



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:45 AM EDT

PDB ID : 8TFN / pdb_00008tfn
Title : Structure of anti-TCR β 6-5 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

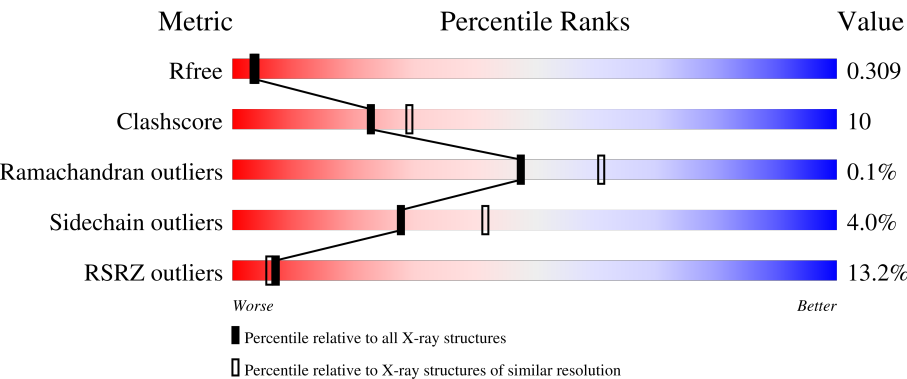
1 Overall quality at a glance i

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	204	8% 79% 17% ••
2	B	242	% 76% 23% ••
3	H	225	21% 58% 29% 12%
4	L	214	20% 65% 28% 7%

2 Entry composition [i](#)

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			

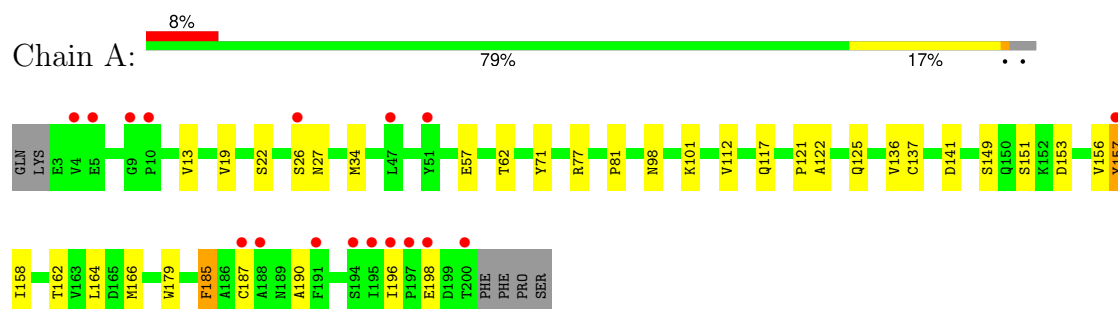
- Molecule 5 is water.

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		

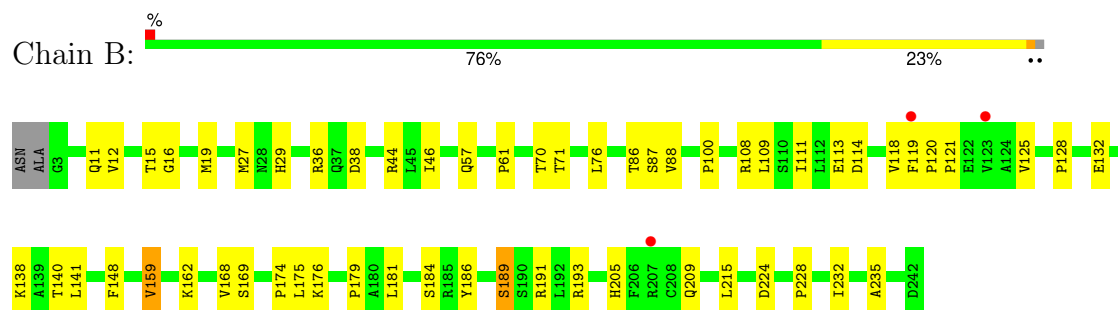
3 Residue-property plots

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.

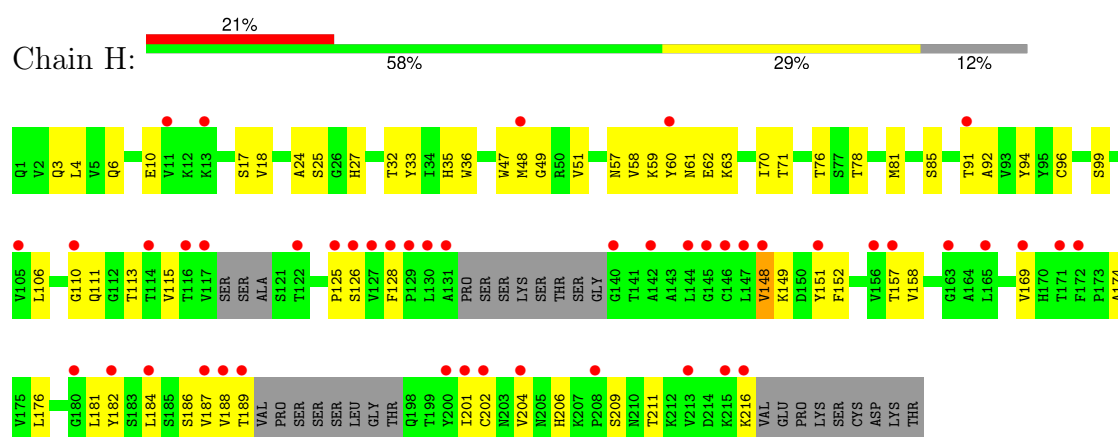
• Molecule 1: TRAV12-3



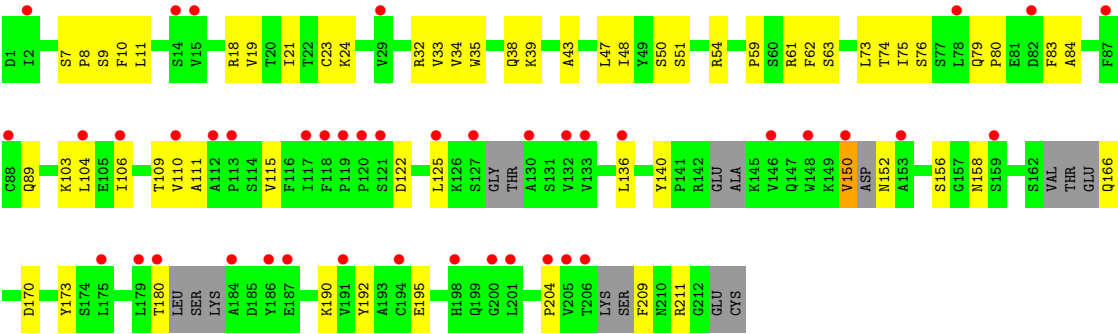
• Molecule 2: TRBV6-5



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



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



4 Data and refinement statistics

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 – 2.54	Depositor EDS
% Data completeness (in resolution range)	78.8 (86.51-2.54) 84.9 (86.51-2.54)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2445 reflections (5.02%)	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)	0.33 , 96.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/1560	0.36	0/2115
2	B	0.12	0/1955	0.33	0/2663
3	H	0.18	0/1478	0.48	0/2013
4	L	0.14	0/1531	0.40	0/2073
All	All	0.15	0/6524	0.39	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 [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	1528	0	1444	23	0
2	B	1899	0	1804	35	0
3	H	1448	0	1363	44	0
4	L	1502	0	1411	36	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	129	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 (129) 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
1:A:34:MET:HE3	2:B:100:PRO:HA	1.75	0.68
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
2:B:27:MET:HE3	2:B:29:HIS:CE1	2.35	0.61
3:H:169:VAL:HA	3:H:188:VAL:HA	1.81	0.61
2:B:11:GLN:CD	2:B:19:MET:HE1	2.26	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:48:MET:HE3	3:H:81:MET:HE3	1.92	0.49
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
1:A:166:MET:HE1	2:B:138:LYS:HG2	1.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:H:209:SER:OG	3:H:211:THR:OG1	2.34	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
2:B:132:GLU:OE2	2:B:140:THR:OG1	2.25	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:8:PRO:O	4:L:9:SER:OG	2.33	0.43
4:L:150:VAL:O	4:L:152:ASN:N	2.51	0.43
2:B:11:GLN:OE1	2:B:19:MET:HE1	2.18	0.43
2:B:38:ASP:OD1	2:B:87:SER:OG	2.33	0.43
4:L:192:TYR:HD2	4:L:209:PHE:CZ	2.37	0.43
3:H:32:THR:C	3:H:33:TYR:HD1	2.28	0.42
3:H:125:PRO:HB3	3:H:151:TYR:CD2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:L:47:LEU:C	4:L:48:ILE:HD13	2.46	0.40
4:L:11:LEU:C	4:L:11:LEU:HD12	2.46	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%)	24	34
4	L	185/214 (86%)	165 (89%)	20 (11%)	0	100	100
All	All	809/885 (91%)	762 (94%)	46 (6%)	1 (0%)	48	61

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%)	169 (97%)	5 (3%)	37	55
2	B	207/207 (100%)	199 (96%)	8 (4%)	28	43
3	H	155/192 (81%)	147 (95%)	8 (5%)	21	32
4	L	165/189 (87%)	158 (96%)	7 (4%)	26	40
All	All	701/768 (91%)	673 (96%)	28 (4%)	28	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	117	GLN
1	A	149	SER
1	A	157	TYR
1	A	185	PHE
2	B	70	THR
2	B	71	THR
2	B	76	LEU
2	B	114	ASP
2	B	159	VAL
2	B	168	VAL
2	B	189	SER
2	B	224	ASP
3	H	27	HIS
3	H	71	THR
3	H	91	THR
3	H	113	THR
3	H	157	THR
3	H	187	VAL
3	H	189	THR
3	H	202	CYS
4	L	21	ILE
4	L	50	SER
4	L	63	SER
4	L	104	LEU
4	L	115	VAL
4	L	150	VAL
4	L	156	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	64	GLN
1	A	80	GLN
1	A	117	GLN
1	A	125	GLN
2	B	85	GLN
2	B	99	GLN
2	B	102	HIS
2	B	165	HIS
2	B	201	ASN
2	B	211	GLN
4	L	38	GLN
4	L	53	HIS
4	L	166	GLN
4	L	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	198/204 (97%)	0.51	17 (8%) 16 15	41, 72, 134, 180	0
2	B	240/242 (99%)	0.23	3 (1%) 75 75	41, 77, 114, 149	1 (0%)
3	H	197/225 (87%)	1.26	47 (23%) 2 1	69, 133, 202, 222	0
4	L	199/214 (92%)	1.18	43 (21%) 2 2	61, 138, 190, 237	0
All	All	834/885 (94%)	0.77	110 (13%) 7 6	41, 91, 183, 237	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	129	PRO	5.1
3	H	130	LEU	5.0
3	H	131	ALA	4.8
3	H	148	VAL	4.5
3	H	140	GLY	4.1
3	H	182	TYR	4.0
3	H	127	VAL	4.0
3	H	128	PHE	3.9
4	L	186	TYR	3.9
4	L	198	HIS	3.8
3	H	200	TYR	3.5
4	L	175	LEU	3.5
3	H	116	THR	3.5
1	A	195	ILE	3.5
4	L	130	ALA	3.4
1	A	5	GLU	3.4
3	H	122	THR	3.3
1	A	4	VAL	3.3
4	L	117	ILE	3.3
4	L	184	ALA	3.3
3	H	144	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
3	H	213	VAL	3.2
4	L	150	VAL	3.2
3	H	184	LEU	3.2
3	H	165	LEU	3.2
3	H	145	GLY	3.2
1	A	198	GLU	3.0
3	H	147	LEU	3.0
1	A	196	ILE	2.9
4	L	179	LEU	2.9
4	L	132	VAL	2.9
4	L	88	CYS	2.9
4	L	136	LEU	2.9
4	L	87	PHE	2.9
4	L	194	CYS	2.9
4	L	148	TRP	2.9
3	H	13	LYS	2.8
1	A	194	SER	2.8
4	L	146	VAL	2.8
4	L	78	LEU	2.8
3	H	216	LYS	2.8
3	H	146	CYS	2.8
4	L	118	PHE	2.8
4	L	204	PRO	2.7
2	B	119	PHE	2.7
4	L	82	ASP	2.7
3	H	110	GLY	2.7
4	L	2	ILE	2.7
3	H	169	VAL	2.6
3	H	188	VAL	2.6
1	A	51	TYR	2.6
4	L	113	PRO	2.6
4	L	121	SER	2.6
3	H	163	GLY	2.6
4	L	104	LEU	2.5
4	L	201	LEU	2.5
3	H	114	THR	2.5
4	L	180	THR	2.5
4	L	206	THR	2.5
4	L	119	PRO	2.5
4	L	112	ALA	2.5
3	H	189	THR	2.5
3	H	60	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	15	VAL	2.5
1	A	191	PHE	2.4
3	H	11	VAL	2.4
4	L	200	GLY	2.4
4	L	125	LEU	2.4
1	A	197	PRO	2.4
4	L	187	GLU	2.4
4	L	205	VAL	2.4
4	L	153	ALA	2.4
3	H	180	GLY	2.4
1	A	9	GLY	2.3
1	A	188	ALA	2.3
1	A	10	PRO	2.3
4	L	127	SER	2.3
2	B	123	VAL	2.3
3	H	151	TYR	2.3
3	H	156	VAL	2.3
1	A	200	THR	2.3
1	A	26	SER	2.3
1	A	187	CYS	2.3
3	H	91	THR	2.2
3	H	105	VAL	2.2
3	H	117	VAL	2.2
3	H	204	VAL	2.2
4	L	191	VAL	2.2
3	H	171	THR	2.2
1	A	157	TYR	2.2
1	A	47	LEU	2.1
3	H	157	THR	2.1
3	H	126	SER	2.1
3	H	172	PHE	2.1
3	H	187	VAL	2.1
4	L	110	VAL	2.1
3	H	201	ILE	2.1
2	B	207[A]	ARG	2.1
4	L	14	SER	2.1
3	H	202	CYS	2.1
3	H	125	PRO	2.1
4	L	29	VAL	2.1
3	H	142	ALA	2.1
3	H	215	LYS	2.1
3	H	48	MET	2.0

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Mol	Chain	Res	Type	RSRZ
4	L	159	SER	2.0
4	L	133	VAL	2.0
4	L	106	ILE	2.0
3	H	208	PRO	2.0
4	L	120	PRO	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 oligosaccharides 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.