Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 05:12 PM EDT

PDB ID	:	8TFN
Title	:	Structure of anti-TCRvbeta6-5 antibody in complex with the cognate TCR
Authors	:	Katragadda, M.; Servatalab, R.; Wirth, J.
Deposited on	:	2023-07-11
Resolution	:	2.54 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:

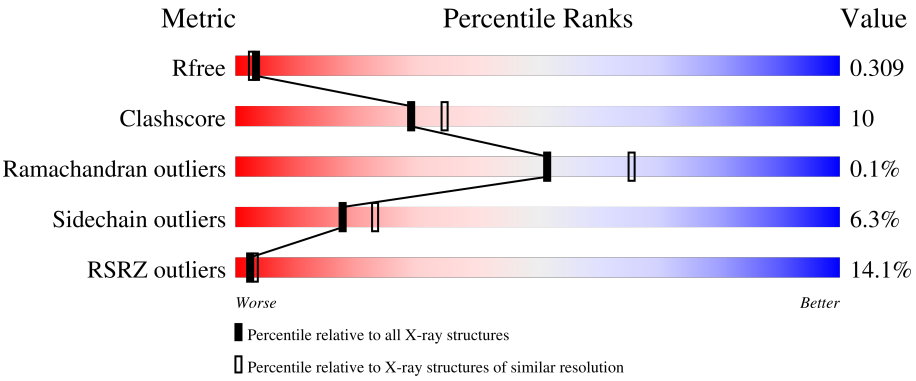
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	204	10% 78% 18%
2	B	242	3% 76% 21%
3	H	225	22% 59% 28% 12%
4	L	214	19% 65% 26% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6387 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 TRAV12-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1528	951	248	320	9			

- Molecule 2 is a protein called TRBV6-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	0	1	0
			1899	1195	332	364	8			

- Molecule 3 is a protein called Anti-TCRVb6-5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	197	Total	C	N	O	S	0	0	0
			1448	910	242	290	6			

- Molecule 4 is a protein called Anti-TCRVb6-5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	199	Total	C	N	O	S	0	0	0
			1502	941	256	300	5			

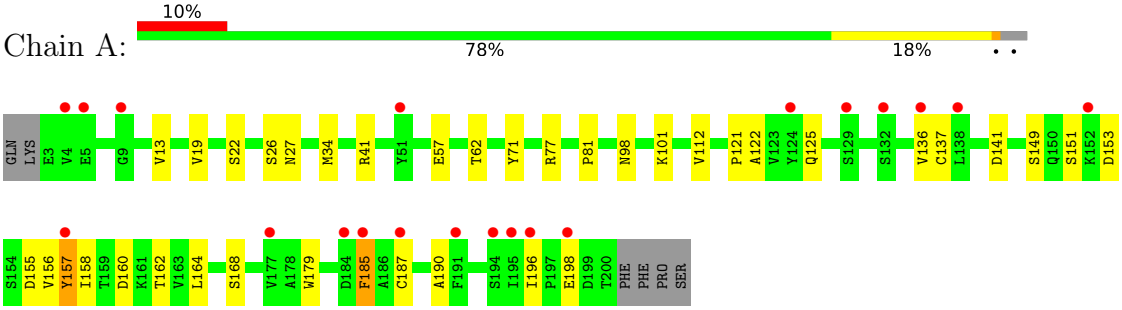
- Molecule 5 is water.

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

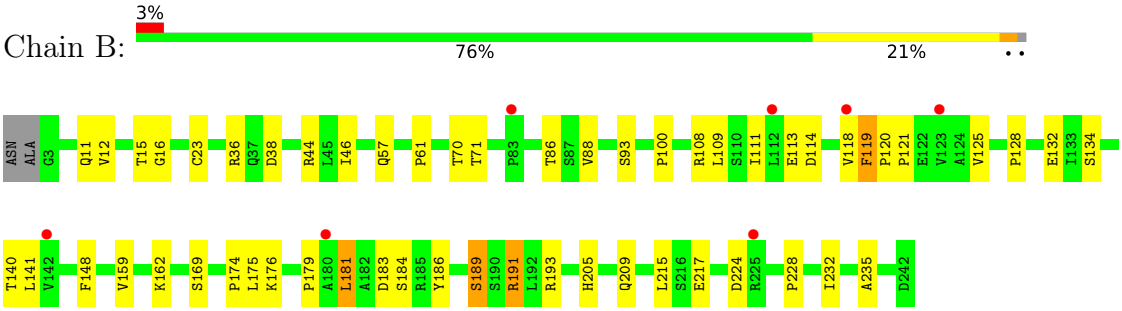
3 Residue-property plots

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.

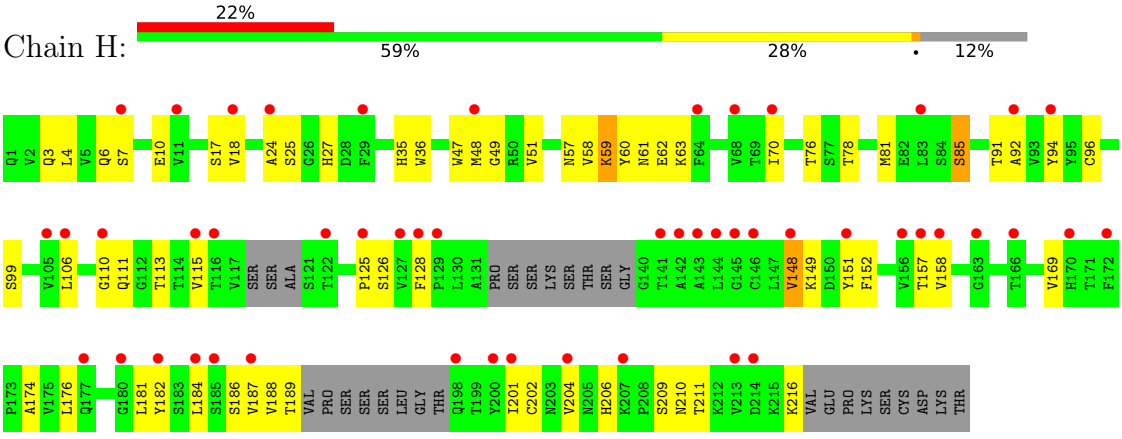
• Molecule 1: TRAV12-3



• Molecule 2: TRBV6-5

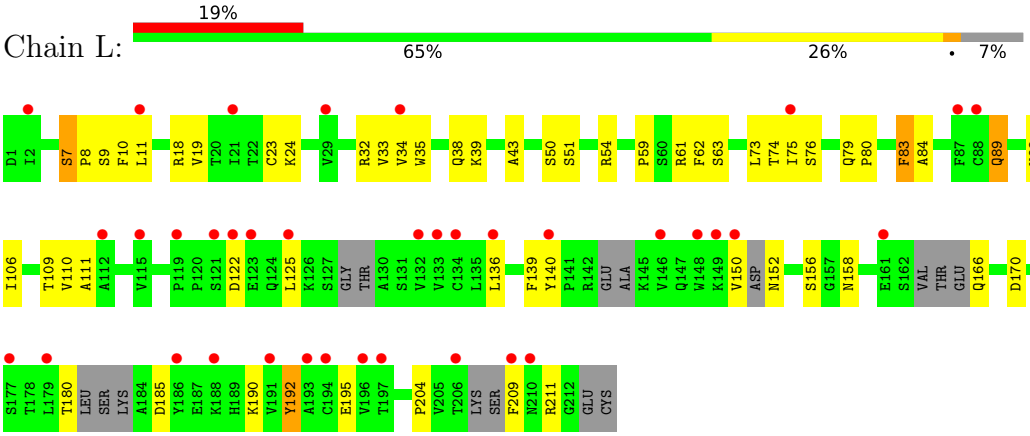


• Molecule 3: Anti-TCRVb6-5 Fab heavy chain



• Molecule 4: Anti-TCRVb6-5 Fab light chain

Chain L:


19%
65%
26%
7%
D1 I2 S7 P8 S9 F10 L11 R18 V19 T20 I21 T22 C23 K24 V29 R32 V33 V34 W35 Q38 K39 A43 S50 S51 R54 P59 S60 R61 F62 S63 L73 T74 I75 S76 Q79 P80 F83 A84 F87 C88 Q89 K92 K103 L104 E105
I106 T109 V110 A111 A112 V115 P119 P120 S121 D122 E123 Q124 L125 K126 S127 GLY THR A130 S131 V132 V133 C134 L135 L136 F139 Y140 P141 R142 GLU ALA K145 V146 Q147 W148 K149 V150 ASP N152 S156 G157 N158 E161 S162 VAL THR GLU Q166 D170 Y173 S174 L175 S176
S177 T178 L179 T180 LEU SER LYS A184 D185 Y186 E187 K188 H189 K190 V191 Y192 A193 C194 E195 V196 T197 P204 V205 T206 LYS SER F209 N210 R211 G212 GLU CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 2	Depositor
Cell constants a, b, c, α, β, γ	64.59Å 118.86Å 173.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.51 – 2.54 86.51 – 2.47	Depositor EDS
% Data completeness (in resolution range)	78.8 (86.51-2.54) 78.8 (86.51-2.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.93 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.245 , 0.294 0.261 , 0.309	Depositor DCC
R_{free} test set	1946 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	81.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6387	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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	0.27	0/1560	0.53	0/2115
2	B	0.26	0/1955	0.53	0/2663
3	H	0.28	0/1478	0.57	0/2013
4	L	0.27	0/1531	0.54	0/2073
All	All	0.27	0/6524	0.54	0/8864

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	1528	0	1444	21	0
2	B	1899	0	1804	29	0
3	H	1448	0	1363	42	0
4	L	1502	0	1411	34	0
5	A	6	0	0	0	0
5	B	2	0	0	0	0
5	H	1	0	0	0	0
5	L	1	0	0	0	0
All	All	6387	0	6022	119	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 10.

All (119) 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:B:86:THR:HG22	2:B:111:ILE:H	1.35	0.91
1:A:164:LEU:HB3	2:B:169:SER:HB2	1.60	0.83
3:H:148:VAL:HB	3:H:149:LYS:HA	1.61	0.81
2:B:120:PRO:HD3	2:B:228:PRO:HB3	1.65	0.78
1:A:121:PRO:HB2	1:A:198:GLU:HG3	1.69	0.74
1:A:185:PHE:CE1	1:A:190:ALA:HB2	2.26	0.70
3:H:99:SER:HB3	3:H:106:LEU:H	1.56	0.67
3:H:128:PHE:CD2	3:H:148:VAL:HG21	2.30	0.67
3:H:51:VAL:HG23	3:H:58:VAL:HG12	1.77	0.66
4:L:18:ARG:HG2	4:L:76:SER:HB2	1.75	0.66
2:B:176:LYS:HD2	2:B:179:PRO:HA	1.78	0.66
4:L:33:VAL:HG22	4:L:51:SER:HB2	1.79	0.64
3:H:6:GLN:H	3:H:111:GLN:HE22	1.46	0.64
1:A:185:PHE:HE1	1:A:190:ALA:HB2	1.62	0.64
2:B:215:LEU:HD12	2:B:228:PRO:HD2	1.80	0.63
3:H:111:GLN:OE1	3:H:111:GLN:N	2.26	0.63
3:H:76:THR:HG23	3:H:78:THR:HG22	1.81	0.62
3:H:169:VAL:HA	3:H:188:VAL:HA	1.81	0.61
1:A:62:THR:OG1	1:A:77:ARG:NH2	2.35	0.60
4:L:195:GLU:OE2	4:L:204:PRO:HB3	2.02	0.59
4:L:10:PHE:HD2	4:L:103:LYS:H	1.51	0.58
3:H:152:PHE:HB2	3:H:181:LEU:HD23	1.86	0.58
1:A:121:PRO:HG3	1:A:196:ILE:HD11	1.85	0.58
4:L:158:ASN:ND2	4:L:180:THR:O	2.37	0.57
2:B:88:VAL:HG22	2:B:108:ARG:HG3	1.85	0.57
1:A:125:GLN:HB2	1:A:187:CYS:HB3	1.87	0.57
1:A:13:VAL:HG11	1:A:19:VAL:HG22	1.87	0.56
3:H:125:PRO:HB3	3:H:151:TYR:HD2	1.70	0.56
4:L:79:GLN:HG2	4:L:80:PRO:HD2	1.87	0.56
1:A:136:VAL:HG12	1:A:179:TRP:HB3	1.86	0.55
2:B:121:PRO:HB3	2:B:148:PHE:HB3	1.88	0.55
1:A:153:ASP:HB2	1:A:156:VAL:HG12	1.89	0.55
2:B:36:ARG:HB3	2:B:46:ILE:HD11	1.89	0.55
1:A:151:SER:HB3	1:A:158:ILE:HD12	1.88	0.55
4:L:34:VAL:HB	4:L:89:GLN:HG2	1.89	0.55
4:L:170:ASP:N	4:L:170:ASP:OD1	2.40	0.55
2:B:189:SER:OG	2:B:191:ARG:NH2	2.40	0.55
3:H:48:MET:HA	3:H:61:ASN:HB2	1.89	0.55
3:H:6:GLN:H	3:H:111:GLN:NE2	2.04	0.54
3:H:201:ILE:HG12	3:H:216:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLY:O	4:L:32:ARG:NH2	2.41	0.54
2:B:38:ASP:OD2	2:B:44:ARG:NH2	2.40	0.54
3:H:92:ALA:HB3	3:H:94:TYR:HE1	1.73	0.54
1:A:122:ALA:HA	1:A:198:GLU:HB3	1.90	0.54
2:B:125:VAL:HG23	2:B:235:ALA:HB3	1.89	0.54
3:H:174:ALA:HA	3:H:184:LEU:HB3	1.89	0.53
4:L:111:ALA:HB3	4:L:140:TYR:H	1.72	0.53
3:H:158:VAL:HG21	3:H:186:SER:HB2	1.91	0.52
2:B:128:PRO:HD3	2:B:141:LEU:HG	1.91	0.52
3:H:148:VAL:HB	3:H:149:LYS:CA	2.36	0.52
4:L:80:PRO:O	4:L:83:PHE:HB2	2.09	0.52
4:L:75:ILE:O	4:L:75:ILE:HG13	2.09	0.51
3:H:36:TRP:CD1	3:H:70:ILE:HD12	2.45	0.51
2:B:12:VAL:HG11	2:B:118:VAL:HG21	1.92	0.51
1:A:137:CYS:SG	1:A:187:CYS:HA	2.51	0.50
4:L:59:PRO:HB2	4:L:61:ARG:HG2	1.93	0.50
3:H:3:GLN:HG2	3:H:25:SER:HB3	1.94	0.50
3:H:111:GLN:HA	4:L:43:ALA:HB2	1.93	0.50
3:H:57:ASN:HD21	3:H:59:LYS:NZ	2.10	0.50
3:H:126:SER:O	3:H:148:VAL:HG23	2.13	0.49
4:L:83:PHE:CZ	4:L:106:ILE:HG13	2.48	0.49
4:L:136:LEU:HA	4:L:136:LEU:HD12	1.67	0.49
1:A:34:MET:HG2	2:B:100:PRO:HB3	1.94	0.48
4:L:7:SER:HA	4:L:9:SER:H	1.78	0.48
4:L:166:GLN:NE2	4:L:173:TYR:CZ	2.81	0.48
2:B:132:GLU:OE2	2:B:140:THR:OG1	2.25	0.48
3:H:85:SER:O	3:H:85:SER:OG	2.29	0.48
3:H:6:GLN:HE21	3:H:110:GLY:HA3	1.79	0.47
3:H:151:TYR:CE1	3:H:182:TYR:HB2	2.49	0.47
3:H:6:GLN:HG2	3:H:96:CYS:SG	2.55	0.47
3:H:6:GLN:NE2	3:H:96:CYS:H	2.12	0.47
1:A:81:PRO:HA	1:A:112:VAL:HB	1.96	0.47
3:H:176:LEU:HD23	3:H:182:TYR:CE2	2.49	0.47
1:A:22:SER:HB2	1:A:71:TYR:CE1	2.49	0.47
3:H:158:VAL:HG12	3:H:204:VAL:HG13	1.95	0.47
4:L:23:CYS:HB2	4:L:35:TRP:CH2	2.50	0.47
4:L:122:ASP:HA	4:L:125:LEU:HB2	1.96	0.47
4:L:35:TRP:CD2	4:L:73:LEU:HD12	2.50	0.46
2:B:15:THR:HG23	2:B:113:GLU:HA	1.97	0.46
4:L:24:LYS:HE3	4:L:24:LYS:HB3	1.65	0.46
3:H:10:GLU:HB2	3:H:115:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:OD1	1:A:101:LYS:NZ	2.49	0.45
1:A:141:ASP:OD1	2:B:193:ARG:NH1	2.44	0.45
2:B:181:LEU:HB2	2:B:184:SER:HB2	1.98	0.45
3:H:17:SER:OG	3:H:18:VAL:N	2.49	0.45
3:H:49:GLY:HA2	3:H:60:TYR:HA	1.97	0.45
3:H:35:HIS:HB3	3:H:47:TRP:HE1	1.81	0.45
2:B:159:VAL:HA	2:B:205:HIS:O	2.16	0.45
1:A:157:TYR:HB2	2:B:175:LEU:HD13	1.97	0.45
4:L:54:ARG:NH1	4:L:62:PHE:O	2.49	0.45
3:H:61:ASN:OD1	3:H:62:GLU:N	2.50	0.45
3:H:125:PRO:HD3	3:H:206:HIS:HD2	1.82	0.44
3:H:63:LYS:N	3:H:63:LYS:HD2	2.32	0.44
4:L:190:LYS:HA	4:L:211:ARG:HG3	1.99	0.44
1:A:162:THR:HG21	2:B:191:ARG:NH1	2.33	0.43
4:L:150:VAL:O	4:L:152:ASN:N	2.51	0.43
4:L:192:TYR:HD2	4:L:209:PHE:CZ	2.37	0.43
4:L:8:PRO:C	4:L:9:SER:HG	2.22	0.42
3:H:125:PRO:HB3	3:H:151:TYR:CD2	2.51	0.42
3:H:209:SER:OG	3:H:211:THR:OG1	2.34	0.42
4:L:111:ALA:HB3	4:L:140:TYR:N	2.34	0.42
4:L:38:GLN:O	4:L:84:ALA:HB1	2.20	0.42
2:B:109:LEU:HA	2:B:109:LEU:HD12	1.81	0.41
2:B:209:GLN:HG3	2:B:232:ILE:HG23	2.02	0.41
3:H:57:ASN:ND2	3:H:59:LYS:NZ	2.68	0.41
3:H:60:TYR:CE1	3:H:70:ILE:HG12	2.55	0.41
2:B:119:PHE:HD1	2:B:119:PHE:HA	1.78	0.41
2:B:57:GLN:HB3	2:B:61:PRO:HG3	2.02	0.41
2:B:162:LYS:HB2	2:B:162:LYS:HE2	1.65	0.41
4:L:11:LEU:HD11	4:L:19:VAL:HG21	2.02	0.41
2:B:11:GLN:HG3	2:B:12:VAL:N	2.35	0.41
3:H:4:LEU:HD23	3:H:24:ALA:HA	2.02	0.41
4:L:109:THR:HG22	4:L:110:VAL:H	1.85	0.41
1:A:26:SER:O	1:A:27:ASN:HB3	2.21	0.41
4:L:74:THR:HG22	4:L:76:SER:H	1.85	0.41
4:L:39:LYS:HD2	4:L:39:LYS:HA	1.84	0.40
4:L:35:TRP:CG	4:L:73:LEU:HD12	2.56	0.40
2:B:174:PRO:HB2	2:B:186:TYR:HB3	2.03	0.40
3:H:6:GLN:N	3:H:111:GLN:HE22	2.16	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	196/204 (96%)	185 (94%)	11 (6%)	0	100 100
2	B	239/242 (99%)	235 (98%)	4 (2%)	0	100 100
3	H	189/225 (84%)	177 (94%)	11 (6%)	1 (0%)	29 40
4	L	185/214 (86%)	165 (89%)	20 (11%)	0	100 100
All	All	809/885 (91%)	762 (94%)	46 (6%)	1 (0%)	51 65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	148	VAL

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	174/180 (97%)	166 (95%)	8 (5%)	27 36
2	B	207/207 (100%)	194 (94%)	13 (6%)	18 23
3	H	155/192 (81%)	143 (92%)	12 (8%)	13 16
4	L	165/189 (87%)	154 (93%)	11 (7%)	16 21
All	All	701/768 (91%)	657 (94%)	44 (6%)	18 23

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	57	GLU
1	A	149	SER
1	A	155	ASP
1	A	157	TYR
1	A	160	ASP
1	A	168	SER
1	A	185	PHE
2	B	23	CYS
2	B	70	THR
2	B	71	THR
2	B	93	SER
2	B	114	ASP
2	B	119	PHE
2	B	134	SER
2	B	181	LEU
2	B	183	ASP
2	B	189	SER
2	B	191	ARG
2	B	217	GLU
2	B	224	ASP
3	H	7	SER
3	H	27	HIS
3	H	59	LYS
3	H	81	MET
3	H	85	SER
3	H	91	THR
3	H	113	THR
3	H	157	THR
3	H	187	VAL
3	H	189	THR
3	H	202	CYS
3	H	210	ASN
4	L	7	SER
4	L	50	SER
4	L	63	SER
4	L	83	PHE
4	L	89	GLN
4	L	92	LYS
4	L	105	GLU
4	L	139	PHE
4	L	156	SER
4	L	185	ASP

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Mol	Chain	Res	Type
4	L	192	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	117	GLN
1	A	125	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

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	198/204 (97%)	0.82	20 (10%) 7 8	41, 72, 134, 180	0
2	B	240/242 (99%)	0.45	7 (2%) 51 59	41, 77, 114, 149	0
3	H	197/225 (87%)	1.13	50 (25%) 0 0	69, 133, 202, 222	0
4	L	199/214 (92%)	1.04	41 (20%) 1 1	61, 138, 190, 237	0
All	All	834/885 (94%)	0.84	118 (14%) 2 3	41, 91, 183, 237	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	144	LEU	6.7
4	L	122	ASP	6.5
4	L	136	LEU	5.8
3	H	116	THR	5.7
4	L	193	ALA	5.7
4	L	175	LEU	5.3
4	L	209	PHE	5.2
3	H	185	SER	5.1
3	H	129	PRO	5.0
4	L	133	VAL	5.0
3	H	207	LYS	4.8
4	L	115	VAL	4.7
3	H	115	VAL	4.7
4	L	191	VAL	4.7
4	L	186	TYR	4.6
4	L	149	LYS	4.6
4	L	121	SER	4.6
3	H	148	VAL	4.5
4	L	125	LEU	4.5
1	A	187	CYS	4.5
3	H	187	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
3	H	143	ALA	4.2
3	H	182	TYR	4.2
4	L	150	VAL	4.1
3	H	158	VAL	4.1
4	L	132	VAL	3.9
3	H	201	ILE	3.8
4	L	104	LEU	3.8
3	H	180	GLY	3.7
4	L	119	PRO	3.7
3	H	213	VAL	3.6
3	H	125	PRO	3.6
3	H	83	LEU	3.5
3	H	128	PHE	3.5
4	L	2	ILE	3.4
1	A	136	VAL	3.3
3	H	156	VAL	3.3
1	A	196	ILE	3.3
3	H	11	VAL	3.2
3	H	105	VAL	3.2
1	A	191	PHE	3.2
4	L	196	VAL	3.2
4	L	206	THR	3.1
3	H	142	ALA	3.1
1	A	152	LYS	3.1
3	H	184	LEU	3.1
3	H	204	VAL	3.1
3	H	151	TYR	3.1
4	L	194	CYS	3.0
4	L	112	ALA	3.0
3	H	172	PHE	3.0
3	H	70	ILE	2.9
1	A	195	ILE	2.9
1	A	5	GLU	2.9
3	H	157	THR	2.9
4	L	11	LEU	2.8
4	L	210	ASN	2.8
3	H	163	GLY	2.8
1	A	194	SER	2.8
3	H	146	CYS	2.7
4	L	75	ILE	2.7
4	L	161	GLU	2.7
3	H	166	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	H	48	MET	2.7
3	H	92	ALA	2.6
4	L	197	THR	2.6
4	L	148	TRP	2.6
2	B	83	PRO	2.6
3	H	94	TYR	2.6
3	H	127	VAL	2.5
3	H	122	THR	2.5
3	H	106	LEU	2.5
4	L	146	VAL	2.5
1	A	9	GLY	2.5
1	A	51	TYR	2.5
2	B	180	ALA	2.5
1	A	177	VAL	2.4
4	L	123	GLU	2.4
1	A	198	GLU	2.4
1	A	124	TYR	2.4
3	H	177	GLN	2.4
1	A	129	SER	2.4
1	A	184	ASP	2.4
1	A	138	LEU	2.4
3	H	200	TYR	2.4
3	H	18	VAL	2.3
3	H	141	THR	2.3
4	L	29	VAL	2.3
3	H	68	VAL	2.3
3	H	24	ALA	2.3
3	H	145	GLY	2.3
3	H	198	GLN	2.3
4	L	21	ILE	2.3
1	A	157	TYR	2.3
2	B	225	ARG	2.2
4	L	88	CYS	2.2
4	L	179	LEU	2.2
4	L	134	CYS	2.2
4	L	34	VAL	2.2
3	H	214	ASP	2.2
4	L	177	SER	2.1
4	L	140	TYR	2.1
3	H	110	GLY	2.1
4	L	103	LYS	2.1
3	H	64	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	142	VAL	2.1
3	H	29	PHE	2.1
2	B	123	VAL	2.1
1	A	132	SER	2.1
1	A	185	PHE	2.1
3	H	7	SER	2.1
1	A	4	VAL	2.0
2	B	118	VAL	2.0
4	L	176	SER	2.0
2	B	112	LEU	2.0
4	L	87	PHE	2.0
3	H	170	HIS	2.0
4	L	188	LYS	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.