Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 08:41 PM JST

PDB ID	:	7BQ5
Title	:	ZIKV sE bound to mAb Z6
Authors	:	Dai, L.; Qi, J.; Gao, G.F.
Deposited on	:	2020-03-24
Resolution	:	2.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

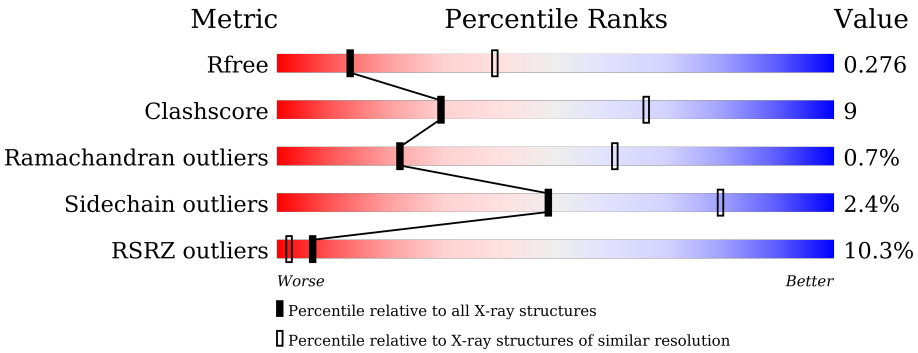
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	415	14% 76% 18% · 6%
1	B	415	13% 74% 19% · 6%
2	C	219	6% 70% 27% ·
2	H	219	6% 76% 21% ·
3	D	215	6% 73% 24% ··
3	L	215	7% 73% 24% ··

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12474 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 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			
1	B	390	Total	C	N	O	S	0	0	0
			2976	1861	519	571	25			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	410	HIS	-	expression tag	UNP A0A142I5B9
A	411	HIS	-	expression tag	UNP A0A142I5B9
A	412	HIS	-	expression tag	UNP A0A142I5B9
A	413	HIS	-	expression tag	UNP A0A142I5B9
A	414	HIS	-	expression tag	UNP A0A142I5B9
A	415	HIS	-	expression tag	UNP A0A142I5B9
B	410	HIS	-	expression tag	UNP A0A142I5B9
B	411	HIS	-	expression tag	UNP A0A142I5B9
B	412	HIS	-	expression tag	UNP A0A142I5B9
B	413	HIS	-	expression tag	UNP A0A142I5B9
B	414	HIS	-	expression tag	UNP A0A142I5B9
B	415	HIS	-	expression tag	UNP A0A142I5B9

- Molecule 2 is a protein called Z6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1637	1038	273	322	4			
2	C	218	Total	C	N	O	S	0	0	0
			1637	1038	273	322	4			

- Molecule 3 is a protein called Z6 Light Chain.

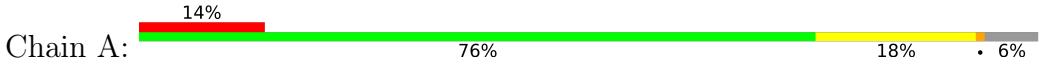
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1624	1025	270	325	4			
3	D	211	Total	C	N	O	S	0	0	0
			1624	1025	270	325	4			

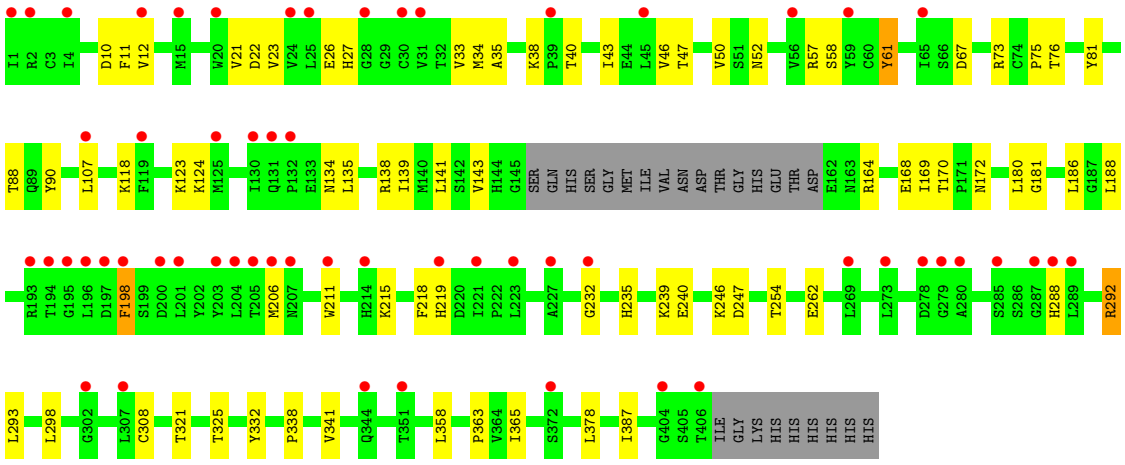
3 Residue-property plots (i)

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

• Molecule 1: envelope protein

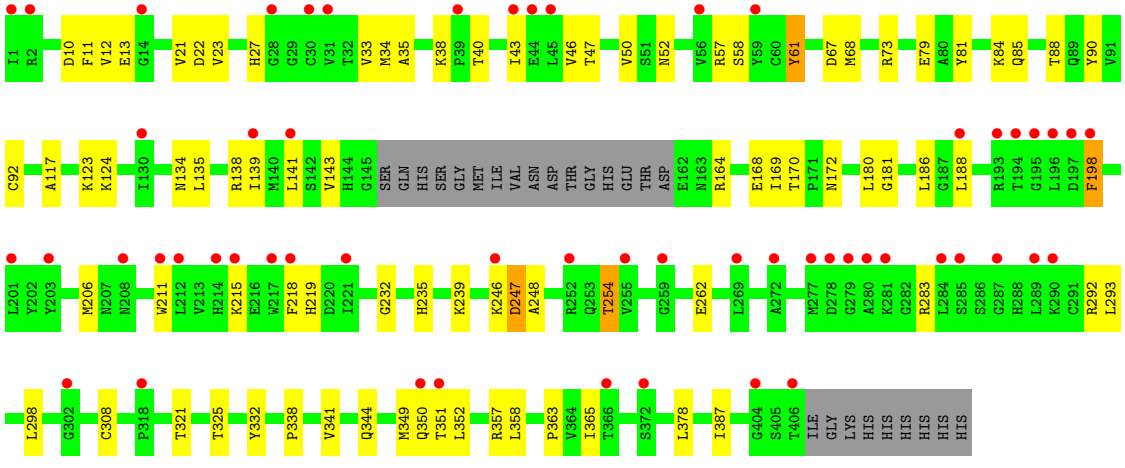
Chain A:



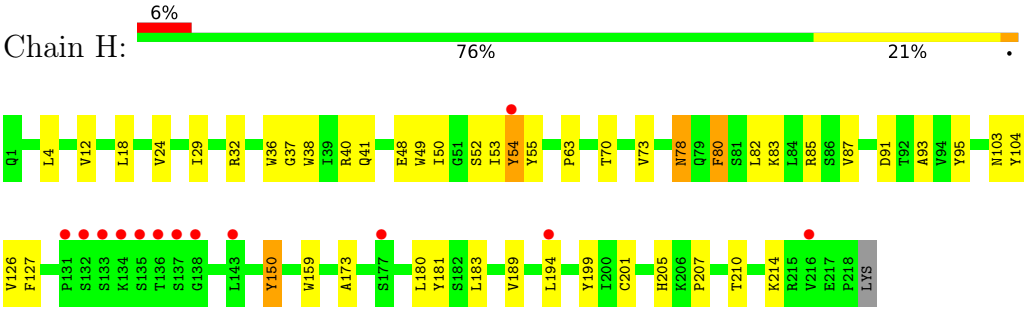


• Molecule 1: envelope protein

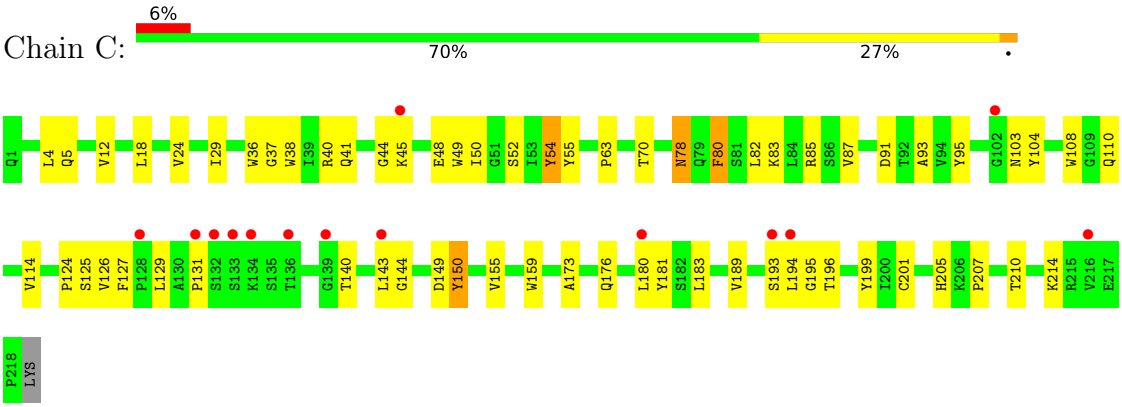
Chain B:



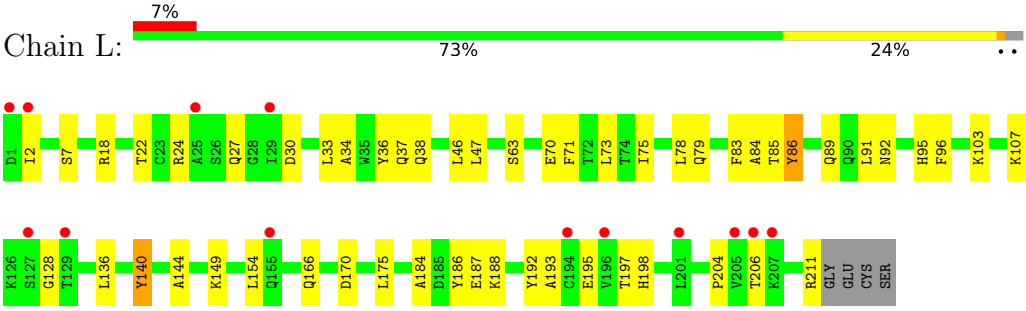
• Molecule 2: Z6 heavy chain



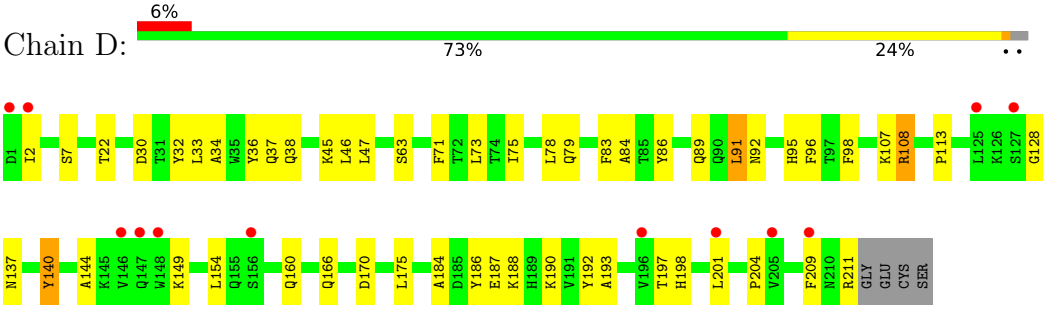
• Molecule 2: Z6 heavy chain



• Molecule 3: Z6 Light Chain



• Molecule 3: Z6 Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.25Å 153.67Å 115.20Å 90.00° 125.49° 90.00°	Depositor
Resolution (Å)	39.23 – 2.99 49.39 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.23-2.99) 98.9 (49.39-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.261 , 0.275 0.261 , 0.276	Depositor DCC
R_{free} test set	2264 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12474	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.26	0/3038	0.50	0/4114
1	B	0.26	0/3038	0.51	0/4114
2	C	0.27	0/1681	0.54	0/2297
2	H	0.27	0/1681	0.53	0/2297
3	D	0.26	0/1661	0.53	1/2258 (0.0%)
3	L	0.27	0/1661	0.52	0/2258
All	All	0.26	0/12760	0.52	1/17338 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	91	LEU	CA-CB-CG	5.34	127.58	115.30

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	2976	0	2917	42	0
1	B	2976	0	2917	46	0
2	C	1637	0	1590	52	0
2	H	1637	0	1590	38	0
3	D	1624	0	1582	38	0
3	L	1624	0	1582	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12474	0	12178	234	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 9.

All (234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:TYR:HE2	2:C:181:TYR:HB2	1.44	0.82
2:H:150:TYR:HE2	2:H:181:TYR:HB2	1.44	0.80
1:B:351:THR:HB	1:B:352:LEU:HB2	1.65	0.78
2:H:104:TYR:HD2	3:L:34:ALA:HB2	1.49	0.77
1:B:186:LEU:HD21	1:B:298:LEU:HD22	1.66	0.77
1:A:186:LEU:HD21	1:A:298:LEU:HD22	1.67	0.75
1:A:88:THR:O	1:A:239:LYS:NZ	2.19	0.74
1:A:47:THR:HB	1:A:138:ARG:HB2	1.70	0.73
1:B:47:THR:HB	1:B:138:ARG:HB2	1.73	0.71
1:B:88:THR:O	1:B:239:LYS:NZ	2.24	0.71
2:C:104:TYR:HD2	3:D:34:ALA:HB2	1.56	0.70
3:L:136:LEU:HB2	3:L:175:LEU:HB3	1.75	0.69
3:L:195:GLU:HG2	3:L:206:THR:HG22	1.76	0.68
1:A:206:MET:HB3	1:A:211:TRP:HZ3	1.59	0.67
1:B:206:MET:HB3	1:B:211:TRP:HZ3	1.58	0.67
3:D:149:LYS:HB2	3:D:193:ALA:HB3	1.75	0.67
1:A:138:ARG:HG2	1:A:168:GLU:HG2	1.76	0.67
1:B:138:ARG:HG2	1:B:168:GLU:HG2	1.76	0.67
3:D:108:ARG:NH1	3:D:170:ASP:O	2.29	0.66
2:C:103:ASN:HD21	3:D:32:TYR:HB3	1.60	0.66
2:H:93:ALA:HB3	2:H:95:TYR:HE1	1.62	0.64
2:C:24:VAL:HB	2:C:78:ASN:ND2	2.12	0.64
2:H:104:TYR:CD2	3:L:34:ALA:HB2	2.33	0.64
2:C:176:GLN:HB3	3:D:160:GLN:HE22	1.63	0.63
3:L:149:LYS:HZ2	3:L:154:LEU:HD21	1.64	0.62
3:D:136:LEU:HB2	3:D:175:LEU:HB3	1.82	0.62
2:H:36:TRP:HB3	2:H:80:PHE:CE1	2.35	0.62
2:C:36:TRP:HB3	2:C:80:PHE:CE1	2.34	0.62
3:D:149:LYS:HZ2	3:D:154:LEU:HD21	1.65	0.62
2:H:150:TYR:CE2	2:H:181:TYR:HB2	2.31	0.61
2:H:70:THR:OG1	2:H:85:ARG:NH2	2.33	0.61
2:C:149:ASP:OD1	2:C:176:GLN:NE2	2.32	0.61
2:C:150:TYR:CE2	2:C:181:TYR:HB2	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.66	0.60
2:C:104:TYR:CD2	3:D:34:ALA:HB2	2.35	0.60
3:L:187:GLU:HA	3:L:211:ARG:HH12	1.65	0.60
2:C:44:GLY:H	2:C:45:LYS:HA	1.65	0.60
2:H:205:HIS:CE1	2:H:207:PRO:HG2	2.37	0.59
2:C:205:HIS:CE1	2:C:207:PRO:HG2	2.37	0.59
2:H:24:VAL:HB	2:H:78:ASN:ND2	2.18	0.59
2:C:93:ALA:HB3	2:C:95:TYR:HE1	1.67	0.59
1:A:34:MET:HG2	1:A:40:THR:HG23	1.84	0.58
2:C:40:ARG:HB3	2:C:50:ILE:HD11	1.84	0.58
2:H:40:ARG:HB3	2:H:50:ILE:HD11	1.85	0.58
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.83	0.58
3:L:108:ARG:NH1	3:L:170:ASP:O	2.36	0.58
3:D:187:GLU:HA	3:D:211:ARG:HH12	1.69	0.58
3:D:144:ALA:HB2	3:D:198:HIS:HD2	1.68	0.58
1:B:246:LYS:HB3	1:B:254:THR:OG1	2.05	0.57
2:C:125:SER:HB3	2:C:127:PHE:HE1	1.69	0.57
1:A:246:LYS:HB3	1:A:254:THR:OG1	2.04	0.57
1:B:21:VAL:HG23	1:B:293:LEU:HG	1.85	0.57
1:B:34:MET:HG2	1:B:40:THR:HG23	1.88	0.56
2:H:205:HIS:HB3	2:H:210:THR:HB	1.87	0.56
1:A:215:LYS:O	1:A:219:HIS:ND1	2.38	0.56
2:C:70:THR:OG1	2:C:85:ARG:NH2	2.39	0.55
1:A:43:ILE:HG12	1:A:141:LEU:HG	1.88	0.55
3:L:2:ILE:HD11	3:L:92:ASN:HD22	1.73	0.54
2:C:5:GLN:HG3	2:C:110:GLN:HE22	1.72	0.54
2:C:29:ILE:HB	2:C:78:ASN:ND2	2.23	0.54
2:C:150:TYR:HE1	2:C:155:VAL:HG22	1.72	0.54
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.89	0.54
1:B:22:ASP:OD1	1:B:292:ARG:HG2	2.08	0.53
1:A:21:VAL:HG23	1:A:293:LEU:HG	1.90	0.53
2:C:44:GLY:N	2:C:45:LYS:HA	2.24	0.53
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.44	0.53
3:D:2:ILE:HD11	3:D:92:ASN:HD22	1.75	0.52
1:B:43:ILE:HG12	1:B:141:LEU:HG	1.92	0.52
2:C:150:TYR:O	2:C:180:LEU:HA	2.09	0.52
1:B:206:MET:HE2	1:B:262:GLU:HG3	1.91	0.52
1:A:206:MET:HE2	1:A:262:GLU:HG3	1.92	0.52
2:H:150:TYR:O	2:H:180:LEU:HA	2.09	0.52
1:B:141:LEU:HD11	1:B:188:LEU:HD11	1.92	0.51
1:B:215:LYS:O	1:B:219:HIS:ND1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:OE2	1:B:357:ARG:NH1	2.43	0.51
1:B:61:TYR:HE2	1:B:123:LYS:HB3	1.76	0.51
3:D:83:PHE:CD1	3:D:166:GLN:HB2	2.46	0.51
2:H:29:ILE:HG13	2:H:36:TRP:CE2	2.46	0.51
2:C:108:TRP:HZ2	3:D:36:TYR:HE2	1.58	0.51
1:A:50:VAL:HG12	1:A:135:LEU:HD23	1.92	0.50
3:L:107:LYS:HA	3:L:140:TYR:OH	2.10	0.50
2:C:205:HIS:HB3	2:C:210:THR:HB	1.93	0.50
1:B:84:LYS:HB3	1:B:90:TYR:CD2	2.45	0.50
3:L:149:LYS:HB2	3:L:193:ALA:HB3	1.92	0.50
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.94	0.50
3:L:83:PHE:CD1	3:L:166:GLN:HB2	2.47	0.49
3:D:107:LYS:HA	3:D:140:TYR:OH	2.11	0.49
2:C:54:TYR:HD2	2:C:55:TYR:H	1.60	0.49
3:D:37:GLN:O	3:D:45:LYS:N	2.44	0.49
3:L:36:TYR:CE1	3:L:46:LEU:HD23	2.47	0.49
1:B:12:VAL:HG21	1:B:23:VAL:HG12	1.94	0.49
2:C:41:GLN:HE22	3:D:38:GLN:HE22	1.60	0.49
2:C:4:LEU:HD22	2:C:24:VAL:HG22	1.94	0.49
2:C:37:GLY:HA2	2:C:52:SER:HA	1.95	0.49
3:D:7:SER:OG	3:D:22:THR:OG1	2.30	0.49
1:A:170:THR:HG22	1:A:172:ASN:H	1.78	0.49
2:H:54:TYR:HD2	2:H:55:TYR:H	1.61	0.49
3:L:186:TYR:HA	3:L:192:TYR:OH	2.13	0.48
3:D:84:ALA:HB3	3:D:86:TYR:HE1	1.78	0.48
2:C:129:LEU:HB2	2:C:144:GLY:HA3	1.95	0.48
1:B:358:LEU:HD22	1:B:378:LEU:HD22	1.95	0.48
1:B:50:VAL:HG12	1:B:135:LEU:HD23	1.95	0.48
2:H:103:ASN:HA	3:L:91:LEU:HD12	1.95	0.48
1:B:27:HIS:NE2	1:B:46:VAL:O	2.46	0.48
2:H:41:GLN:HE22	3:L:38:GLN:HE22	1.61	0.48
2:H:49:TRP:CD2	3:L:96:PHE:HB2	2.50	0.47
1:B:170:THR:HG22	1:B:172:ASN:H	1.79	0.47
3:L:78:LEU:HD23	3:L:79:GLN:N	2.29	0.47
3:L:84:ALA:HB3	3:L:86:TYR:HE1	1.79	0.47
2:C:12:VAL:HG21	2:C:18:LEU:HD13	1.97	0.47
1:A:341:VAL:HB	1:A:363:PRO:HG2	1.96	0.47
3:L:83:PHE:CE1	3:L:166:GLN:HB2	2.49	0.47
3:L:24:ARG:HG2	3:L:70:GLU:HG2	1.97	0.47
3:D:36:TYR:CE1	3:D:46:LEU:HD23	2.49	0.47
3:D:83:PHE:CE1	3:D:166:GLN:HB2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:TYR:HA	3:D:192:TYR:OH	2.14	0.47
1:B:52:ASN:O	1:B:134:ASN:ND2	2.48	0.47
1:B:344:GLN:NE2	1:B:352:LEU:O	2.47	0.47
2:C:40:ARG:HG2	2:C:48:GLU:HB3	1.97	0.47
2:H:40:ARG:HG2	2:H:48:GLU:HB3	1.97	0.47
1:B:57:ARG:HB2	1:B:218:PHE:CE2	2.49	0.47
1:A:27:HIS:NE2	1:A:46:VAL:O	2.48	0.47
1:A:75:PRO:O	1:A:76:THR:OG1	2.31	0.46
2:H:12:VAL:HG21	2:H:18:LEU:HD13	1.97	0.46
2:H:87:VAL:HG13	2:H:91:ASP:HB2	1.98	0.46
3:L:84:ALA:HB3	3:L:86:TYR:CE1	2.50	0.46
2:C:29:ILE:HG21	2:C:78:ASN:HA	1.97	0.46
2:C:194:LEU:HA	2:C:195:GLY:HA2	1.48	0.46
2:H:53:ILE:HD13	2:H:73:VAL:HG23	1.98	0.46
2:H:125:SER:HB3	2:H:127:PHE:HE1	1.79	0.46
3:D:78:LEU:HD23	3:D:79:GLN:N	2.30	0.46
3:L:7:SER:OG	3:L:22:THR:OG1	2.28	0.46
3:L:197:THR:HG22	3:L:204:PRO:HG3	1.96	0.46
1:B:61:TYR:HE2	1:B:123:LYS:CB	2.29	0.46
3:D:84:ALA:HB3	3:D:86:TYR:CE1	2.51	0.46
1:B:85:GLN:HA	1:B:92:CYS:SG	2.56	0.45
1:A:141:LEU:HD11	1:A:188:LEU:HD11	1.97	0.45
1:A:139:ILE:HD12	1:A:169:ILE:HD12	1.99	0.45
2:C:131:PRO:HD3	2:C:143:LEU:HD23	1.99	0.45
1:B:308:CYS:HB3	1:B:332:TYR:CE1	2.52	0.45
2:H:29:ILE:HB	2:H:78:ASN:ND2	2.31	0.45
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.98	0.45
1:A:198:PHE:N	1:A:198:PHE:CD1	2.85	0.44
1:A:321:THR:OG1	1:A:325:THR:OG1	2.30	0.44
2:H:82:LEU:HD23	2:H:83:LYS:N	2.31	0.44
1:A:57:ARG:HB3	1:A:218:PHE:CE2	2.53	0.44
1:B:341:VAL:HB	1:B:363:PRO:HG2	1.98	0.44
2:C:82:LEU:HD23	2:C:83:LYS:N	2.33	0.44
1:A:90:TYR:CZ	1:A:118:LYS:HB2	2.52	0.44
2:H:38:TRP:CD2	2:H:82:LEU:HD12	2.52	0.44
2:C:103:ASN:HB3	2:C:104:TYR:CE1	2.52	0.44
1:A:61:TYR:HE2	1:A:123:LYS:CB	2.31	0.44
2:H:37:GLY:HA2	2:H:52:SER:HA	2.00	0.44
3:D:197:THR:HG22	3:D:204:PRO:HG3	1.99	0.44
2:C:87:VAL:HG13	2:C:91:ASP:HB2	1.99	0.44
3:L:33:LEU:HD22	3:L:89:GLN:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:GLN:NE2	2:C:45:LYS:HG2	2.33	0.44
1:A:22:ASP:OD1	1:A:292:ARG:HG3	2.18	0.44
2:H:173:ALA:HA	2:H:183:LEU:HB3	2.00	0.44
2:H:126:VAL:HG12	2:H:214:LYS:HG3	1.99	0.43
1:B:35:ALA:HB3	1:B:38:LYS:HG3	1.99	0.43
2:C:49:TRP:CD2	3:D:96:PHE:HB2	2.52	0.43
1:A:338:PRO:HA	1:A:365:ILE:O	2.18	0.43
1:A:358:LEU:HD22	1:A:378:LEU:HD22	1.99	0.43
3:D:63:SER:O	3:D:73:LEU:HD12	2.18	0.43
1:A:35:ALA:HB3	1:A:38:LYS:HG3	2.01	0.43
2:C:40:ARG:NH2	2:C:91:ASP:HA	2.34	0.43
1:B:349:MET:HA	1:B:352:LEU:HD12	1.99	0.43
2:C:63:PRO:HD2	3:D:95:HIS:CD2	2.53	0.43
2:C:124:PRO:HB3	2:C:150:TYR:HB3	2.00	0.43
2:C:173:ALA:HA	2:C:183:LEU:HB3	2.01	0.43
1:A:10:ASP:C	1:A:11:PHE:HD1	2.22	0.43
1:A:61:TYR:HE2	1:A:123:LYS:HB2	1.83	0.43
3:L:63:SER:O	3:L:73:LEU:HD12	2.19	0.43
2:H:32:ARG:HG2	2:H:54:TYR:OH	2.19	0.43
3:D:75:ILE:HD11	3:D:86:TYR:CE2	2.53	0.43
3:D:184:ALA:O	3:D:188:LYS:HG3	2.19	0.43
1:A:12:VAL:HG21	1:A:23:VAL:HG12	1.99	0.43
1:B:10:ASP:C	1:B:11:PHE:HD1	2.22	0.43
2:C:126:VAL:HG12	2:C:214:LYS:HG3	2.01	0.42
1:A:143:VAL:HG23	1:A:180:LEU:HD13	2.01	0.42
1:B:143:VAL:HG23	1:B:180:LEU:HD13	2.00	0.42
2:C:41:GLN:NE2	3:D:38:GLN:HE22	2.16	0.42
2:H:150:TYR:O	2:H:150:TYR:HD2	2.03	0.42
1:B:88:THR:HB	1:B:235:HIS:CE1	2.53	0.42
2:C:18:LEU:HD22	2:C:114:VAL:HG11	2.00	0.42
3:D:33:LEU:HD22	3:D:89:GLN:O	2.20	0.42
3:L:144:ALA:HB2	3:L:198:HIS:CD2	2.50	0.42
3:D:190:LYS:HG2	3:D:211:ARG:HH21	1.84	0.42
1:A:107:LEU:HD21	3:L:91:LEU:O	2.19	0.42
2:H:159:TRP:CH2	2:H:201:CYS:HB3	2.55	0.42
1:B:338:PRO:HA	1:B:365:ILE:O	2.18	0.42
2:C:54:TYR:HD2	2:C:55:TYR:N	2.18	0.42
1:B:58:SER:OG	1:B:124:LYS:HD3	2.20	0.42
2:C:38:TRP:CD2	2:C:82:LEU:HD12	2.55	0.42
2:C:193:SER:O	2:C:196:THR:N	2.53	0.42
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD12	1:A:387:ILE:HG12	2.00	0.42
3:L:85:THR:HG22	3:L:103:LYS:HA	2.02	0.42
2:H:189:VAL:HG11	2:H:199:TYR:CE1	2.55	0.42
3:L:27:GLN:HB3	1:B:79:GLU:HG3	2.02	0.42
3:L:184:ALA:O	3:L:188:LYS:HG3	2.20	0.42
1:A:246:LYS:HG2	1:A:247:ASP:H	1.85	0.41
2:H:108:TRP:HZ2	3:L:36:TYR:HE2	1.67	0.41
1:B:198:PHE:N	1:B:198:PHE:CD1	2.87	0.41
2:C:108:TRP:HZ2	3:D:36:TYR:CE2	2.37	0.41
1:A:88:THR:HB	1:A:235:HIS:CE1	2.55	0.41
2:H:40:ARG:NH2	2:H:91:ASP:HA	2.36	0.41
3:D:113:PRO:HG2	3:D:201:LEU:HD11	2.02	0.41
1:B:68:MET:HG2	1:B:117:ALA:HB2	2.02	0.41
2:H:63:PRO:HD2	3:L:95:HIS:CD2	2.55	0.41
1:B:247:ASP:OD1	1:B:248:ALA:N	2.54	0.41
2:C:189:VAL:HG11	2:C:199:TYR:CE1	2.55	0.41
2:H:41:GLN:NE2	3:L:38:GLN:HE22	2.18	0.41
3:L:136:LEU:HD13	3:L:175:LEU:HD12	2.02	0.41
1:B:139:ILE:HD12	1:B:169:ILE:HD12	2.02	0.41
1:B:321:THR:OG1	1:B:325:THR:OG1	2.27	0.41
1:A:26:GLU:OE1	1:A:288:HIS:ND1	2.53	0.41
3:D:86:TYR:N	3:D:86:TYR:CD1	2.89	0.41
1:A:52:ASN:O	1:A:134:ASN:ND2	2.54	0.40
1:A:240:GLU:CD	1:A:240:GLU:H	2.24	0.40
2:C:41:GLN:HE22	3:D:38:GLN:NE2	2.18	0.40
2:C:159:TRP:CH2	2:C:201:CYS:HB3	2.55	0.40
1:A:43:ILE:HD12	1:A:293:LEU:HD22	2.04	0.40
1:B:350:GLN:HA	1:B:351:THR:HG23	2.02	0.40
1:B:378:LEU:HD12	1:B:387:ILE:HG12	2.03	0.40
1:A:33:VAL:O	1:A:40:THR:HA	2.21	0.40
1:A:58:SER:OG	1:A:124:LYS:HD3	2.20	0.40
2:C:80:PHE:N	2:C:80:PHE:CD2	2.87	0.40
3:L:2:ILE:CD1	3:L:92:ASN:HD22	2.34	0.40
3:L:75:ILE:HD11	3:L:86:TYR:CE2	2.56	0.40
3:L:86:TYR:N	3:L:86:TYR:CD1	2.89	0.40
1:B:33:VAL:O	1:B:40:THR:HA	2.21	0.40
3:D:98:PHE:N	3:D:98:PHE:CD1	2.90	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	386/415 (93%)	360 (93%)	23 (6%)	3 (1%)	19	57
1	B	386/415 (93%)	358 (93%)	24 (6%)	4 (1%)	15	53
2	C	216/219 (99%)	198 (92%)	18 (8%)	0	100	100
2	H	216/219 (99%)	198 (92%)	18 (8%)	0	100	100
3	D	209/215 (97%)	198 (95%)	9 (4%)	2 (1%)	15	53
3	L	209/215 (97%)	195 (93%)	12 (6%)	2 (1%)	15	53
All	All	1622/1698 (96%)	1507 (93%)	104 (6%)	11 (1%)	22	60

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	ASP
1	A	67	ASP
1	A	181	GLY
1	A	232	GLY
3	L	30	ASP
1	B	67	ASP
1	B	181	GLY
1	B	232	GLY
3	D	30	ASP
3	L	128	GLY
3	D	128	GLY

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	325/347 (94%)	319 (98%)	6 (2%)	59 85
1	B	325/347 (94%)	318 (98%)	7 (2%)	52 81
2	C	185/188 (98%)	180 (97%)	5 (3%)	44 77
2	H	185/188 (98%)	180 (97%)	5 (3%)	44 77
3	D	184/188 (98%)	178 (97%)	6 (3%)	38 73
3	L	184/188 (98%)	179 (97%)	5 (3%)	44 77
All	All	1388/1446 (96%)	1354 (98%)	34 (2%)	49 79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	TYR
1	A	73	ARG
1	A	81	TYR
1	A	164	ARG
1	A	198	PHE
1	A	292	ARG
2	H	54	TYR
2	H	78	ASN
2	H	80	PHE
2	H	150	TYR
2	H	194	LEU
3	L	18	ARG
3	L	71	PHE
3	L	86	TYR
3	L	108	ARG
3	L	140	TYR
1	B	61	TYR
1	B	73	ARG
1	B	81	TYR
1	B	164	ARG
1	B	198	PHE
1	B	254	THR
1	B	283	ARG
2	C	54	TYR
2	C	78	ASN
2	C	80	PHE
2	C	140	THR
2	C	150	TYR
3	D	71	PHE
3	D	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	108	ARG
3	D	137	ASN
3	D	140	TYR
3	D	209	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
3	L	38	GLN
1	B	266	HIS
2	C	41	GLN
2	C	78	ASN
3	D	38	GLN
3	D	160	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 monosaccharides 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 (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^{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	390/415 (93%)	1.01	58 (14%) 2 1	37, 95, 171, 249	0
1	B	390/415 (93%)	1.00	56 (14%) 2 1	38, 100, 167, 240	0
2	C	218/219 (99%)	0.64	14 (6%) 19 6	25, 59, 129, 202	0
2	H	218/219 (99%)	0.64	13 (5%) 21 7	25, 60, 129, 216	0
3	D	211/215 (98%)	0.59	13 (6%) 20 7	28, 71, 134, 189	0
3	L	211/215 (98%)	0.59	15 (7%) 16 5	28, 74, 137, 196	0
All	All	1638/1698 (96%)	0.80	169 (10%) 6 2	25, 81, 157, 249	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	ASP	14.5
1	A	302	GLY	13.6
3	L	1	ASP	11.8
1	B	279	GLY	11.2
1	B	280	ALA	9.2
1	B	302	GLY	9.1
1	B	194	THR	8.9
1	A	198	PHE	8.8
1	A	196	LEU	8.3
1	A	194	THR	8.3
1	A	195	GLY	8.2
1	A	278	ASP	8.1
1	B	196	LEU	7.9
1	A	279	GLY	7.8
1	B	195	GLY	7.2
2	C	132	SER	6.9
2	H	132	SER	6.8
1	A	280	ALA	6.5
1	A	201	LEU	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	134	LYS	6.2
1	A	197	ASP	6.1
3	D	1	ASP	6.0
1	B	406	THR	6.0
1	B	198	PHE	5.8
1	A	130	ILE	5.8
3	D	2	ILE	5.8
2	C	216	VAL	5.3
1	A	406	THR	5.2
1	B	193	ARG	5.2
2	C	133	SER	5.1
1	B	277	MET	5.1
1	A	289	LEU	4.9
2	C	136	THR	4.7
1	B	287	GLY	4.6
1	B	197	ASP	4.5
1	A	214	HIS	4.4
1	B	255	VAL	4.1
1	B	2	ARG	4.1
2	H	133	SER	4.1
1	B	281	LYS	4.1
1	B	201	LEU	4.0
1	B	259	GLY	3.9
1	A	232	GLY	3.9
3	D	196	VAL	3.8
1	B	269	LEU	3.8
2	C	131	PRO	3.8
3	L	2	ILE	3.8
1	B	221	ILE	3.8
1	B	130	ILE	3.8
2	C	134	LYS	3.7
1	B	285	SER	3.7
3	L	155	GLN	3.7
1	B	1	ILE	3.7
1	B	404	GLY	3.7
3	D	201	LEU	3.7
2	H	143	LEU	3.6
2	C	143	LEU	3.5
3	D	205	VAL	3.5
1	B	208	ASN	3.4
1	A	59	TYR	3.4
1	A	285	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	216	VAL	3.2
1	B	31	VAL	3.2
1	B	217	TRP	3.2
1	A	45	LEU	3.2
1	B	14	GLY	3.2
1	A	2	ARG	3.1
2	H	137	SER	3.1
1	A	30	CYS	3.1
1	A	31	VAL	3.0
1	B	350	GLN	3.0
1	A	25	LEU	3.0
1	A	206	MET	3.0
1	A	125	MET	3.0
2	H	131	PRO	3.0
1	B	214	HIS	3.0
2	C	180	LEU	2.9
1	A	205	THR	2.9
1	A	221	ILE	2.9
3	L	29	ILE	2.9
1	B	45	LEU	2.9
2	H	136	THR	2.8
1	A	15	MET	2.8
1	B	289	LEU	2.8
1	A	207	ASN	2.8
1	B	139	ILE	2.8
3	L	196	VAL	2.8
1	A	4	ILE	2.8
1	A	20	TRP	2.8
1	B	372	SER	2.8
3	L	125	LEU	2.8
1	A	372	SER	2.7
1	A	56	VAL	2.7
1	A	203	TYR	2.7
2	C	102	GLY	2.7
3	L	207	LYS	2.7
1	A	24	VAL	2.7
1	A	219	HIS	2.7
1	A	193	ARG	2.6
1	A	227	ALA	2.6
3	L	201	LEU	2.6
1	B	252	ARG	2.6
1	A	269	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	127	SER	2.6
1	A	119	PHE	2.6
2	C	139	GLY	2.5
3	L	129	THR	2.5
1	A	28	GLY	2.5
2	H	135	SER	2.5
3	L	205	VAL	2.5
3	L	206	THR	2.5
1	B	59	TYR	2.5
1	A	287	GLY	2.4
1	B	211	TRP	2.4
1	B	215	LYS	2.4
3	L	194	CYS	2.4
1	A	12	VAL	2.4
3	D	147	GLN	2.4
1	B	188	LEU	2.4
3	D	127	SER	2.4
1	B	30	CYS	2.4
1	B	246	LYS	2.4
1	B	318	PRO	2.4
1	A	273	LEU	2.4
1	A	404	GLY	2.4
1	B	284	LEU	2.4
1	B	290	LYS	2.3
1	B	272	ALA	2.3
1	B	212	LEU	2.3
1	B	39	PRO	2.3
1	B	366	THR	2.3
3	D	148	TRP	2.3
1	B	141	LEU	2.3
2	C	194	LEU	2.3
3	D	125	LEU	2.3
1	A	65	ILE	2.3
3	D	133	VAL	2.3
1	A	39	PRO	2.3
1	B	28	GLY	2.3
3	L	121	SER	2.2
1	A	132	PRO	2.2
1	B	56	VAL	2.2
2	C	128	PRO	2.2
2	H	138	GLY	2.2
3	D	146	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	2.2
2	C	193	SER	2.2
1	A	351	THR	2.2
1	A	107	LEU	2.2
1	A	131	GLN	2.2
1	A	223	LEU	2.1
1	B	203	TYR	2.1
1	A	211	TRP	2.1
1	B	44	GLU	2.1
3	D	156	SER	2.1
1	A	307	LEU	2.1
1	B	43	ILE	2.1
3	D	209	PHE	2.1
2	C	45	LYS	2.1
3	L	25	ALA	2.1
1	A	204	LEU	2.1
2	H	177	SER	2.1
1	A	344	GLN	2.0
2	H	194	LEU	2.0
2	H	54	TYR	2.0
1	B	218	PHE	2.0
1	A	1	ILE	2.0
1	A	200	ASP	2.0
1	A	288	HIS	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 monosaccharides 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.