



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 4P5T / pdb_00004p5t
Title : 14.C6 TCR complexed with MHC class II I-Ab/3K peptide
Authors : Trenh, P.; Stadinski, B.; Huseby, E.S.; Stern, L.J.
Deposited on : 2014-03-19
Resolution : 3.26 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

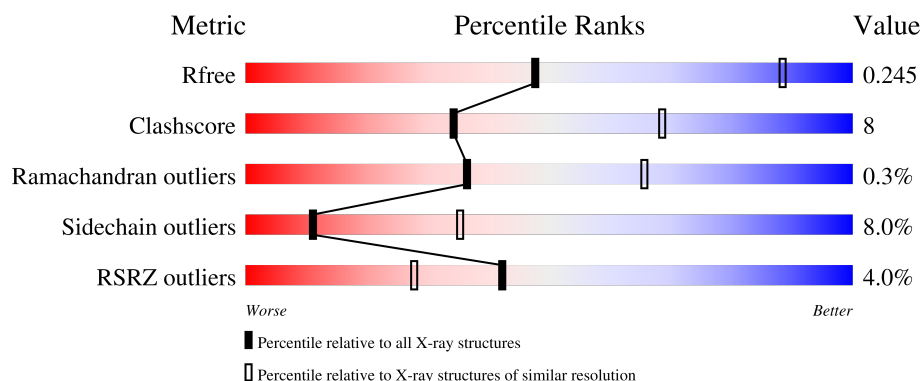
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	206	11% 77% 18% .
1	E	206	11% 69% 18% . 9%
2	B	241	10% 76% 20% . .
2	F	241	10% 72% 22% . 5%
3	C	182	79% 19% . .

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Mol	Chain	Length	Quality of chain
3	G	182	 3% 82% 16% ..
4	D	217	 69% 21% . 8%
4	H	217	 2% 69% 19% . 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12366 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 TRA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1488	948	241	292	7			
1	E	188	Total	C	N	O	S	0	0	0
			1403	902	223	272	6			

- Molecule 2 is a protein called Human nkt tcr beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1815	1146	318	345	6			
2	F	229	Total	C	N	O	S	0	0	0
			1725	1091	300	328	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1381	897	215	266	3			
3	G	179	Total	C	N	O	S	0	0	0
			1377	895	214	265	3			

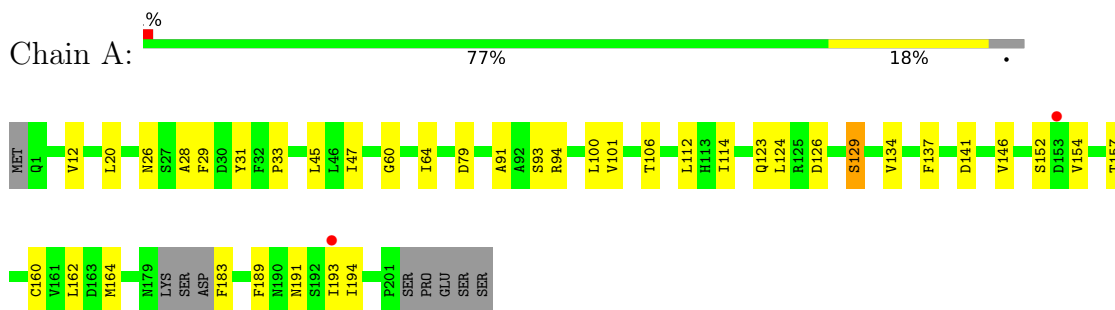
- Molecule 4 is a protein called protein of 3K peptide (FEAQKAKANKAVD), Linker region - GGGGSLVPRGSGGGG, H-2 class II histocompatibility antigen, A beta chain, H-2 class II histocompatibility antigen, A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1593	1001	279	307	6			
4	H	199	Total	C	N	O	S	0	0	0
			1584	997	275	306	6			

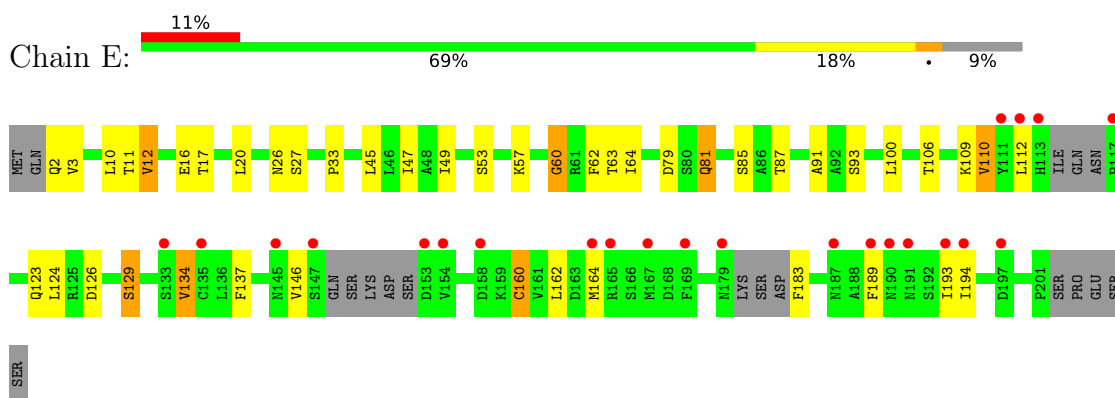
3 Residue-property plots [i](#)

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.

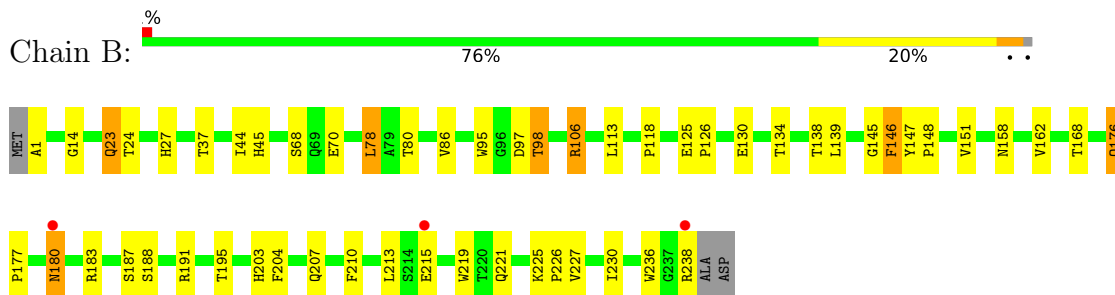
- Molecule 1: TRA protein



- Molecule 1: TRA protein

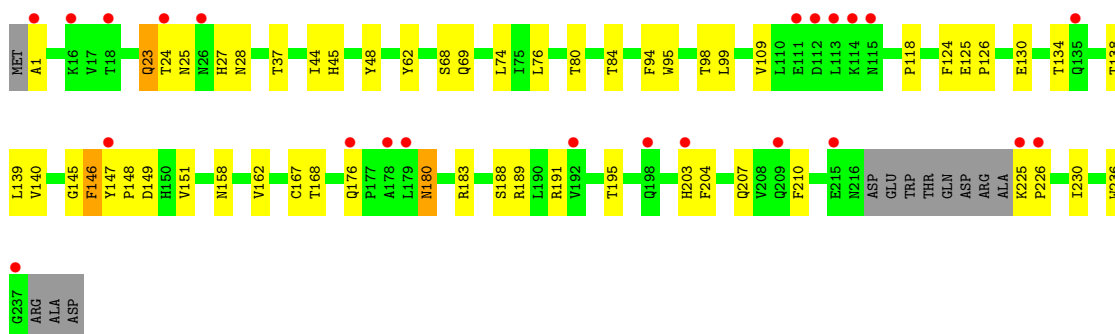


- Molecule 2: Human nkt tcr beta chain

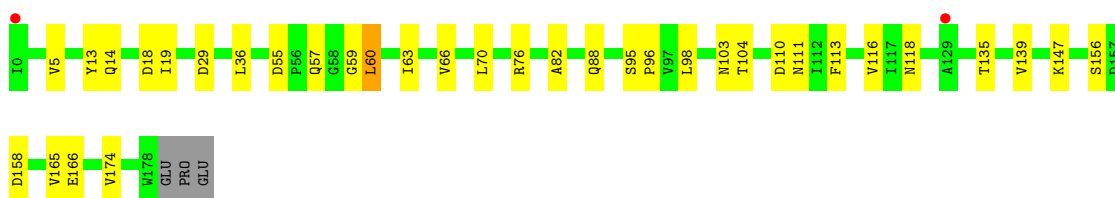
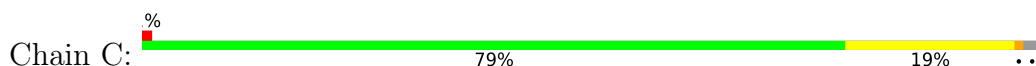


- Molecule 2: Human nkt tcr beta chain

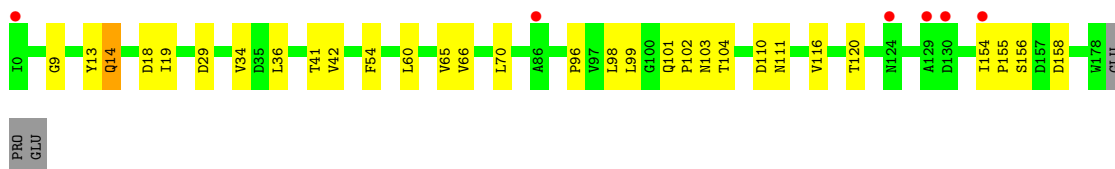
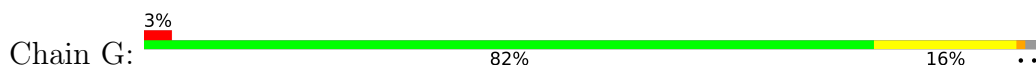




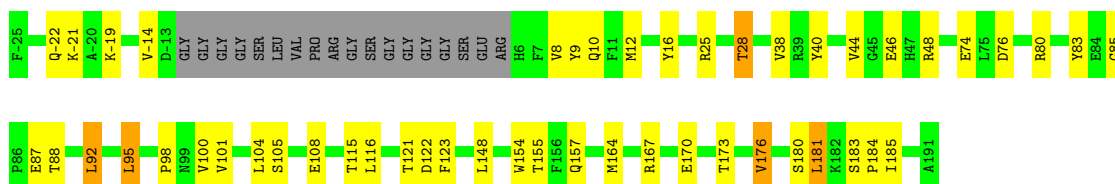
- Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain



- Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

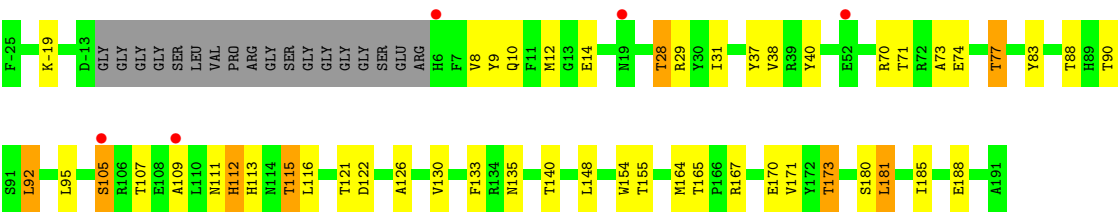


- Molecule 4: protein of 3K peptide (FEAQKAKANKAVD),Linker region - GGGGSLVPRGSGGGG,H-2 class II histocompatibility antigen, A beta chain,H-2 class II histocompatibility antigen, A beta chain



- Molecule 4: protein of 3K peptide (FEAQKAKANKAVD),Linker region - GGGGSLVPRGSGGGG,H-2 class II histocompatibility antigen, A beta chain,H-2 class II histocompatibility antigen, A beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.01Å 74.14Å 259.29Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	47.05 – 3.26 47.05 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.05-3.26) 98.9 (47.05-3.26)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.186 , 0.236 0.201 , 0.245	Depositor DCC
R_{free} test set	1957 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12366	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

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

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	0.29	0/1525	0.70	0/2078
1	E	0.28	0/1438	0.67	0/1960
2	B	0.29	0/1868	0.76	2/2558 (0.1%)
2	F	0.27	0/1775	0.76	4/2432 (0.2%)
3	C	0.28	0/1425	0.71	0/1957
3	G	0.26	0/1420	0.70	0/1949
4	D	0.28	0/1632	0.72	2/2225 (0.1%)
4	H	0.28	0/1623	0.72	0/2214
All	All	0.28	0/12706	0.72	8/17373 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	176	GLN	CA-C-N	6.27	125.96	119.56
2	F	176	GLN	C-N-CA	6.27	125.96	119.56
2	B	176	GLN	CA-C-N	6.15	125.83	119.56
2	B	176	GLN	C-N-CA	6.15	125.83	119.56
2	F	125	GLU	CA-C-N	5.09	125.10	119.90
2	F	125	GLU	C-N-CA	5.09	125.10	119.90
4	D	85	GLY	CA-C-N	5.01	124.80	119.28
4	D	85	GLY	C-N-CA	5.01	124.80	119.28

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	1488	0	1353	19	0
1	E	1403	0	1255	18	0
2	B	1815	0	1654	35	0
2	F	1725	0	1561	42	0
3	C	1381	0	1263	19	0
3	G	1377	0	1256	16	0
4	D	1593	0	1471	30	0
4	H	1584	0	1456	29	0
All	All	12366	0	11269	179	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 8.

All (179) 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:F:84:THR:HG22	2:F:109:VAL:H	1.46	0.80
4:D:116:LEU:HG	4:D:164:MET:HE2	1.66	0.77
1:E:45:LEU:HD22	2:F:98:THR:HG22	1.69	0.74
2:B:130:GLU:OE2	2:B:191:ARG:NH1	2.20	0.74
2:F:130:GLU:OE2	2:F:191:ARG:NH1	2.20	0.74
4:H:116:LEU:HG	4:H:164:MET:HE2	1.69	0.74
3:C:139:VAL:HG11	4:D:12:MET:HE1	1.70	0.73
2:F:145:GLY:HA2	2:F:183:ARG:HD3	1.71	0.73
2:B:145:GLY:HA2	2:B:183:ARG:HD3	1.72	0.71
3:G:34:VAL:HG22	3:G:41:THR:HG22	1.74	0.69
1:E:49:ILE:HD13	1:E:57:LYS:HB2	1.75	0.68
4:H:14:GLU:OE1	4:H:29:ARG:NH1	2.26	0.68
3:C:118:ASN:HB2	3:C:166:GLU:HB2	1.79	0.64
4:D:46:GLU:OE2	4:D:48:ARG:NH1	2.30	0.64
1:E:93:SER:HB2	1:E:100:LEU:HD23	1.82	0.61
3:C:14:GLN:HG2	4:D:8:VAL:HG22	1.82	0.61
4:H:113:HIS:H	4:H:165:THR:HG23	1.66	0.61
4:H:111:ASN:OD1	4:H:167:ARG:NH1	2.34	0.60
4:D:95:LEU:HG	4:D:180:SER:HA	1.83	0.60
4:D:100:VAL:HG21	4:D:176:VAL:HG11	1.84	0.60
3:G:103:ASN:OD1	3:G:104:THR:N	2.34	0.59
3:G:13:TYR:OH	3:G:18:ASP:OD1	2.20	0.59
2:F:180:ASN:OD1	2:F:180:ASN:N	2.34	0.57
1:A:20:LEU:HD22	1:A:106:THR:HG21	1.87	0.56
1:A:94:ARG:NH2	3:C:55:ASP:OD2	2.38	0.56
4:H:37:TYR:CD2	4:H:38:VAL:HG23	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:ALA:H2	2:B:24:THR:HB	1.69	0.56
3:C:70:LEU:HD13	4:D:9:TYR:HB2	1.87	0.56
4:D:76:ASP:OD1	4:D:80:ARG:NH1	2.39	0.56
1:A:114:ILE:HG13	1:A:141:ASP:HA	1.88	0.55
2:F:23:GLN:HG2	2:F:25:ASN:H	1.71	0.55
2:B:68:SER:OG	2:B:70:GLU:OE1	2.25	0.55
1:A:152:SER:C	1:A:154:VAL:H	2.14	0.55
1:E:49:ILE:HD11	1:E:53:SER:HB2	1.88	0.55
2:B:225:LYS:HG2	2:B:227:VAL:HG13	1.88	0.55
2:F:158:ASN:HA	2:F:203:HIS:CE1	2.42	0.55
2:F:28:ASN:ND2	2:F:48:TYR:O	2.40	0.54
1:A:28:ALA:O	4:D:-22:GLN:NE2	2.41	0.54
4:D:10:GLN:HE21	4:D:12:MET:HE3	1.73	0.54
1:E:134:VAL:HB	2:F:124:PHE:CD2	2.41	0.54
1:A:33:PRO:HG2	1:A:91:ALA:HB3	1.89	0.53
2:B:158:ASN:HA	2:B:203:HIS:CE1	2.42	0.53
2:B:95:TRP:CE2	4:D:-19:LYS:HB2	2.43	0.53
2:F:1:ALA:N	2:F:25:ASN:OD1	2.43	0.52
2:B:180:ASN:OD1	2:B:180:ASN:N	2.36	0.52
4:H:10:GLN:HB3	4:H:31:ILE:HB	1.91	0.52
3:G:110:ASP:OD1	3:G:111:ASN:N	2.39	0.51
3:G:41:THR:HG21	3:G:54:PHE:HD2	1.75	0.51
1:E:47:ILE:HG23	1:E:64:ILE:HD11	1.92	0.51
2:B:23:GLN:OE1	2:B:27:HIS:N	2.42	0.51
2:B:147:TYR:HD2	2:B:148:PRO:HA	1.76	0.51
2:F:147:TYR:CD2	2:F:148:PRO:HA	2.46	0.51
4:D:28:THR:HB	4:D:40:TYR:HB3	1.93	0.51
4:H:173:THR:HG23	4:H:188:GLU:HG2	1.92	0.51
2:F:147:TYR:HD2	2:F:148:PRO:HA	1.76	0.50
2:F:68:SER:OG	2:F:69:GLN:N	2.44	0.50
2:B:147:TYR:CD2	2:B:148:PRO:HA	2.46	0.50
3:C:110:ASP:OD1	3:C:111:ASN:N	2.38	0.50
4:D:121:THR:HG22	4:D:157:GLN:HG3	1.93	0.50
4:H:122:ASP:HA	4:H:155:THR:HB	1.93	0.50
4:D:122:ASP:HA	4:D:155:THR:HB	1.93	0.50
1:E:162:LEU:HB3	2:F:167:CYS:HB3	1.94	0.49
1:E:126:ASP:HA	2:F:124:PHE:HD1	1.77	0.49
2:B:146:PHE:HE1	2:B:151:VAL:HG21	1.78	0.49
2:B:146:PHE:HD2	2:B:146:PHE:H	1.60	0.49
2:F:94:PHE:CG	3:G:65:VAL:HG22	2.47	0.49
2:F:146:PHE:HE1	2:F:151:VAL:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:203:HIS:HB3	2:F:236:TRP:CE3	2.47	0.48
2:B:203:HIS:HB3	2:B:236:TRP:CE3	2.47	0.48
3:C:165:VAL:HB	3:C:174:VAL:HG12	1.95	0.48
2:F:27:HIS:O	2:F:69:GLN:NE2	2.46	0.48
2:B:86:VAL:HG22	2:B:106:ARG:HD3	1.95	0.48
4:D:16:TYR:HB2	4:D:25:ARG:HB3	1.96	0.48
2:F:146:PHE:HD2	2:F:146:PHE:H	1.60	0.48
1:A:47:ILE:HG23	1:A:64:ILE:HD11	1.96	0.48
1:E:126:ASP:HB3	1:E:129:SER:O	2.14	0.48
1:A:93:SER:HB2	1:A:100:LEU:HD23	1.95	0.47
3:C:135:THR:O	3:C:147:LYS:HE3	2.14	0.47
4:D:176:VAL:HG13	4:D:185:ILE:HB	1.95	0.47
2:B:44:ILE:HG22	2:B:45:HIS:CD2	2.48	0.47
2:F:23:GLN:HG2	2:F:24:THR:N	2.30	0.47
2:B:168:THR:HG23	2:B:188:SER:HB2	1.97	0.47
2:F:168:THR:HG23	2:F:188:SER:HB2	1.96	0.47
2:F:158:ASN:HA	2:F:203:HIS:HE1	1.81	0.46
4:H:167:ARG:O	4:H:170:GLU:HG2	2.15	0.46
1:E:20:LEU:HD22	1:E:106:THR:HG21	1.97	0.46
2:F:23:GLN:OE1	2:F:27:HIS:N	2.40	0.46
3:C:66:VAL:HG13	4:D:9:TYR:CD2	2.51	0.46
1:A:126:ASP:HB3	1:A:129:SER:O	2.16	0.46
2:B:158:ASN:HA	2:B:203:HIS:HE1	1.81	0.46
3:C:96:PRO:HD3	4:D:121:THR:HG21	1.98	0.46
3:C:82:ALA:HB1	3:C:113:PHE:CE2	2.51	0.46
4:D:-19:LYS:HG2	4:D:74:GLU:OE1	2.16	0.46
4:D:181:LEU:HD22	4:D:185:ILE:HG13	1.97	0.45
4:H:105:SER:OG	4:H:115:THR:HG23	2.15	0.45
2:F:23:GLN:HE21	2:F:23:GLN:HB3	1.52	0.45
1:A:29:PHE:HD1	1:A:94:ARG:HG2	1.81	0.45
1:A:137:PHE:HB2	1:A:189:PHE:CE2	2.50	0.45
1:E:137:PHE:HB2	1:E:189:PHE:CE2	2.51	0.45
2:F:28:ASN:HA	2:F:69:GLN:HE22	1.82	0.45
2:B:207:GLN:HG3	2:B:230:ILE:HG23	1.99	0.45
3:C:156:SER:OG	3:C:158:ASP:OD1	2.28	0.45
4:H:-19:LYS:HG2	4:H:74:GLU:OE1	2.17	0.45
3:G:66:VAL:HG13	4:H:9:TYR:CD2	2.52	0.45
3:G:14:GLN:HG2	3:G:19:ILE:HD12	1.99	0.45
3:C:57:GLN:HA	3:C:60:LEU:HB2	1.98	0.45
1:A:31:TYR:OH	2:B:97:ASP:HB2	2.17	0.44
2:F:151:VAL:HG12	2:F:210:PHE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:83:TYR:O	4:H:88:THR:HG23	2.17	0.44
2:B:118:PRO:HD3	2:B:226:PRO:HB3	2.00	0.44
2:F:118:PRO:HD3	2:F:226:PRO:HB3	1.99	0.44
2:F:207:GLN:HG3	2:F:230:ILE:HG23	1.99	0.44
3:G:156:SER:OG	3:G:158:ASP:OD1	2.24	0.44
1:A:29:PHE:CD1	1:A:94:ARG:HG2	2.53	0.44
2:B:219:TRP:CE2	2:B:221:GLN:HB2	2.52	0.44
2:F:149:ASP:OD1	2:F:149:ASP:N	2.50	0.44
4:H:9:TYR:OH	4:H:37:TYR:OH	2.31	0.44
2:B:151:VAL:HG12	2:B:210:PHE:HA	2.00	0.44
2:F:225:LYS:HA	2:F:226:PRO:HD3	1.77	0.43
4:D:95:LEU:HD12	4:D:95:LEU:HA	1.83	0.43
4:H:73:ALA:O	4:H:77:THR:OG1	2.37	0.43
2:B:23:GLN:HE21	2:B:23:GLN:HB3	1.62	0.43
3:C:103:ASN:OD1	3:C:104:THR:N	2.45	0.43
2:B:14:GLY:HA2	2:B:78:LEU:HD23	2.01	0.43
3:G:99:LEU:HA	3:G:155:PRO:HB2	1.99	0.43
3:C:76:ARG:NH2	4:D:-14:VAL:O	2.52	0.43
4:H:28:THR:HG22	4:H:40:TYR:HB3	2.01	0.43
1:A:162:LEU:HD21	2:B:191:ARG:HD3	2.01	0.43
1:E:81:GLN:O	1:E:110:VAL:HG21	2.19	0.43
3:G:70:LEU:HD13	4:H:9:TYR:HB2	2.01	0.42
3:G:29:ASP:HB3	4:H:154:TRP:CE2	2.54	0.42
4:H:135:ASN:ND2	4:H:171:VAL:H	2.17	0.42
4:D:98:PRO:HB3	4:D:123:PHE:HB3	2.01	0.42
1:E:126:ASP:HA	2:F:124:PHE:CD1	2.54	0.42
2:F:62:TYR:HD1	2:F:74:LEU:HD21	1.84	0.42
3:C:29:ASP:HB3	4:D:154:TRP:CE2	2.55	0.42
4:H:181:LEU:HD22	4:H:185:ILE:HG13	2.01	0.42
4:D:183:SER:HA	4:D:184:PRO:HD3	1.89	0.42
3:C:59:GLY:O	3:C:63:ILE:HG12	2.20	0.42
2:F:44:ILE:HG22	2:F:45:HIS:CD2	2.55	0.42
1:A:45:LEU:HD22	2:B:98:THR:HG22	2.01	0.41
2:B:125:GLU:HA	2:B:126:PRO:HD3	1.96	0.41
2:F:140:VAL:HG22	2:F:189:ARG:HG3	2.02	0.41
3:G:96:PRO:HD3	4:H:121:THR:HG21	2.02	0.41
1:A:157:THR:HG21	2:B:187:SER:OG	2.20	0.41
2:B:95:TRP:CD2	4:D:-19:LYS:HB2	2.55	0.41
3:G:9:GLY:O	4:H:12:MET:HA	2.20	0.41
4:H:88:THR:HA	4:H:92:LEU:HB2	2.02	0.41
1:A:152:SER:O	1:A:154:VAL:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101:GLN:HA	3:G:102:PRO:HD2	1.83	0.41
2:F:76:LEU:HD12	2:F:76:LEU:HA	1.83	0.41
2:F:146:PHE:N	2:F:146:PHE:CD2	2.88	0.41
1:E:26:ASN:OD1	1:E:27:SER:N	2.54	0.41
4:D:83:TYR:O	4:D:88:THR:HG23	2.21	0.41
2:F:130:GLU:OE2	2:F:138:THR:OG1	2.37	0.41
1:A:26:ASN:HB3	1:A:29:PHE:CE2	2.56	0.41
2:B:146:PHE:N	2:B:146:PHE:CD2	2.88	0.41
3:C:13:TYR:OH	3:C:18:ASP:OD1	2.22	0.41
4:D:92:LEU:HD12	4:D:92:LEU:HA	1.88	0.41
2:F:126:PRO:HD3	2:F:139:LEU:HG	2.02	0.41
4:H:109:ALA:O	4:H:112:HIS:HB2	2.21	0.41
4:H:126:ALA:HB1	4:H:148:LEU:HD21	2.03	0.41
1:A:152:SER:C	1:A:154:VAL:N	2.79	0.41
2:B:138:THR:OG1	2:B:191:ARG:HD2	2.21	0.41
1:E:12:VAL:HG13	1:E:16:GLU:HB2	2.03	0.41
1:E:33:PRO:HG2	1:E:91:ALA:HB3	2.03	0.41
2:F:188:SER:C	2:F:189:ARG:HD3	2.46	0.41
2:B:126:PRO:HD3	2:B:139:LEU:HG	2.03	0.40
2:B:176:GLN:HA	2:B:177:PRO:HD2	1.94	0.40
4:D:104:LEU:HD21	4:D:108:GLU:HB2	2.03	0.40
4:D:167:ARG:HB2	4:D:170:GLU:HG3	2.03	0.40
2:B:113:LEU:HD21	2:B:213:LEU:HD21	2.02	0.40
4:H:133:PHE:HB2	4:H:173:THR:HB	2.02	0.40
1:E:160:CYS:HB3	2:F:189:ARG:NH2	2.36	0.40
2:F:95:TRP:CE2	4:H:19:LYS:HB2	2.57	0.40
3:C:14:GLN:OE1	3:C:116:VAL:HG23	2.21	0.40
1:E:60:GLY:C	1:E:62:PHE:H	2.29	0.40
4:H:95:LEU:HD23	4:H:180:SER:HA	2.03	0.40
3:G:14:GLN:HB2	4:H:8:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	193/206 (94%)	182 (94%)	9 (5%)	2 (1%)	12	40
1	E	180/206 (87%)	172 (96%)	6 (3%)	2 (1%)	11	38
2	B	236/241 (98%)	225 (95%)	11 (5%)	0	100	100
2	F	225/241 (93%)	213 (95%)	12 (5%)	0	100	100
3	C	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
3	G	175/182 (96%)	168 (96%)	7 (4%)	0	100	100
4	D	195/217 (90%)	185 (95%)	9 (5%)	1 (0%)	24	55
4	H	195/217 (90%)	189 (97%)	6 (3%)	0	100	100
All	All	1576/1692 (93%)	1506 (96%)	65 (4%)	5 (0%)	36	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY
1	E	60	GLY
1	E	79	ASP
1	A	79	ASP
4	D	105	SER

5.3.2 Protein sidechains ⓘ

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	157/185 (85%)	143 (91%)	14 (9%)	9	30
1	E	143/185 (77%)	120 (84%)	23 (16%)	2	11
2	B	185/206 (90%)	171 (92%)	14 (8%)	12	36
2	F	175/206 (85%)	165 (94%)	10 (6%)	18	46
3	C	147/163 (90%)	140 (95%)	7 (5%)	23	50
3	G	146/163 (90%)	138 (94%)	8 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	168/189 (89%)	155 (92%)	13 (8%)	12	36
4	H	166/189 (88%)	152 (92%)	14 (8%)	10	33
All	All	1287/1486 (87%)	1184 (92%)	103 (8%)	11	35

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	101	VAL
1	A	112	LEU
1	A	123	GLN
1	A	124	LEU
1	A	129	SER
1	A	134	VAL
1	A	146	VAL
1	A	160	CYS
1	A	164	MET
1	A	183	PHE
1	A	191	ASN
1	A	193	ILE
1	A	194	ILE
2	B	23	GLN
2	B	37	THR
2	B	78	LEU
2	B	80	THR
2	B	98	THR
2	B	106	ARG
2	B	134	THR
2	B	146	PHE
2	B	162	VAL
2	B	180	ASN
2	B	195	THR
2	B	204	PHE
2	B	215	GLU
2	B	238	ARG
3	C	5	VAL
3	C	19	ILE
3	C	36	LEU
3	C	60	LEU
3	C	88	GLN
3	C	95	SER

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Mol	Chain	Res	Type
3	C	98	LEU
4	D	-21	LYS
4	D	28	THR
4	D	38	VAL
4	D	44	VAL
4	D	87	GLU
4	D	92	LEU
4	D	95	LEU
4	D	101	VAL
4	D	115	THR
4	D	148	LEU
4	D	173	THR
4	D	176	VAL
4	D	181	LEU
1	E	2	GLN
1	E	3	VAL
1	E	10	LEU
1	E	11	THR
1	E	12	VAL
1	E	17	THR
1	E	63	THR
1	E	81	GLN
1	E	85	SER
1	E	87	THR
1	E	109	LYS
1	E	110	VAL
1	E	112	LEU
1	E	123	GLN
1	E	124	LEU
1	E	129	SER
1	E	134	VAL
1	E	146	VAL
1	E	160	CYS
1	E	164	MET
1	E	183	PHE
1	E	193	ILE
1	E	194	ILE
2	F	23	GLN
2	F	37	THR
2	F	80	THR
2	F	99	LEU
2	F	134	THR

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Mol	Chain	Res	Type
2	F	146	PHE
2	F	162	VAL
2	F	180	ASN
2	F	195	THR
2	F	204	PHE
3	G	14	GLN
3	G	36	LEU
3	G	42	VAL
3	G	60	LEU
3	G	98	LEU
3	G	116	VAL
3	G	120	THR
3	G	154	ILE
4	H	28	THR
4	H	70	ARG
4	H	71	THR
4	H	77	THR
4	H	90	THR
4	H	92	LEU
4	H	105	SER
4	H	107	THR
4	H	112	HIS
4	H	115	THR
4	H	130	VAL
4	H	140	THR
4	H	173	THR
4	H	181	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	76	HIS
1	A	113	HIS
2	B	8	ASN
2	B	27	HIS
2	B	69	GLN
2	B	133	HIS
3	C	84	ASN
3	C	101	GLN
4	D	10	GLN
4	D	47	HIS

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Mol	Chain	Res	Type
1	E	76	HIS
2	F	22	ASN
2	F	27	HIS
2	F	69	GLN
3	G	78	ASN
4	H	6	HIS
4	H	81	HIS
4	H	157	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	85:GLU	C	86:ALA	N	3.12

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	197/206 (95%)	-0.11	2 (1%) 79 62	22, 40, 83, 109	0
1	E	188/206 (91%)	0.93	23 (12%) 8 7	62, 99, 133, 142	0
2	B	238/241 (98%)	-0.20	3 (1%) 75 56	20, 38, 70, 107	0
2	F	229/241 (95%)	0.76	23 (10%) 12 10	60, 92, 123, 153	0
3	C	179/182 (98%)	-0.25	2 (1%) 78 60	23, 41, 72, 95	0
3	G	179/182 (98%)	0.35	6 (3%) 48 32	53, 79, 113, 132	0
4	D	199/217 (91%)	-0.28	0 100 100	27, 44, 71, 100	0
4	H	199/217 (91%)	0.27	5 (2%) 58 39	54, 73, 96, 114	0
All	All	1608/1692 (95%)	0.18	64 (3%) 42 28	20, 65, 113, 153	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	153	ASP	5.0
1	E	190	ASN	5.0
1	E	197	ASP	4.9
2	F	225	LYS	4.7
1	E	145	ASN	4.5
1	E	193	ILE	4.1
2	F	112	ASP	4.1
2	F	215	GLU	4.0
2	F	111	GLU	3.9
1	E	187	ASN	3.8
1	E	194	ILE	3.6
3	G	124	ASN	3.5
1	E	147	SER	3.5
3	G	86	ALA	3.4
2	F	179	LEU	3.3
1	E	167	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	178	ALA	3.0
1	E	154	VAL	3.0
1	A	193	ILE	3.0
3	G	129	ALA	2.9
2	F	26	ASN	2.9
1	E	169	PHE	2.9
2	F	113	LEU	2.8
1	E	165	ARG	2.8
2	F	135	GLN	2.8
2	F	237	GLY	2.7
1	E	189	PHE	2.7
1	E	117	PRO	2.7
2	B	215	GLU	2.6
4	H	19	ASN	2.6
4	H	52	GLU	2.6
1	E	191	ASN	2.6
3	C	0	ILE	2.5
4	H	6	HIS	2.5
1	E	113	HIS	2.5
1	E	111	TYR	2.4
2	F	198	GLN	2.4
1	E	112	LEU	2.4
1	E	135	CYS	2.4
4	H	109	ALA	2.4
3	G	130	ASP	2.4
2	F	24	THR	2.3
1	A	153	ASP	2.3
2	F	176	GLN	2.3
2	B	238	ARG	2.3
3	G	0	ILE	2.3
2	F	1	ALA	2.3
1	E	133	SER	2.3
4	H	105	SER	2.3
1	E	179	ASN	2.3
2	F	203	HIS	2.2
2	F	115	ASN	2.2
1	E	164	MET	2.2
2	F	16	LYS	2.2
2	B	180	ASN	2.2
2	F	192	VAL	2.2
2	F	209	GLN	2.2
3	G	154	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	147	TYR	2.1
2	F	114	LYS	2.1
2	F	226	PRO	2.1
3	C	129	ALA	2.1
1	E	158	ASP	2.0
2	F	18	THR	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.