:LYS:HG3	2.03	0.41
1:L:27:GLN:HB3	1:L:27:GLN:HE21	1.69	0.40
3:Q:94:LYS:H	3:Q:94:LYS:CD	2.32	0.40
3:R:94:LYS:H	3:R:94:LYS:HD3	1.86	0.40
1:A:14:SER:O	1:A:15:ALA:C	2.59	0.40
3:Q:36:CYS:SG	3:Q:102:CYS:HB2	2.61	0.40
3:R:36:CYS:SG	3:R:102:CYS:HB2	2.61	0.40
2:H:66:ARG:NH1	2:H:82(A):ASN:O	2.54	0.40
3:R:14:MET:HE2	3:R:20:GLN:HE22	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	209/211 (99%)	195 (93%)	12 (6%)	2 (1%)	19	52
1	L	209/211 (99%)	196 (94%)	11 (5%)	2 (1%)	19	52
2	B	208/215 (97%)	188 (90%)	16 (8%)	4 (2%)	10	33
2	H	208/215 (97%)	196 (94%)	7 (3%)	5 (2%)	7	27
3	Q	111/123 (90%)	99 (89%)	4 (4%)	8 (7%)	1	3
3	R	112/123 (91%)	98 (88%)	6 (5%)	8 (7%)	1	3
All	All	1057/1098 (96%)	972 (92%)	56 (5%)	29 (3%)	6	23

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	168	SER
2	H	198	PRO
2	H	227	PRO
2	B	150	GLU
2	B	151	PRO
3	R	31	SER
3	R	81	THR
3	R	122	VAL
3	Q	31	SER
3	Q	81	THR
3	Q	121	LYS
1	L	2	ILE
2	B	168	SER
3	R	59	SER
1	A	77	SER
3	R	34	GLN
3	R	80	ASP
3	Q	34	GLN
3	Q	59	SER
3	Q	83	ASN

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Mol	Chain	Res	Type
2	H	128	CYS
2	B	85	ASP
3	R	48	PRO
1	L	77	SER
2	H	196	TRP
1	A	2	ILE
3	R	82	ASN
3	Q	48	PRO
3	Q	80	ASP

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	185/185 (100%)	163 (88%)	22 (12%)	6 17
1	L	185/185 (100%)	164 (89%)	21 (11%)	7 19
2	B	184/187 (98%)	156 (85%)	28 (15%)	3 9
2	H	184/187 (98%)	159 (86%)	25 (14%)	5 12
3	Q	107/115 (93%)	90 (84%)	17 (16%)	3 8
3	R	108/115 (94%)	91 (84%)	17 (16%)	3 8
All	All	953/974 (98%)	823 (86%)	130 (14%)	5 12

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	19	VAL
1	L	20	THR
1	L	27	GLN
1	L	29	VAL
1	L	30	ARG
1	L	31	ASN
1	L	54	ARG
1	L	61	ARG

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Mol	Chain	Res	Type
1	L	63	THR
1	L	65	ASP
1	L	70	ASP
1	L	81	ASP
1	L	94	SER
1	L	106	LEU
1	L	115	VAL
1	L	131	SER
1	L	142	ARG
1	L	159	VAL
1	L	168	SER
1	L	211	ARG
2	H	4	LEU
2	H	19	SER
2	H	24	VAL
2	H	29	LEU
2	H	43	LYS
2	H	60	ASN
2	H	81	LYS
2	H	96	ILE
2	H	107	THR
2	H	108	MET
2	H	136	SER
2	H	142	CYS
2	H	143	LEU
2	H	152	VAL
2	H	153	THR
2	H	154	VAL
2	H	173	THR
2	H	178	LEU
2	H	181	GLN
2	H	191	VAL
2	H	202	THR
2	H	210	VAL
2	H	226	VAL
2	H	227	PRO
2	H	228	ARG
1	A	7	SER
1	A	14	SER
1	A	19	VAL
1	A	30	ARG
1	A	31	ASN

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Mol	Chain	Res	Type
1	A	33	ILE
1	A	39	LYS
1	A	63	THR
1	A	76	ASN
1	A	81	ASP
1	A	90	ARG
1	A	91	ILE
1	A	94	SER
1	A	106	LEU
1	A	115	VAL
1	A	131	SER
1	A	142	ARG
1	A	145	SER
1	A	176	SER
1	A	184	VAL
1	A	199	LYS
1	A	207	LYS
2	B	4	LEU
2	B	19	SER
2	B	29	LEU
2	B	43	LYS
2	B	56	ASP
2	B	60	ASN
2	B	81	LYS
2	B	82(C)	LEU
2	B	96	ILE
2	B	107	THR
2	B	108	MET
2	B	126	PRO
2	B	142	CYS
2	B	143	LEU
2	B	149	PRO
2	B	151	PRO
2	B	152	VAL
2	B	154	VAL
2	B	169	ASP
2	B	173	THR
2	B	178	LEU
2	B	181	GLN
2	B	187	LEU
2	B	191	VAL
2	B	194	SER

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Mol	Chain	Res	Type
2	B	202	THR
2	B	206	ASN
2	B	210	VAL
3	R	6	GLU
3	R	9	ILE
3	R	13	LYS
3	R	25	VAL
3	R	32	VAL
3	R	46	LYS
3	R	63	ILE
3	R	66	ASP
3	R	80	ASP
3	R	83	ASN
3	R	88	THR
3	R	89	LEU
3	R	94	LYS
3	R	96	ASN
3	R	97	GLU
3	R	105	ILE
3	R	120	GLN
3	Q	6	GLU
3	Q	7	LEU
3	Q	9	ILE
3	Q	13	LYS
3	Q	25	VAL
3	Q	32	VAL
3	Q	34	GLN
3	Q	63	ILE
3	Q	64	THR
3	Q	74	LEU
3	Q	81	THR
3	Q	89	LEU
3	Q	94	LYS
3	Q	96	ASN
3	Q	97	GLU
3	Q	105	ILE
3	Q	120	GLN

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

Mol	Chain	Res	Type
1	L	27	GLN

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Mol	Chain	Res	Type
1	L	31	ASN
1	L	76	ASN
1	L	124	GLN
1	L	198	HIS
1	L	210	ASN
2	H	13	GLN
2	H	60	ASN
2	H	82(A)	ASN
2	H	221	GLN
1	A	31	ASN
1	A	76	ASN
1	A	124	GLN
1	A	138	ASN
1	A	198	HIS
1	A	210	ASN
2	B	16	GLN
2	B	82(A)	ASN
2	B	172	HIS
2	B	221	GLN
3	R	20	GLN
3	R	34	GLN
3	R	41	GLN
3	R	96	ASN
3	R	107	ASN
3	R	120	GLN
3	Q	20	GLN
3	Q	34	GLN
3	Q	96	ASN
3	Q	120	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	211/211 (100%)	0.04	2 (0%) 85 84	35, 41, 48, 55	0
1	L	211/211 (100%)	0.09	3 (1%) 78 76	34, 41, 48, 55	0
2	B	212/215 (98%)	0.02	1 (0%) 91 90	32, 42, 51, 58	0
2	H	212/215 (98%)	0.23	10 (4%) 35 30	30, 41, 50, 59	0
3	Q	115/123 (93%)	0.73	14 (12%) 5 3	30, 42, 51, 60	0
3	R	116/123 (94%)	0.58	10 (8%) 13 8	32, 42, 50, 65	0
All	All	1077/1098 (98%)	0.21	40 (3%) 45 39	30, 41, 50, 65	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	129	GLY	7.8
3	R	31	SER	5.9
3	Q	62	LYS	4.4
3	Q	59	SER	3.9
3	R	73	LYS	3.9
2	H	1	GLN	3.8
3	R	30	GLY	3.8
3	Q	61	ASN	3.7
2	H	127	GLY	3.7
2	H	167	SER	3.6
3	R	61	ASN	3.4
3	Q	31	SER	3.3
3	Q	46	LYS	3.3
3	Q	98	GLY	3.2
2	H	227	PRO	3.2
3	Q	60	HIS	3.2
3	R	123	ASN	3.1
1	L	1	ASP	3.0
3	Q	32	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
3	R	44	SER	2.8
3	Q	34	GLN	2.8
2	H	228	ARG	2.7
2	H	223	ILE	2.7
1	A	65	ASP	2.5
3	Q	65	TRP	2.5
3	Q	30	GLY	2.4
3	R	33	SER	2.4
3	Q	74	LEU	2.4
3	Q	63	ILE	2.3
3	R	81	THR	2.2
3	Q	44	SER	2.2
1	L	65	ASP	2.2
1	A	1	ASP	2.2
1	L	190	ASN	2.2
3	R	65	TRP	2.1
2	B	13	GLN	2.1
2	H	222	LYS	2.1
3	R	109	VAL	2.1
2	H	128	CYS	2.1
2	H	193	SER	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)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.