Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 PM GMT

PDB ID	:	4P5T
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

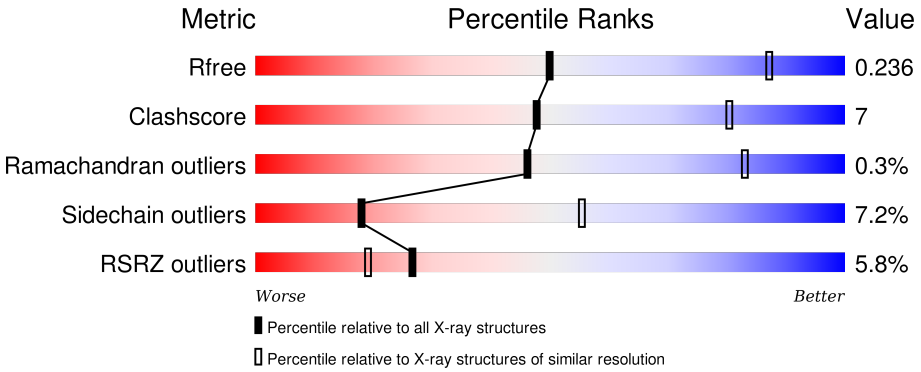
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	206	77% 18% •
1	E	206	17% 70% 18% • 9%
2	B	241	76% 20% ••
2	F	241	11% 74% 20% • 5%
3	C	182	% 81% 16% ••

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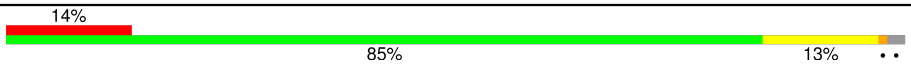
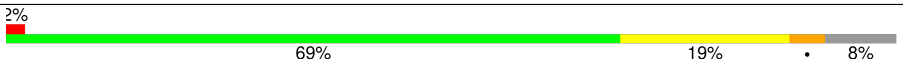
Mol	Chain	Length	Quality of chain
3	G	182	
4	D	217	
4	H	217	

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.

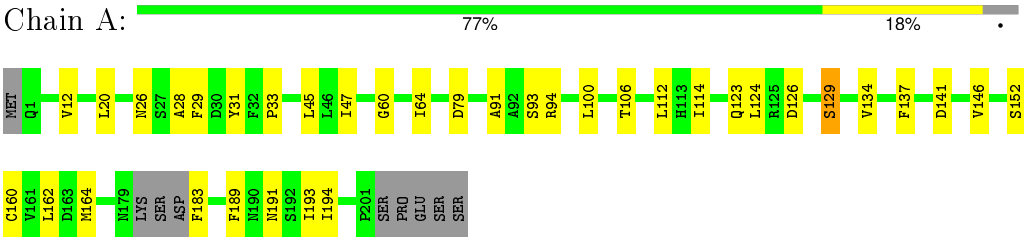
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	199	Total	C	N	O	S	0	0	0
			1593	1001	279	307	6			
4	H	199	Total	C	N	O	S	0	0	0
			1584	997	275	306	6			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

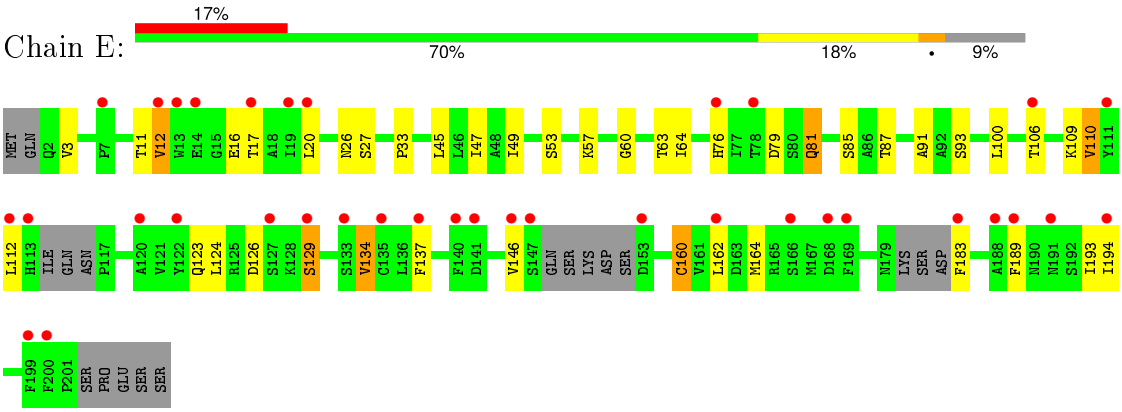
- Molecule 1: TRA protein

Chain A:



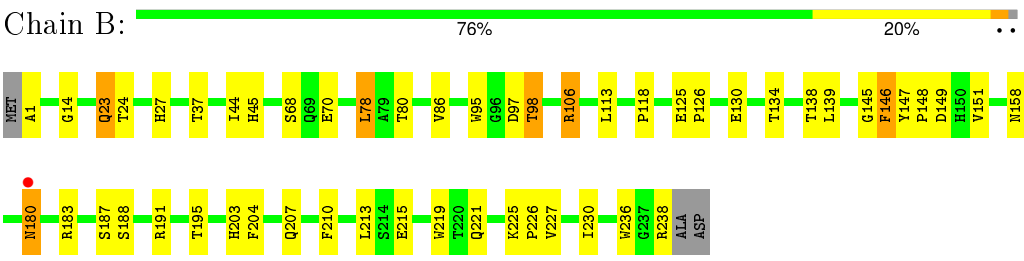
- Molecule 1: TRA protein

Chain E:



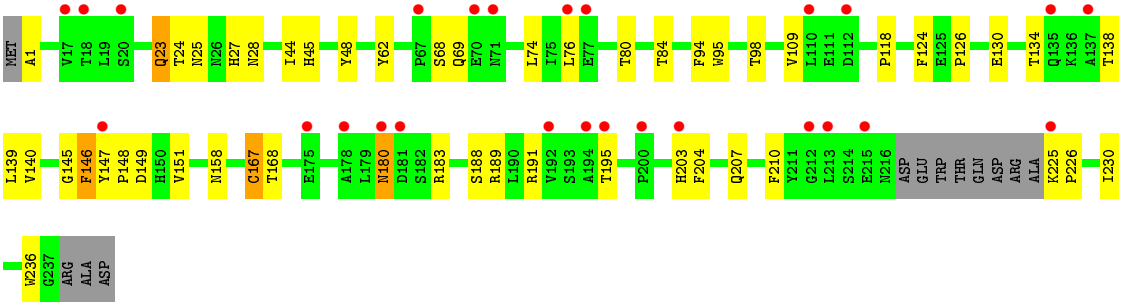
- Molecule 2: Human nkt tcr beta chain

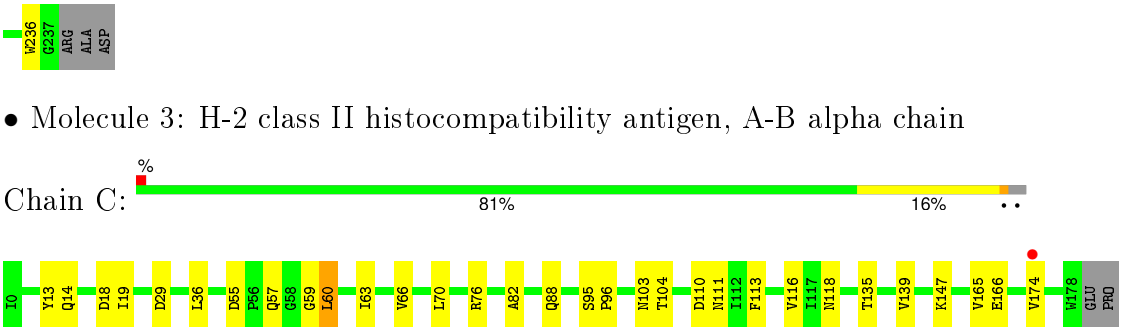
Chain B:



- Molecule 2: Human nkt tcr beta chain

Chain F:

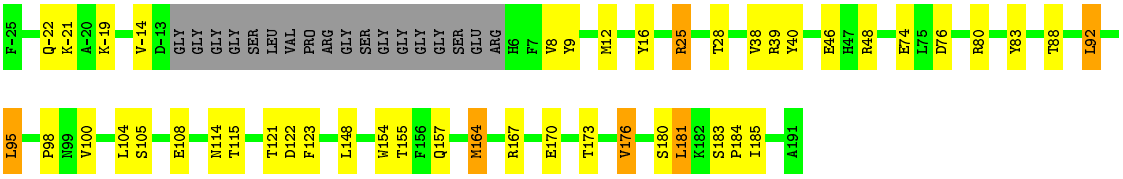




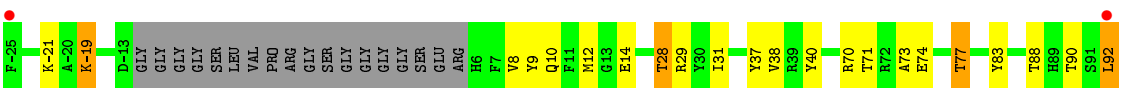
• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

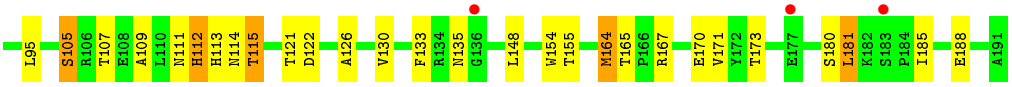
• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

• 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




L95
S105
R106
T107
E108
A109
L110
N111
H112
H113
N114
T115
T121
D122
A126
V130
F133
R134
N135
G136
L148
W154
T155
M164
T165
P166
R167
E170
V171
Y172
T173
E177
S180
L181
K182
S183
P184
I185
E188
A191

4 Data and refinement statistics (i)

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 48.78 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.05-3.26) 99.0 (48.78-3.26)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.42 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.186 , 0.236 0.186 , 0.236	Depositor DCC
R_{free} test set	1957 reflections (5.01%)	DCC
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 , 66.5	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 39092 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0/1525	0.40	0/2078
1	E	0.24	0/1438	0.38	0/1960
2	B	0.25	0/1868	0.44	0/2558
2	F	0.23	0/1775	0.41	0/2432
3	C	0.25	0/1425	0.40	0/1957
3	G	0.22	0/1420	0.38	0/1949
4	D	0.24	0/1632	0.40	0/2225
4	H	0.24	0/1623	0.40	0/2214
All	All	0.24	0/12706	0.40	0/17373

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	1488	0	1353	18	0
1	E	1403	0	1255	17	0
2	B	1815	0	1654	36	0
2	F	1725	0	1561	41	0
3	C	1381	0	1263	18	0
3	G	1377	0	1256	15	0
4	D	1593	0	1471	30	0
4	H	1584	0	1456	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12366	0	11269	174	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 7.

All (174) 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
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
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
3:C:139:VAL:HG11	4:D:12:MET:HE1	1.75	0.68
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
4:D:114:ASN:HB3	4:D:164:MET:HE1	1.80	0.62
1:E:93:SER:HB2	1:E:100:LEU:HD23	1.82	0.61
4:H:113:HIS:H	4:H:165:THR:HG23	1.66	0.61
3:C:14:GLN:HG2	4:D:8:VAL:HG22	1.82	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:B:1:ALA:H3	2:B:24:THR:HB	1.68	0.58
2:F:180:ASN:N	2:F:180:ASN:OD1	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
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
4:H:114:ASN:HB3	4:H:164:MET:HE1	1.87	0.55
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:E:49:ILE:HD11	1:E:53:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:134:VAL:HB	2:F:124:PHE:CD2	2.41	0.54
2:B:158:ASN:HA	2:B:203:HIS:CE1	2.42	0.53
1:A:33:PRO:HG2	1:A:91:ALA:HB3	1.89	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:N	2:B:180:ASN:OD1	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
1:A:152:SER:C	1:A:154:VAL:H	2.14	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:H	2:B:146:PHE:HD2	1.60	0.49
2:F:94:PHE:CG	3:G:65:VAL:HG22	2.47	0.49
2:F:203:HIS:HB3	2:F:236:TRP:CE3	2.47	0.48
2:F:146:PHE:HE1	2:F:151:VAL:HG21	1.78	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:F:146:PHE:HD2	2:F:146:PHE:H	1.60	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
1:A:47:ILE:HG23	1:A:64:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ASP:HB3	1:E:129:SER:O	2.14	0.48
4:D:176:VAL:HG13	4:D:185:ILE:HB	1.95	0.47
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
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
4:H:167:ARG:O	4:H:170:GLU:HG2	2.15	0.46
2:F:158:ASN:HA	2:F:203:HIS:HE1	1.81	0.46
2:F:23:GLN:OE1	2:F:27:HIS:N	2.40	0.46
1:E:20:LEU:HD22	1:E:106:THR:HG21	1.97	0.46
3:C:66:VAL:HG13	4:D:9:TYR:CD2	2.51	0.46
2:B:158:ASN:HA	2:B:203:HIS:HE1	1.81	0.46
1:A:126:ASP:HB3	1:A:129:SER:O	2.16	0.46
3:C:96:PRO:HD3	4:D:121:THR:HG21	1.98	0.46
4:D:-19:LYS:HG2	4:D:74:GLU:OE1	2.16	0.46
3:C:82:ALA:HB1	3:C:113:PHE:CE2	2.51	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:HB3	2:F:23:GLN:HE21	1.52	0.45
1:A:29:PHE:HD1	1:A:94:ARG:HG2	1.81	0.45
2:F:28:ASN:HA	2:F:69:GLN:HE22	1.82	0.45
1:E:137:PHE:HB2	1:E:189:PHE:CE2	2.51	0.45
1:A:137:PHE:HB2	1:A:189:PHE:CE2	2.50	0.45
4:H:-19:LYS:HG2	4:H:74:GLU:OE1	2.17	0.45
2:B:207:GLN:HG3	2:B:230:ILE:HG23	1.99	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
2:F:138:THR:HG1	2:F:191:ARG:HH11	1.64	0.45
3:C:57:GLN:HA	3:C:60:LEU:HB2	1.98	0.45
2:F:151:VAL:HG12	2:F:210:PHE:HA	1.99	0.44
4:H:83:TYR:O	4:H:88:THR:HG23	2.17	0.44
1:A:31:TYR:OH	2:B:97:ASP:HB2	2.17	0.44
2:F:118:PRO:HD3	2:F:226:PRO:HB3	1.99	0.44
2:B:118:PRO:HD3	2:B:226:PRO:HB3	2.00	0.44
2:F:207:GLN:HG3	2:F:230:ILE:HG23	1.99	0.44
1:A:29:PHE:CD1	1:A:94:ARG:HG2	2.53	0.44
2:F:149:ASP:N	2:F:149:ASP:OD1	2.50	0.44
2:B:219:TRP:CE2	2:B:221:GLN:HB2	2.52	0.44
2:B:151:VAL:HG12	2:B:210:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:ASP:OD1	2:B:149:ASP:N	2.50	0.43
3:G:99:LEU:HA	3:G:155:PRO:HB2	1.99	0.43
2:B:14:GLY:HA2	2:B:78:LEU:HD23	2.01	0.43
4:H:28:THR:HG22	4:H:40:TYR:HB3	2.01	0.43
3:C:76:ARG:NH2	4:D:-14:VAL:O	2.52	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
1:E:126:ASP:HA	2:F:124:PHE:CD1	2.54	0.42
4:D:98:PRO:HB3	4:D:123:PHE:HB3	2.01	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
3:G:96:PRO:HD3	4:H:121:THR:HG21	2.02	0.41
2:B:125:GLU:HA	2:B:126:PRO:HD3	1.96	0.41
1:A:45:LEU:HD22	2:B:98:THR:HG22	2.01	0.41
2:F:140:VAL:HG22	2:F:189:ARG:HG3	2.02	0.41
2:B:95:TRP:CD2	4:D:-19:LYS:HB2	2.55	0.41
4:H:88:THR:HA	4:H:92:LEU:HB2	2.02	0.41
1:A:157:THR:HG21	2:B:187:SER:OG	2.20	0.41
3:G:9:GLY:O	4:H:12:MET:HA	2.20	0.41
1:A:152:SER:O	1:A:154:VAL:N	2.51	0.41
3:G:101:GLN:HA	3:G:102:PRO:HD2	1.83	0.41
2:F:146:PHE:CD2	2:F:146:PHE:N	2.88	0.41
2:F:76:LEU:HA	2:F:76:LEU:HD12	1.83	0.41
1:E:26:ASN:OD1	1:E:27:SER:N	2.54	0.41
4:D:12:MET:HB3	4:D:12:MET:HE3	1.92	0.41
4:D:83:TYR:O	4:D:88:THR:HG23	2.21	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
2:F:126:PRO:HD3	2:F:139:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:TYR:OH	3:C:18:ASP:OD1	2.22	0.41
4:D:92:LEU:HA	4:D:92:LEU:HD12	1.88	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
2:B:138:THR:OG1	2:B:191:ARG:HD2	2.21	0.41
1:E:33:PRO:HG2	1:E:91:ALA:HB3	2.03	0.41
1:E:12:VAL:HG13	1:E:16:GLU:HB2	2.03	0.41
2:B:126:PRO:HD3	2:B:139:LEU:HG	2.03	0.40
4:D:167:ARG:HB2	4:D:170:GLU:HG3	2.03	0.40
4:D:104:LEU:HD21	4:D:108:GLU:HB2	2.03	0.40
2:B:176:GLN:HA	2:B:177:PRO:HD2	1.94	0.40
4:H:133:PHE:HB2	4:H:173:THR:HB	2.02	0.40
2:B:113:LEU:HD21	2:B:213:LEU:HD21	2.02	0.40
2:F:95:TRP:CE2	4:H:-19:LYS:HB2	2.57	0.40
1:E:160:CYS:HB3	2:F:189:ARG:NH2	2.36	0.40
3:C:14:GLN:OE1	3:C:116:VAL:HG23	2.21	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 (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	193/206 (94%)	182 (94%)	9 (5%)	2 (1%)	19	62
1	E	180/206 (87%)	172 (96%)	6 (3%)	2 (1%)	17	60
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	195/217 (90%)	185 (95%)	9 (5%)	1 (0%)	34 75
4	H	195/217 (90%)	189 (97%)	6 (3%)	0	100 100
All	All	1576/1692 (93%)	1506 (96%)	65 (4%)	5 (0%)	46 83

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%)	144 (92%)	13 (8%)	14 48
1	E	143/185 (77%)	121 (85%)	22 (15%)	3 16
2	B	185/206 (90%)	172 (93%)	13 (7%)	19 57
2	F	175/206 (85%)	167 (95%)	8 (5%)	33 72
3	C	147/163 (90%)	142 (97%)	5 (3%)	44 79
3	G	146/163 (90%)	141 (97%)	5 (3%)	44 79
4	D	168/189 (89%)	156 (93%)	12 (7%)	18 56
4	H	166/189 (88%)	151 (91%)	15 (9%)	12 42
All	All	1287/1486 (87%)	1194 (93%)	93 (7%)	18 55

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	112	LEU

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Mol	Chain	Res	Type
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	180	ASN
2	B	195	THR
2	B	204	PHE
2	B	215	GLU
2	B	238	ARG
3	C	19	ILE
3	C	36	LEU
3	C	60	LEU
3	C	88	GLN
3	C	95	SER
4	D	-21	LYS
4	D	25	ARG
4	D	38	VAL
4	D	39	ARG
4	D	92	LEU
4	D	95	LEU
4	D	115	THR
4	D	148	LEU
4	D	164	MET
4	D	173	THR
4	D	176	VAL
4	D	181	LEU
1	E	3	VAL

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Mol	Chain	Res	Type
1	E	11	THR
1	E	12	VAL
1	E	17	THR
1	E	63	THR
1	E	76	HIS
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	80	THR
2	F	134	THR
2	F	146	PHE
2	F	167	CYS
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	116	VAL
3	G	120	THR
4	H	-21	LYS
4	H	-19	LYS
4	H	28	THR
4	H	70	ARG
4	H	71	THR
4	H	77	THR
4	H	90	THR
4	H	92	LEU

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Mol	Chain	Res	Type
4	H	105	SER
4	H	107	THR
4	H	112	HIS
4	H	115	THR
4	H	130	VAL
4	H	164	MET
4	H	181	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	69	GLN
4	D	10	GLN
2	F	27	HIS
2	F	69	GLN
4	H	157	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 carbohydrates 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

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, 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	197/206 (95%)	0.02	0 100 100	22, 40, 83, 109	0
1	E	188/206 (91%)	1.14	36 (19%) 2 1	62, 99, 133, 142	0
2	B	238/241 (98%)	0.05	1 (0%) 93 91	20, 38, 70, 107	0
2	F	229/241 (95%)	0.95	26 (11%) 7 5	60, 92, 123, 153	0
3	C	179/182 (98%)	0.12	1 (0%) 90 86	23, 41, 72, 95	0
3	G	179/182 (98%)	0.83	25 (13%) 4 3	53, 79, 113, 132	0
4	D	199/217 (91%)	-0.02	0 100 100	27, 44, 71, 100	0
4	H	199/217 (91%)	0.24	5 (2%) 61 51	54, 73, 96, 114	0
All	All	1608/1692 (95%)	0.41	94 (5%) 26 19	20, 65, 113, 153	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	146	VAL	4.6
3	G	86	ALA	4.5
2	F	194	ALA	4.3
3	G	173	PRO	4.2
1	E	166	SER	4.0
1	E	147	SER	4.0
1	E	111	TYR	3.9
1	E	113	HIS	3.9
3	G	177	HIS	3.7
1	E	191	ASN	3.6
2	F	215	GLU	3.5
1	E	153	ASP	3.5
2	F	112	ASP	3.4
1	E	168	ASP	3.3
1	E	199	PHE	3.3
2	F	135	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	112	LEU	3.2
2	F	180	ASN	3.1
2	F	192	VAL	3.1
1	E	122	TYR	3.0
3	G	157	ASP	3.0
3	G	155	PRO	2.9
3	G	178	TRP	2.9
1	E	140	PHE	2.9
1	E	141	ASP	2.9
3	G	129	ALA	2.9
2	F	70	GLU	2.9
3	G	84	ASN	2.8
1	E	7	PRO	2.8
2	F	18	THR	2.8
1	E	135	CYS	2.8
2	F	181	ASP	2.8
3	G	162	ASP	2.7
2	F	203	HIS	2.7
3	G	121	TRP	2.7
3	G	156	SER	2.7
3	G	164	LYS	2.7
3	G	160	ILE	2.7
1	E	129	SER	2.6
1	E	133	SER	2.6
1	E	200	PHE	2.6
2	F	212	GLY	2.6
1	E	127	SER	2.6
3	G	122	LEU	2.6
2	F	17	VAL	2.5
3	G	161	TYR	2.5
1	E	188	ALA	2.5
2	F	213	LEU	2.5
2	F	200	PRO	2.5
3	G	172	GLU	2.4
2	F	175	GLU	2.4
4	H	136	GLY	2.4
3	G	125	SER	2.4
2	F	147	TYR	2.4
2	F	67	PRO	2.4
1	E	137	PHE	2.4
1	E	189	PHE	2.4
1	E	106	THR	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	183	SER	2.3
2	F	110	LEU	2.3
1	E	78	THR	2.3
3	G	175	LEU	2.3
3	G	166	GLU	2.3
1	E	162	LEU	2.3
1	E	169	PHE	2.3
4	H	92	LEU	2.2
4	H	-25	PHE	2.2
1	E	19	ILE	2.2
2	F	178	ALA	2.2
1	E	120	ALA	2.2
2	F	77	GLU	2.2
2	F	225	LYS	2.2
3	G	120	THR	2.2
3	G	149	SER	2.2
1	E	76	HIS	2.2
1	E	12	VAL	2.2
1	E	14	GLU	2.2
1	E	20	LEU	2.2
2	F	76	LEU	2.2
2	F	71	ASN	2.2
1	E	17	THR	2.1
1	E	13	TRP	2.1
2	F	137	ALA	2.1
3	G	153	PHE	2.1
3	G	128	VAL	2.1
3	G	174	VAL	2.1
1	E	183	PHE	2.1
2	F	20	SER	2.1
1	E	194	ILE	2.1
2	B	180	ASN	2.1
3	G	133	TYR	2.1
4	H	177	GLU	2.0
3	C	174	VAL	2.0
2	F	195	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.