



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 PM UTC

PDB ID : 7F5K / pdb_00007f5k
Title : Crystal structure of TCR4-1 ectodomain
Authors : Nagae, M.; Yamasaki, S.
Deposited on : 2021-06-22
Resolution : 3.00 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

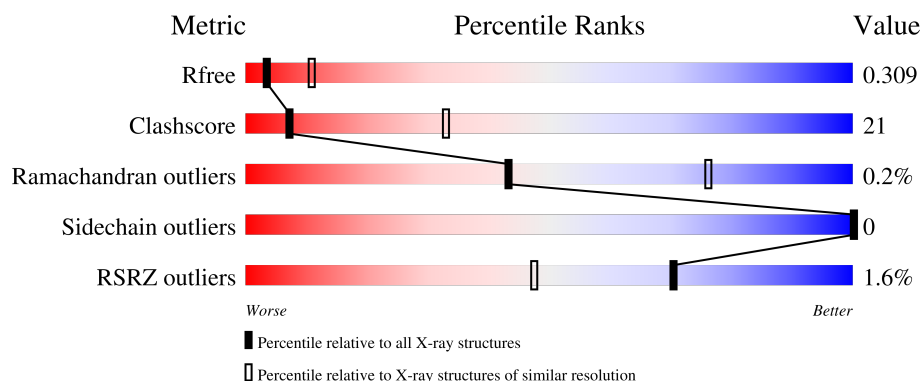
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	200	2% 50% 46% .
1	C	200	4% 56% 40% .
2	B	238	% 60% 39% .
2	D	238	65% 34% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6678 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 T cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	0	0
			1486	931	251	295	9			
1	C	192	Total	C	N	O	S	0	0	0
			1486	931	251	295	9			

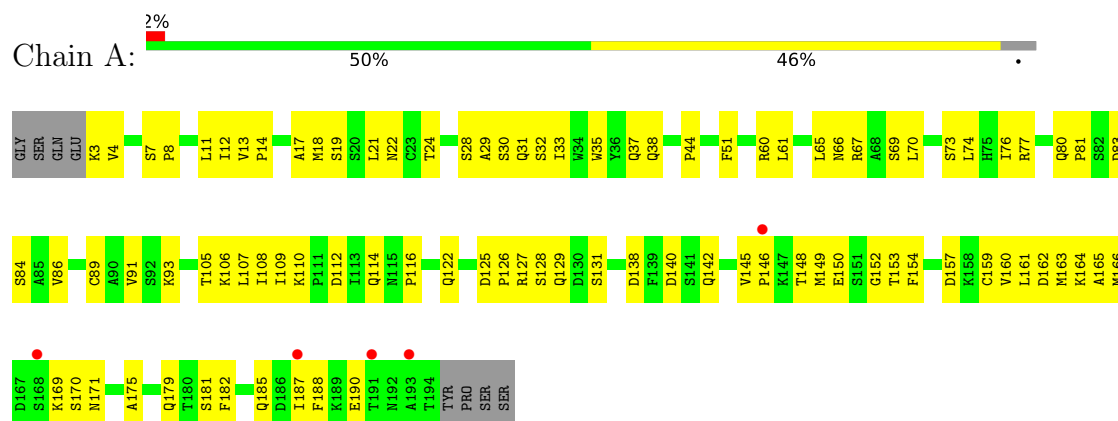
- Molecule 2 is a protein called T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1853	1163	331	352	7			
2	D	236	Total	C	N	O	S	0	0	0
			1853	1163	331	352	7			

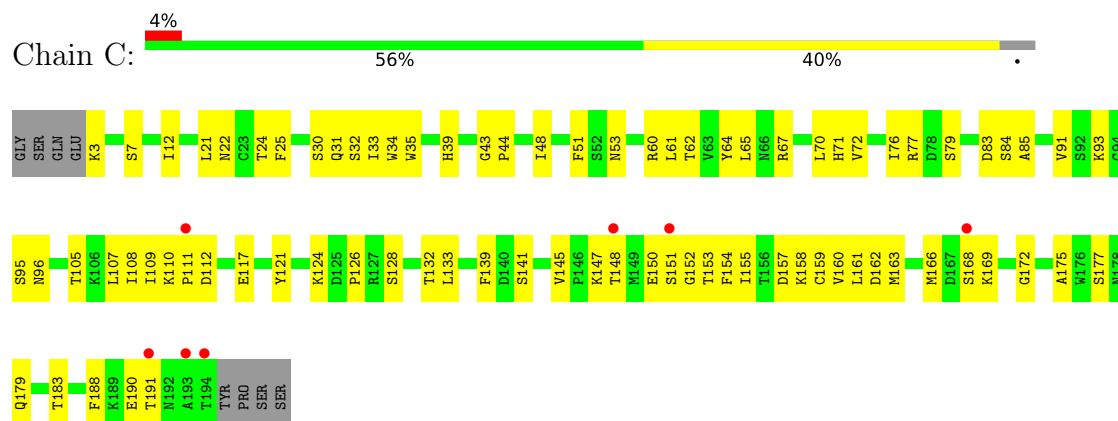
3 Residue-property plots [i](#)

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.

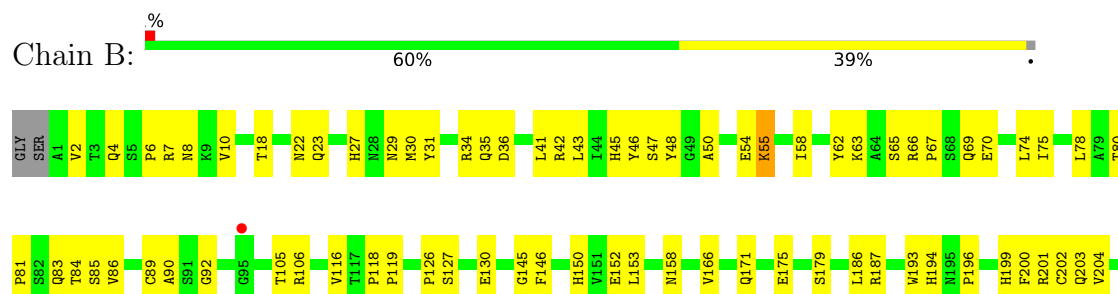
• Molecule 1: T cell receptor alpha chain

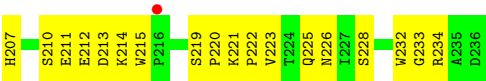


• Molecule 1: T cell receptor alpha chain



• Molecule 2: T cell receptor beta chain





● Molecule 2: T cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.87Å 73.79Å 170.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 3.00 48.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.72-3.00) 99.8 (48.72-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.225 , 0.311 0.227 , 0.309	Depositor DCC
R_{free} test set	848 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6678	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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	0.51	0/1518	0.83	0/2059
1	C	0.43	0/1518	0.72	0/2059
2	B	0.52	0/1904	0.74	0/2587
2	D	0.52	0/1904	0.74	0/2587
All	All	0.50	0/6844	0.75	0/9292

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	A	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Peptide
1	A	128	SER	Peptide
1	A	165	ALA	Peptide
1	C	7	SER	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	1486	0	1448	81	0
1	C	1486	0	1448	72	0
2	B	1853	0	1768	75	0
2	D	1853	0	1768	66	0
All	All	6678	0	6432	271	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 21.

All (271) 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:145:GLY:HA2	2:B:179:SER:HB2	1.35	1.05
1:A:108:ILE:HG21	1:A:160:VAL:HG21	1.41	1.02
1:A:65:LEU:HD21	1:A:67:ARG:HG3	1.43	1.01
1:A:170:SER:HB3	2:B:187:ARG:HB2	1.45	0.98
2:D:23:GLN:NE2	2:D:25:ASN:O	2.02	0.93
1:C:62:THR:OG1	1:C:77:ARG:NH2	2.07	0.88
2:B:63:LYS:HB3	2:B:75:ILE:HD11	1.58	0.85
2:D:66:ARG:NH2	2:D:69:GLN:O	2.11	0.83
1:A:30:SER:O	1:A:67:ARG:NH2	2.14	0.80
2:B:18:THR:OG1	2:B:75:ILE:HG22	1.82	0.80
1:A:66:ASN:HB3	1:A:69:SER:HB2	1.64	0.78
2:D:80:THR:HG22	2:D:82:SER:H	1.50	0.77
2:B:42:ARG:HD2	2:B:58:ILE:HD11	1.65	0.76
1:A:60:ARG:NH1	1:A:83:ASP:OD2	2.14	0.76
1:A:187:ILE:O	1:A:187:ILE:HD12	1.86	0.75
1:A:33:ILE:HG13	1:A:91:VAL:HG12	1.68	0.75
2:D:94:MET:HG3	2:D:95:GLY:H	1.50	0.74
1:A:106:LYS:HD3	1:A:108:ILE:HD11	1.69	0.74
2:D:29:ASN:HB2	2:D:92:GLY:O	1.87	0.74
1:C:51:PHE:O	1:C:67:ARG:NH1	2.19	0.74
2:D:47:SER:OG	2:D:52:SER:O	2.02	0.73
1:A:108:ILE:CG2	1:A:160:VAL:HG21	2.17	0.73
2:B:145:GLY:HA2	2:B:179:SER:CB	2.16	0.72
1:A:108:ILE:HG21	1:A:160:VAL:CG2	2.19	0.72
2:D:205:GLN:NE2	2:D:226:ASN:OD1	2.23	0.70
1:C:148:THR:HG22	1:C:155:ILE:H	1.58	0.69
1:A:84:SER:HB3	1:A:109:ILE:HG12	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:ASN:ND2	2:B:70:GLU:O	2.27	0.68
1:C:60:ARG:NH2	1:C:83:ASP:OD2	2.26	0.68
1:A:7:SER:HB2	1:A:22:ASN:HB2	1.76	0.67
1:A:31:GLN:NE2	1:A:93:LYS:O	2.26	0.67
2:D:167:CYS:HB3	2:D:185:ARG:HG3	1.76	0.67
1:A:61:LEU:HD22	1:A:74:LEU:HD11	1.76	0.67
1:A:163:MET:SD	1:A:164:LYS:N	2.69	0.66
1:A:22:ASN:HD22	1:A:73:SER:HB2	1.59	0.66
2:B:226:ASN:HB2	2:D:225:GLN:HG2	1.78	0.66
1:A:148:THR:OG1	1:A:149:MET:N	2.27	0.66
1:C:93:LYS:HD2	1:C:95:SER:HB3	1.76	0.66
1:A:108:ILE:CG2	1:A:160:VAL:CG2	2.73	0.65
1:C:31:GLN:H	1:C:93:LYS:HA	1.61	0.65
1:C:126:PRO:C	1:C:128:SER:H	2.04	0.65
1:C:111:PRO:HG3	1:C:160:VAL:HG11	1.78	0.65
1:C:121:TYR:CE2	2:D:130:GLU:HB2	2.33	0.64
1:C:161:LEU:O	1:C:169:LYS:HA	1.98	0.64
2:D:151:VAL:HG12	2:D:206:PHE:HA	1.79	0.64
2:B:80:THR:HG23	2:B:83:GLN:HG3	1.78	0.64
1:C:21:LEU:HD22	1:C:105:THR:HG21	1.80	0.63
1:C:117:GLU:HG2	1:C:117:GLU:O	1.97	0.63
2:D:119:PRO:HB3	2:D:146:PHE:CD2	2.34	0.63
1:A:21:LEU:HD22	1:A:105:THR:HG21	1.80	0.63
1:C:147:LYS:HG3	1:C:148:THR:HG23	1.81	0.62
1:C:177:SER:OG	1:C:179:GLN:OE1	2.17	0.62
2:D:128:LYS:HA	2:D:131:ILE:HD12	1.81	0.62
1:C:32:SER:HB3	1:C:34:TRP:CZ3	2.35	0.62
2:B:127:SER:HB3	2:B:130:GLU:HB2	1.79	0.62
1:C:154:PHE:CZ	2:D:175:GLU:HG3	2.35	0.62
1:C:65:LEU:HD21	1:C:67:ARG:HD3	1.81	0.62
1:A:146:PRO:HD2	1:A:190:GLU:HG3	1.82	0.62
1:A:11:LEU:HD23	1:A:107:LEU:HD12	1.80	0.62
1:C:35:TRP:HB2	1:C:48:ILE:HG22	1.82	0.61
2:B:62:TYR:HB3	2:B:74:LEU:HD11	1.82	0.61
2:D:52:SER:OG	2:D:53:THR:N	2.32	0.61
1:A:80:GLN:O	1:A:109:ILE:HG13	2.00	0.60
2:D:34:ARG:HH12	2:D:83:GLN:HA	1.66	0.60
1:A:138:ASP:H	1:A:171:ASN:HD21	1.47	0.60
1:C:65:LEU:HD12	1:C:72:VAL:HG12	1.82	0.60
2:B:23:GLN:NE2	2:B:69:GLN:O	2.34	0.60
2:B:212:GLU:OE1	2:B:212:GLU:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PRO:HD3	2:B:222:PRO:HB3	1.84	0.59
1:A:159:CYS:SG	1:A:160:VAL:N	2.76	0.59
1:A:51:PHE:O	1:A:67:ARG:NH1	2.34	0.59
1:C:44:PRO:HD2	2:D:101:PHE:CG	2.38	0.59
2:B:126:PRO:HD2	2:B:193:TRP:CZ2	2.38	0.59
1:A:179:GLN:HB3	1:A:182:PHE:HE1	1.66	0.59
1:C:163:MET:HB2	1:C:166:MET:O	2.03	0.58
2:D:84:THR:HG23	2:D:108:THR:HA	1.85	0.57
2:B:58:ILE:HG22	2:B:58:ILE:O	2.05	0.56
1:C:53:ASN:HA	1:C:65:LEU:O	2.05	0.56
1:C:84:SER:HA	1:C:107:LEU:O	2.06	0.56
2:B:45:HIS:HB3	2:B:55:LYS:C	2.31	0.55
1:C:79:SER:HB3	1:C:109:ILE:HD13	1.87	0.55
1:C:12:ILE:HB	1:C:108:ILE:HG23	1.89	0.55
2:D:108:THR:HG22	2:D:150:HIS:CE1	2.42	0.55
2:B:63:LYS:HB3	2:B:75:ILE:CD1	2.32	0.55
1:A:22:ASN:ND2	1:A:73:SER:HB2	2.21	0.55
2:B:196:PRO:HA	2:B:233:GLY:O	2.07	0.55
1:A:33:ILE:HD13	1:A:65:LEU:HD12	1.89	0.55
2:D:213:ASP:O	2:D:221:LYS:NZ	2.39	0.55
1:C:188:PHE:C	1:C:190:GLU:H	2.15	0.54
2:B:106:ARG:NH2	2:B:152:GLU:OE2	2.40	0.54
2:D:26:ASN:OD1	2:D:69:GLN:NE2	2.40	0.54
1:C:161:LEU:HD23	2:D:185:ARG:CZ	2.38	0.54
1:C:150:GLU:O	1:C:152:GLY:N	2.41	0.53
1:A:138:ASP:N	1:A:171:ASN:HD21	2.07	0.53
1:C:83:ASP:HB2	1:C:109:ILE:HD12	1.90	0.53
1:C:183:THR:O	1:C:183:THR:OG1	2.24	0.53
2:D:117:THR:HG22	2:D:118:PRO:O	2.09	0.52
1:C:61:LEU:CD2	1:C:76:ILE:HG12	2.39	0.52
1:C:62:THR:CB	1:C:77:ARG:HH22	2.20	0.52
1:A:38:GLN:HB3	1:A:86:VAL:HB	1.91	0.52
2:B:10:VAL:HG11	2:B:116:VAL:HG21	1.90	0.52
1:C:126:PRO:HG3	2:D:125:GLU:CD	2.35	0.52
1:C:53:ASN:HA	1:C:65:LEU:HD23	1.90	0.52
2:D:157:VAL:HG22	2:D:162:VAL:HG11	1.92	0.52
2:B:158:ASN:OD1	2:B:199:HIS:N	2.38	0.51
2:D:108:THR:HG21	2:D:148:PRO:CB	2.39	0.51
2:D:189:SER:OG	2:D:192:PHE:N	2.39	0.51
1:A:7:SER:CB	1:A:8:PRO:HD3	2.40	0.51
2:B:30:MET:HE1	2:B:69:GLN:O	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HD12	1:A:110:LYS:HD2	1.91	0.51
2:D:29:ASN:ND2	2:D:94:MET:O	2.43	0.51
1:C:12:ILE:HD11	1:C:110:LYS:HD3	1.92	0.51
1:C:61:LEU:HD23	1:C:76:ILE:HG12	1.93	0.51
2:D:76:LEU:HD23	2:D:83:GLN:OE1	2.09	0.51
1:A:154:PHE:O	1:A:175:ALA:HA	2.11	0.51
1:C:117:GLU:HG2	2:D:134:LYS:HZ3	1.76	0.51
1:A:7:SER:HB3	1:A:8:PRO:HD3	1.92	0.51
1:A:185:GLN:HA	1:A:188:PHE:CZ	2.45	0.51
2:D:4:GLN:OE1	2:D:89:CYS:N	2.43	0.51
1:C:145:VAL:HA	1:C:190:GLU:OE1	2.11	0.51
1:A:161:LEU:HD21	1:A:169:LYS:HB3	1.93	0.51
2:B:45:HIS:HE2	2:B:63:LYS:C	2.19	0.51
1:C:43:GLY:HA2	2:D:88:PHE:CE1	2.46	0.50
2:D:177:ASN:C	2:D:178:TYR:HD1	2.19	0.50
2:B:81:PRO:O	2:B:84:THR:HG22	2.12	0.50
2:B:219:SER:HB2	2:B:220:PRO:HD2	1.93	0.50
2:B:116:VAL:O	2:B:222:PRO:HG3	2.12	0.50
2:B:153:LEU:HD12	2:B:204:VAL:HG22	1.93	0.50
2:D:139:LEU:HD13	2:D:186:LEU:HD23	1.93	0.50
1:A:148:THR:HG21	1:A:153:THR:HB	1.93	0.49
1:A:19:SER:HB3	1:A:107:LEU:HD11	1.93	0.49
2:B:207:HIS:HD2	2:D:211:GLU:OE1	1.94	0.49
1:A:108:ILE:HG22	1:A:160:VAL:HG22	1.94	0.49
1:A:14:PRO:HB2	1:A:112:ASP:HB2	1.94	0.49
1:A:122:GLN:O	1:A:122:GLN:HG3	2.13	0.49
2:B:6:PRO:HB2	2:B:8:ASN:O	2.11	0.49
2:B:85:SER:OG	2:B:86:VAL:N	2.46	0.49
1:A:31:GLN:H	1:A:93:LYS:HA	1.78	0.49
1:C:162:ASP:OD1	1:C:163:MET:N	2.46	0.49
2:D:215:TRP:CD1	2:D:217:GLU:HG2	2.47	0.49
1:A:19:SER:HB3	1:A:107:LEU:CD1	2.43	0.48
2:B:30:MET:HE3	2:B:66:ARG:CZ	2.44	0.48
1:C:161:LEU:HD23	2:D:185:ARG:NH2	2.28	0.48
2:B:23:GLN:O	2:B:70:GLU:HG2	2.14	0.48
2:B:31:TYR:HB2	2:B:90:ALA:HB3	1.94	0.48
2:B:34:ARG:NH1	2:B:36:ASP:OD2	2.47	0.48
2:B:65:SER:OG	2:B:67:PRO:HD3	2.13	0.48
1:A:28:SER:O	1:A:67:ARG:HB3	2.14	0.48
1:A:108:ILE:HG22	1:A:160:VAL:CG2	2.44	0.48
1:C:148:THR:HA	1:C:155:ILE:HD12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:THR:HG21	2:D:148:PRO:HB3	1.96	0.48
1:C:43:GLY:HA2	2:D:88:PHE:HE1	1.78	0.47
1:C:157:ASP:HB2	2:D:173:TYR:OH	2.14	0.47
2:D:90:ALA:HA	2:D:100:PHE:O	2.14	0.47
2:B:30:MET:HE3	2:B:30:MET:HB2	1.60	0.47
2:D:174:LYS:HB2	2:D:174:LYS:HE3	1.71	0.47
1:A:129:GLN:HG3	1:A:131:SER:N	2.30	0.47
2:B:43:LEU:HD21	2:B:46:TYR:CD2	2.50	0.47
1:C:154:PHE:O	1:C:175:ALA:HA	2.15	0.47
2:D:33:TYR:CE2	2:D:43:LEU:HB2	2.50	0.47
2:D:106:ARG:HG2	2:D:150:HIS:CD2	2.50	0.47
1:A:146:PRO:CD	1:A:190:GLU:HG3	2.44	0.47
2:B:214:LYS:HG3	2:B:214:LYS:O	2.14	0.47
1:A:12:ILE:HA	1:A:108:ILE:O	2.15	0.46
1:A:125:ASP:OD2	1:A:126:PRO:HD2	2.14	0.46
2:B:2:VAL:HG22	2:B:23:GLN:HB3	1.96	0.46
2:B:119:PRO:HB3	2:B:146:PHE:HB3	1.96	0.46
2:B:207:HIS:CD2	2:D:211:GLU:OE1	2.68	0.46
2:B:210:SER:HG	2:B:213:ASP:CG	2.22	0.46
1:C:126:PRO:O	1:C:128:SER:N	2.45	0.46
2:D:205:GLN:OE1	2:D:226:ASN:ND2	2.48	0.46
1:A:3:LYS:HE3	1:A:3:LYS:HB3	1.67	0.46
1:C:139:PHE:HD1	1:C:139:PHE:H	1.61	0.46
2:B:211:GLU:HA	2:B:221:LYS:NZ	2.30	0.46
1:A:166:MET:C	1:A:169:LYS:HD3	2.41	0.46
2:B:215:TRP:CB	2:B:221:LYS:HG3	2.45	0.46
2:D:194:HIS:HB3	2:D:235:ALA:HB2	1.98	0.46
2:B:6:PRO:O	2:B:105:THR:OG1	2.29	0.46
1:A:138:ASP:H	1:A:171:ASN:ND2	2.14	0.46
2:D:94:MET:HG3	2:D:95:GLY:N	2.26	0.46
2:B:47:SER:CB	2:B:66:ARG:HH11	2.29	0.45
1:A:4:VAL:HA	1:A:24:THR:O	2.16	0.45
2:D:146:PHE:CE1	2:D:180:TYR:HB2	2.51	0.45
1:A:80:GLN:O	1:A:81:PRO:C	2.58	0.45
2:D:203:GLN:HG3	2:D:228:SER:HB2	1.99	0.45
1:A:13:VAL:HB	1:A:17:ALA:HB3	1.99	0.45
1:A:140:ASP:C	1:A:142:GLN:H	2.25	0.45
2:B:62:TYR:CD1	2:B:74:LEU:HD11	2.52	0.45
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.83	0.45
1:A:37:GLN:O	1:A:44:PRO:HA	2.17	0.45
1:A:148:THR:OG1	1:A:153:THR:HB	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:CB	2:B:187:ARG:HB2	2.33	0.45
1:C:112:ASP:HA	1:C:141:SER:OG	2.16	0.45
1:A:150:GLU:HG3	1:A:152:GLY:H	1.81	0.44
1:A:18:MET:HE3	1:A:18:MET:HB2	1.79	0.44
1:A:162:ASP:CG	1:A:162:ASP:O	2.60	0.44
1:C:158:LYS:H	1:C:158:LYS:HG2	1.32	0.44
2:B:7:ARG:O	2:B:105:THR:HA	2.17	0.44
2:B:50:ALA:HB2	2:B:69:GLN:HB3	1.99	0.44
2:D:43:LEU:HD21	2:D:46:TYR:CD2	2.52	0.44
2:D:215:TRP:HE1	2:D:219:SER:HB2	1.82	0.44
1:C:159:CYS:C	2:D:167:CYS:SG	3.01	0.44
1:C:33:ILE:HD13	1:C:65:LEU:CD1	2.47	0.44
2:B:201:ARG:NH2	2:B:203:GLN:HB2	2.33	0.44
1:C:39:HIS:CE1	1:C:85:ALA:HB2	2.53	0.44
1:C:64:TYR:O	1:C:72:VAL:HA	2.18	0.44
1:A:19:SER:CB	1:A:107:LEU:HD11	2.48	0.43
1:A:154:PHE:CE1	2:B:175:GLU:HG2	2.53	0.43
2:D:114:ARG:H	2:D:114:ARG:HG2	1.52	0.43
1:C:22:ASN:CB	1:C:71:HIS:HE1	2.31	0.43
1:C:117:GLU:HG2	2:D:134:LYS:NZ	2.32	0.43
2:B:202:CYS:O	2:B:228:SER:HA	2.18	0.43
1:C:12:ILE:HA	1:C:108:ILE:O	2.18	0.43
1:C:30:SER:HA	1:C:93:LYS:CB	2.48	0.43
1:C:168:SER:OG	2:D:136:LYS:HD3	2.19	0.43
1:A:84:SER:HA	1:A:107:LEU:HD23	2.01	0.43
1:A:114:GLN:C	1:A:116:PRO:HD3	2.43	0.43
2:B:47:SER:HB3	2:B:66:ARG:HH11	1.83	0.43
2:B:211:GLU:HA	2:B:221:LYS:HZ2	1.84	0.43
1:C:126:PRO:C	1:C:128:SER:N	2.75	0.43
2:B:54:GLU:O	2:B:55:LYS:HB2	2.17	0.43
1:C:3:LYS:HA	1:C:3:LYS:HD2	1.78	0.43
2:B:29:ASN:OD1	2:B:48:TYR:HD1	2.02	0.43
1:A:32:SER:C	1:A:33:ILE:HD12	2.44	0.42
2:B:34:ARG:HH11	2:B:85:SER:HB2	1.83	0.42
2:B:36:ASP:OD1	2:B:85:SER:OG	2.24	0.42
2:D:36:ASP:HB2	2:D:39:HIS:HB2	2.01	0.42
2:B:200:PHE:CD1	2:B:200:PHE:N	2.87	0.42
1:C:33:ILE:HG23	1:C:91:VAL:HG22	2.01	0.42
1:A:11:LEU:CD2	1:A:107:LEU:HD12	2.47	0.42
2:B:27:HIS:HB3	2:B:92:GLY:O	2.20	0.42
1:A:138:ASP:OD1	2:B:187:ARG:NH1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLN:OE1	2:B:89:CYS:N	2.52	0.42
2:B:199:HIS:HB2	2:B:232:TRP:CZ3	2.54	0.42
1:C:24:THR:HA	1:C:70:LEU:O	2.20	0.42
1:C:158:LYS:HA	1:C:172:GLY:O	2.19	0.42
2:D:149:ASP:HB3	2:D:180:TYR:CG	2.54	0.42
1:C:133:LEU:C	1:C:133:LEU:HD12	2.44	0.42
2:D:8:ASN:ND2	2:D:150:HIS:HB3	2.34	0.42
1:A:179:GLN:C	1:A:181:SER:H	2.28	0.42
2:B:62:TYR:HD1	2:B:74:LEU:HD11	1.85	0.42
1:C:188:PHE:HB2	1:C:190:GLU:HG2	2.01	0.42
1:A:7:SER:HB3	1:A:22:ASN:H	1.85	0.41
1:A:106:LYS:HZ1	2:B:171:GLN:HG3	1.84	0.41
1:A:129:GLN:CG	1:A:131:SER:HB2	2.50	0.41
1:C:93:LYS:HG3	1:C:96:ASN:H	1.85	0.41
1:A:60:ARG:HB2	1:A:77:ARG:HG3	2.02	0.41
2:B:43:LEU:HD21	2:B:46:TYR:HD2	1.84	0.41
2:B:225:GLN:HB3	2:D:224:THR:HB	2.02	0.41
1:C:25:PHE:O	1:C:70:LEU:HD13	2.20	0.41
1:C:148:THR:HB	1:C:153:THR:O	2.20	0.41
2:D:22:ASN:OD1	2:D:23:GLN:N	2.53	0.41
2:D:174:LYS:HG2	2:D:176:SER:O	2.20	0.41
1:A:18:MET:HA	1:A:76:ILE:O	2.20	0.41
2:D:9:LYS:HG3	2:D:10:VAL:N	2.35	0.41
1:C:124:LYS:HG2	1:C:132:THR:HG22	2.02	0.41
2:B:223:VAL:O	2:B:225:GLN:HG2	2.20	0.41
1:C:191:THR:O	1:C:191:THR:OG1	2.31	0.41
1:A:29:ALA:O	1:A:30:SER:C	2.63	0.41
2:B:166:VAL:HG22	2:B:186:LEU:HD13	2.02	0.41
2:D:47:SER:HB3	2:D:66:ARG:HD2	2.02	0.41
2:D:194:HIS:O	2:D:235:ALA:HB2	2.20	0.41
1:A:66:ASN:O	1:A:70:LEU:N	2.54	0.41
2:B:194:HIS:HA	2:B:234:ARG:O	2.21	0.41
1:C:33:ILE:HG21	1:C:72:VAL:HG11	2.02	0.40
1:C:34:TRP:CZ3	2:D:97:ALA:HB3	2.57	0.40
2:B:35:GLN:HB2	2:B:41:LEU:HD23	2.02	0.40
1:A:35:TRP:CZ3	1:A:89:CYS:HB2	2.56	0.40
1:A:108:ILE:CG2	1:A:160:VAL:HG22	2.51	0.40
1:A:145:VAL:HB	1:A:157:ASP:OD1	2.22	0.40
2:B:150:HIS:CD2	2:B:150:HIS:N	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	190/200 (95%)	153 (80%)	37 (20%)	0	100	100
1	C	190/200 (95%)	165 (87%)	24 (13%)	1 (0%)	24	60
2	B	234/238 (98%)	212 (91%)	21 (9%)	1 (0%)	30	65
2	D	234/238 (98%)	204 (87%)	30 (13%)	0	100	100
All	All	848/876 (97%)	734 (87%)	112 (13%)	2 (0%)	43	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	55	LYS
1	C	151	SER

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	171/178 (96%)	171 (100%)	0	100	100
1	C	171/178 (96%)	171 (100%)	0	100	100
2	B	200/201 (100%)	200 (100%)	0	100	100
2	D	200/201 (100%)	200 (100%)	0	100	100
All	All	742/758 (98%)	742 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	192	ASN
2	B	22	ASN
2	B	205	GLN
2	B	207	HIS
2	B	226	ASN
1	C	27	ASN
1	C	71	HIS
1	C	96	ASN
1	C	98	GLN
1	C	144	ASN
2	D	135	GLN
2	D	150	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	192/200 (96%)	0.21	5 (2%) 57 34	32, 57, 100, 129	0
1	C	192/200 (96%)	0.32	7 (3%) 46 26	35, 65, 109, 120	0
2	B	236/238 (99%)	-0.10	2 (0%) 82 64	24, 48, 76, 91	0
2	D	236/238 (99%)	-0.11	0 100 100	27, 48, 76, 84	0
All	All	856/876 (97%)	0.06	14 (1%) 70 47	24, 54, 97, 129	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ILE	3.6
1	A	146	PRO	3.1
1	C	193	ALA	3.0
1	C	151	SER	2.8
1	A	193	ALA	2.6
1	A	168	SER	2.4
1	C	111	PRO	2.4
1	C	148	THR	2.4
1	A	191	THR	2.3
1	C	191	THR	2.3
2	B	216	PRO	2.2
1	C	194	THR	2.1
2	B	95	GLY	2.1
1	C	168	SER	2.1

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.