Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 08:21 PM EDT

PDB ID	:	5IW1
Title	:	Crystal Structure of B4.2.3 T-Cell Receptor
Authors	:	Natarajan, K.; Jiang, J.; Margulies, D.
Deposited on	:	2016-03-21
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:

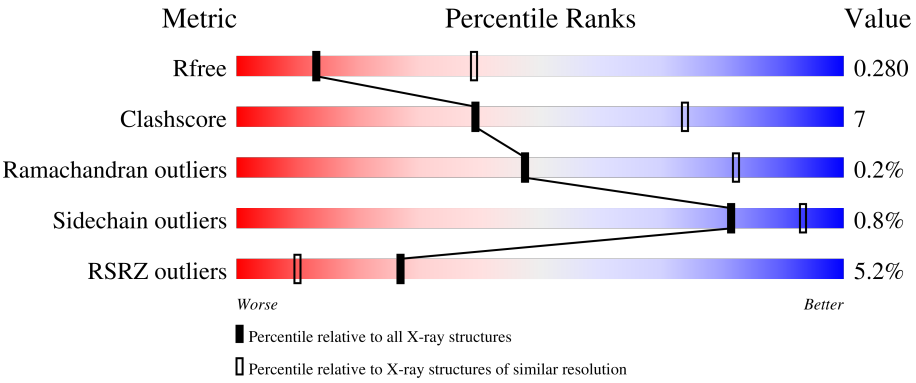
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	194	2% 75% 21%
1	C	194	2% 83% 14%
1	E	194	19% 82% 15%
2	B	235	78% 21%
2	D	235	76% 23%

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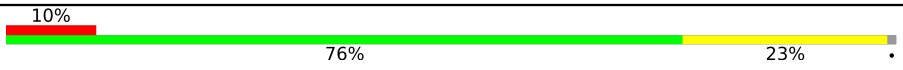
Mol	Chain	Length	Quality of chain
2	F	235	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10062 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	189	Total	C	N	O	S	12	0	0
			1478	934	242	294	8			
1	C	189	Total	C	N	O	S	27	0	0
			1478	934	242	294	8			
1	E	189	Total	C	N	O	S	5	0	0
			1478	934	242	294	8			

- Molecule 2 is a protein called T-CELL RECEPTOR BETA CHAIN.

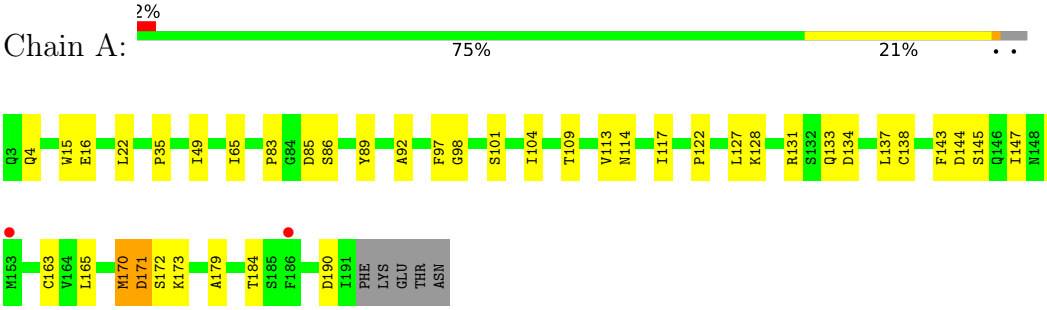
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	2	0	0
			1876	1187	331	349	9			
2	D	233	Total	C	N	O	S	0	0	0
			1876	1187	331	349	9			
2	F	233	Total	C	N	O	S	0	0	0
			1876	1187	331	349	9			

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.

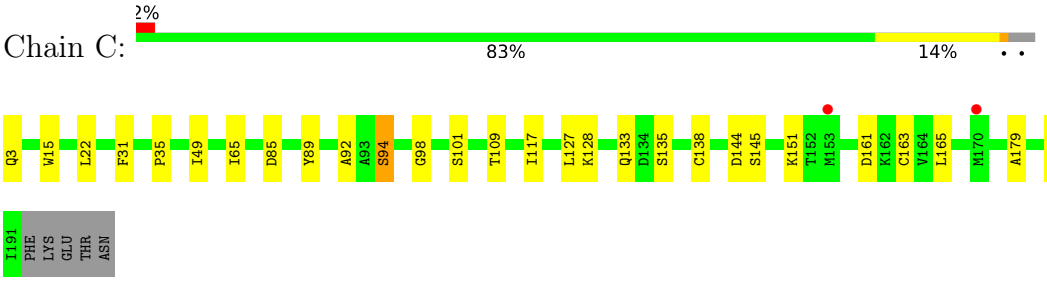
• Molecule 1: T-CELL RECEPTOR ALPHA CHAIN

Chain A:



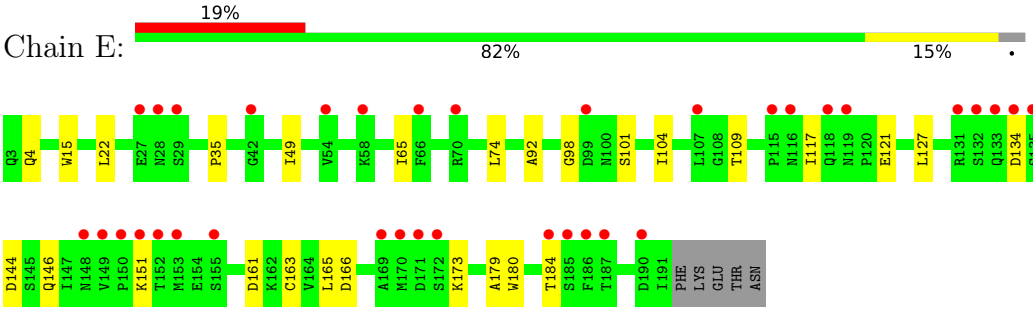
• Molecule 1: T-CELL RECEPTOR ALPHA CHAIN

Chain C:



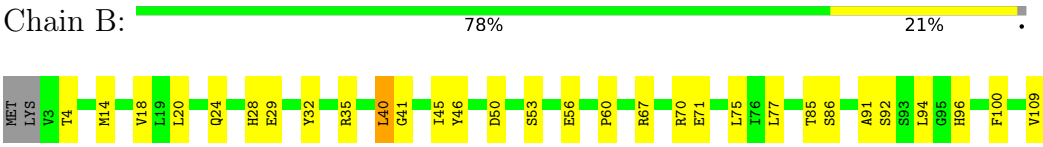
• Molecule 1: T-CELL RECEPTOR ALPHA CHAIN

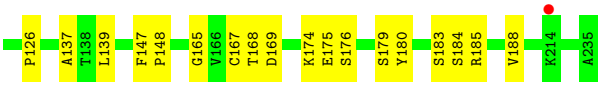
Chain E:



• Molecule 2: T-CELL RECEPTOR BETA CHAIN

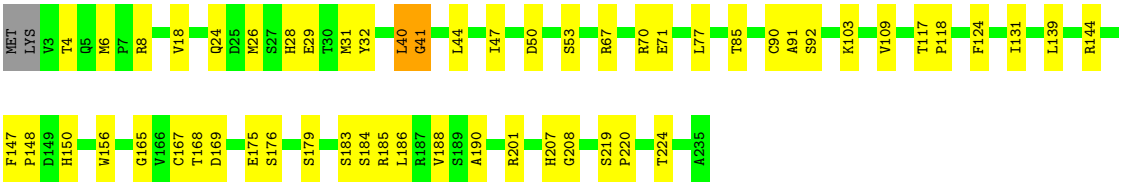
Chain B:





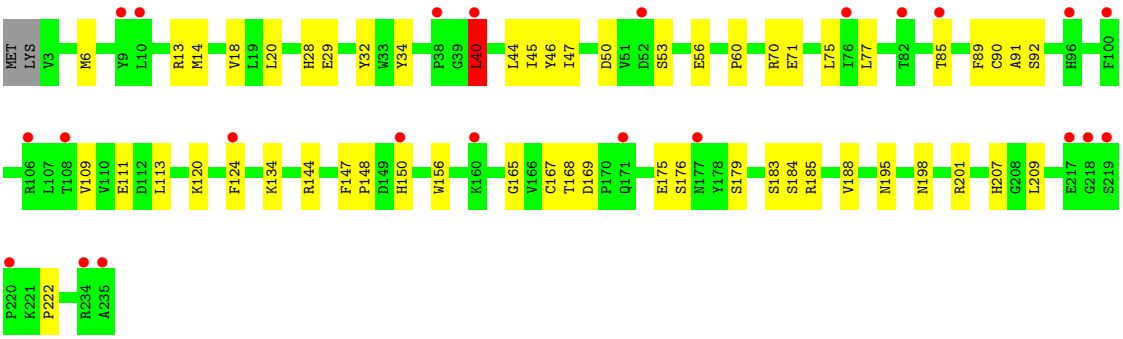
• Molecule 2: T-CELL RECEPTOR BETA CHAIN

Chain D:



• Molecule 2: T-CELL RECEPTOR BETA CHAIN

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	96.11Å 96.11Å 167.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.06 – 3.00 48.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.4 (48.06-3.00) 94.4 (48.06-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.240 , 0.268 0.240 , 0.280	Depositor DCC
R_{free} test set	1934 reflections (5.92%)	wwPDB-VP
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.649	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 10.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.458 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10062	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/1513	0.45	1/2054 (0.0%)
1	C	0.23	0/1513	0.42	1/2054 (0.0%)
1	E	0.22	0/1513	0.41	0/2054
2	B	0.22	0/1927	0.40	0/2611
2	D	0.22	0/1927	0.40	0/2611
2	F	0.21	0/1927	0.56	2/2611 (0.1%)
All	All	0.22	0/10320	0.45	4/13995 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	40	LEU	N-CA-C	16.23	154.84	111.00
2	F	40	LEU	CB-CA-C	-13.48	84.58	110.20
1	C	94	SER	CB-CA-C	6.44	122.34	110.10
1	A	170	MET	N-CA-C	5.38	125.53	111.00

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	1478	0	1414	27	0
1	C	1478	0	1414	18	0
1	E	1478	0	1414	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1876	0	1811	33	0
2	D	1876	0	1811	34	0
2	F	1876	0	1811	32	0
All	All	10062	0	9675	146	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 (146) 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:D:85:THR:HG22	2:D:109:VAL:H	1.44	0.83
2:F:85:THR:HG22	2:F:109:VAL:H	1.48	0.79
2:F:32:TYR:HB2	2:F:91:ALA:HB3	1.65	0.78
2:B:85:THR:HG22	2:B:109:VAL:H	1.49	0.77
1:E:117:ILE:HD11	1:E:144:ASP:HA	1.65	0.76
2:D:32:TYR:HB2	2:D:91:ALA:HB3	1.68	0.76
1:C:117:ILE:HD11	1:C:144:ASP:HA	1.68	0.75
1:A:170:MET:O	1:A:171:ASP:C	2.26	0.73
2:B:32:TYR:HB2	2:B:91:ALA:HB3	1.75	0.67
1:E:35:PRO:HG2	1:E:92:ALA:HB3	1.75	0.67
2:D:28:HIS:HE1	2:D:31:MET:HG2	1.62	0.65
1:A:117:ILE:HD11	1:A:144:ASP:HA	1.79	0.64
1:A:134:ASP:HB2	1:A:184:THR:HG23	1.79	0.64
1:C:127:LEU:HB3	2:D:124:PHE:HB3	1.78	0.64
1:E:98:GLY:O	1:E:101:SER:OG	2.17	0.62
2:B:28:HIS:NE2	2:B:92:SER:HB2	2.15	0.62
2:B:29:GLU:O	2:B:67:ARG:NH2	2.29	0.62
2:D:26:MET:HG3	2:D:28:HIS:HD2	1.66	0.61
1:A:138:CYS:HB2	1:A:179:ALA:HB3	1.83	0.61
1:A:85:ASP:O	1:A:89:TYR:OH	2.12	0.60
1:C:138:CYS:HB2	1:C:179:ALA:HB3	1.83	0.60
1:E:151:LYS:NZ	1:E:161:ASP:OD1	2.33	0.60
1:A:163:CYS:O	2:B:185:ARG:NH2	2.35	0.60
1:A:165:LEU:HD13	2:B:167:CYS:HB2	1.82	0.59
1:E:165:LEU:HD13	2:F:167:CYS:HB2	1.83	0.59
1:A:98:GLY:O	1:A:101:SER:OG	2.17	0.58
1:A:35:PRO:HG2	1:A:92:ALA:HB3	1.83	0.58
2:B:169:ASP:OD2	2:B:183:SER:OG	2.18	0.58
1:C:163:CYS:O	2:D:185:ARG:NH2	2.28	0.58
2:F:18:VAL:HB	2:F:77:LEU:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:LEU:HD12	2:F:75:LEU:HD23	1.84	0.58
1:A:97:PHE:O	2:B:96:HIS:ND1	2.37	0.58
2:B:29:GLU:OE1	2:B:70:ARG:NH1	2.37	0.58
1:E:134:ASP:HB2	1:E:184:THR:HG23	1.84	0.58
2:D:29:GLU:O	2:D:67:ARG:NH2	2.31	0.57
1:C:85:ASP:O	1:C:89:TYR:OH	2.21	0.57
1:C:31:PHE:HA	1:C:94:SER:O	2.05	0.57
2:D:169:ASP:OD2	2:D:183:SER:OG	2.21	0.57
1:C:165:LEU:HD13	2:D:167:CYS:HB2	1.86	0.56
2:F:168:THR:HG23	2:F:184:SER:HB2	1.88	0.56
1:A:22:LEU:HD23	1:A:109:THR:HB	1.88	0.55
2:B:168:THR:HG23	2:B:184:SER:HB2	1.88	0.55
1:E:163:CYS:O	2:F:185:ARG:NH2	2.28	0.55
2:F:28:HIS:CE1	2:F:92:SER:HB2	2.42	0.55
1:C:151:LYS:NZ	1:C:161:ASP:OD1	2.38	0.55
1:E:165:LEU:HD11	2:F:165:GLY:C	2.27	0.55
2:D:150:HIS:HB3	2:D:207:HIS:HB2	1.90	0.54
1:A:49:ILE:HG23	1:A:65:ILE:HD11	1.89	0.54
1:E:49:ILE:HG23	1:E:65:ILE:HD11	1.89	0.54
2:F:169:ASP:OD2	2:F:183:SER:OG	2.22	0.54
2:D:168:THR:HG23	2:D:184:SER:HB2	1.89	0.53
2:D:18:VAL:HB	2:D:77:LEU:HB2	1.90	0.53
2:F:56:GLU:HB3	2:F:60:PRO:HG3	1.91	0.53
1:C:35:PRO:HG2	1:C:92:ALA:HB3	1.90	0.52
2:F:150:HIS:HB3	2:F:207:HIS:HB2	1.92	0.52
1:E:15:TRP:HZ2	1:E:146:GLN:HB3	1.75	0.52
1:C:182:ASN:OD1	2:D:144:ARG:NH2	2.25	0.51
1:C:165:LEU:HD11	2:D:165:GLY:C	2.31	0.51
2:D:131:ILE:HG23	2:D:190:ALA:HB1	1.92	0.51
2:F:6:MET:HE1	2:F:90:CYS:HB3	1.93	0.51
2:F:20:LEU:HB2	2:F:75:LEU:HB3	1.91	0.51
2:F:71:GLU:OE1	2:F:71:GLU:N	2.44	0.51
2:F:45:ILE:HG22	2:F:46:TYR:HD1	1.77	0.50
1:A:165:LEU:HD11	2:B:165:GLY:C	2.32	0.50
2:F:209:LEU:HD13	2:F:222:PRO:HG2	1.93	0.50
1:A:128:LYS:NZ	1:A:133:GLN:HA	2.27	0.49
2:B:176:SER:HB3	2:B:179:SER:HB3	1.94	0.49
2:B:28:HIS:CE1	2:B:92:SER:HB2	2.47	0.49
1:A:131:ARG:HH22	2:B:122:SER:HA	1.77	0.49
2:B:71:GLU:N	2:B:71:GLU:OE1	2.45	0.49
2:D:71:GLU:N	2:D:71:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLU:HB3	2:B:60:PRO:HG3	1.95	0.48
1:A:15:TRP:CH2	1:A:145:SER:HB2	2.47	0.48
2:D:28:HIS:NE2	2:D:92:SER:HB2	2.28	0.48
1:C:15:TRP:CH2	1:C:145:SER:HB2	2.49	0.48
2:B:50:ASP:HB2	2:B:70:ARG:HH12	1.78	0.48
1:A:128:LYS:HZ1	1:A:133:GLN:HA	1.78	0.48
2:B:4:THR:HG22	2:B:24:GLN:HB3	1.96	0.48
1:A:190:ASP:OD2	2:F:195:ASN:ND2	2.47	0.48
2:F:44:LEU:HD21	2:F:47:ILE:HD11	1.96	0.47
1:C:49:ILE:HG23	1:C:65:ILE:HD11	1.95	0.47
2:B:126:PRO:HD3	2:B:139:LEU:HD23	1.96	0.47
1:A:170:MET:O	1:A:172:SER:N	2.47	0.47
1:C:128:LYS:NZ	1:C:133:GLN:HA	2.30	0.47
2:D:175:GLU:OE2	2:D:179:SER:OG	2.29	0.47
2:B:18:VAL:HB	2:B:77:LEU:HB2	1.95	0.47
2:D:29:GLU:OE1	2:D:70:ARG:NH1	2.48	0.47
2:D:176:SER:HB3	2:D:179:SER:HB3	1.96	0.47
2:B:35:ARG:HH21	2:B:86:SER:HB3	1.79	0.46
2:B:40:LEU:HD12	2:B:41:GLY:H	1.79	0.46
1:E:166:ASP:HB2	1:E:173:LYS:HE3	1.96	0.46
2:F:14:MET:HG2	2:F:111:GLU:HA	1.97	0.46
2:B:174:LYS:HD3	2:B:180:TYR:CZ	2.51	0.46
2:D:28:HIS:CE1	2:D:92:SER:HB2	2.51	0.46
1:A:16:GLU:N	1:A:114:ASN:O	2.49	0.46
2:F:147:PHE:HB3	2:F:148:PRO:HD3	1.98	0.46
2:D:4:THR:HG22	2:D:24:GLN:HB3	1.97	0.46
2:F:120:LYS:N	2:F:144:ARG:O	2.35	0.46
2:B:28:HIS:HB3	2:B:94:LEU:HB3	1.98	0.45
2:F:176:SER:HB3	2:F:179:SER:HB3	1.98	0.45
2:B:14:MET:HG2	2:B:111:GLU:HA	1.97	0.45
1:E:138:CYS:HB2	1:E:179:ALA:HB3	1.98	0.45
1:E:121:GLU:HB2	2:F:134:LYS:HE3	1.97	0.45
1:A:83:PRO:HA	1:A:113:VAL:HB	1.99	0.45
2:F:156:TRP:HB2	2:F:201:ARG:HB3	1.99	0.44
1:A:86:SER:HB3	1:A:113:VAL:H	1.82	0.44
2:D:8:ARG:NH2	2:D:103:LYS:HD2	2.33	0.44
2:F:50:ASP:N	2:F:53:SER:OG	2.45	0.44
1:C:98:GLY:O	1:C:101:SER:OG	2.29	0.44
1:E:15:TRP:CZ2	1:E:146:GLN:HB3	2.53	0.44
2:D:50:ASP:N	2:D:53:SER:OG	2.50	0.44
1:A:127:LEU:HB2	1:A:137:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:GLY:H	2:D:224:THR:HG22	1.83	0.43
2:B:175:GLU:OE2	2:B:179:SER:OG	2.30	0.43
1:E:22:LEU:HD23	1:E:109:THR:HB	2.00	0.43
2:D:147:PHE:HB3	2:D:148:PRO:HD3	2.00	0.43
2:F:29:GLU:OE1	2:F:70:ARG:NH1	2.52	0.43
2:D:219:SER:HA	2:D:220:PRO:HD3	1.89	0.43
1:E:127:LEU:HB3	2:F:124:PHE:HB3	2.00	0.43
1:C:128:LYS:HE2	1:C:135:SER:H	1.83	0.43
1:E:4:GLN:HB2	1:E:104:ILE:HG21	1.99	0.43
2:B:50:ASP:N	2:B:53:SER:OG	2.48	0.43
1:C:128:LYS:HZ1	1:C:133:GLN:HA	1.82	0.43
1:E:137:LEU:HD12	1:E:180:TRP:HB3	2.00	0.43
2:B:92:SER:O	2:B:100:PHE:N	2.36	0.43
2:F:13:ARG:NH1	2:F:113:LEU:H	2.16	0.43
2:F:175:GLU:OE2	2:F:179:SER:OG	2.28	0.42
2:D:28:HIS:CE1	2:D:31:MET:HG2	2.49	0.42
2:B:45:ILE:HG22	2:B:46:TYR:HD2	1.84	0.42
2:F:34:TYR:O	2:F:89:PHE:N	2.45	0.42
1:A:143:PHE:HB2	1:A:147:ILE:HD12	2.02	0.42
2:B:147:PHE:HB3	2:B:148:PRO:HD3	2.00	0.42
1:A:149:VAL:HA	1:A:150:PRO:HD3	1.87	0.42
2:D:40:LEU:HB2	2:D:41:GLY:H	1.76	0.42
2:D:139:LEU:N	2:D:186:LEU:O	2.42	0.42
2:B:14:MET:SD	2:B:111:GLU:HG2	2.60	0.41
2:D:44:LEU:HD21	2:D:47:ILE:HD11	2.02	0.41
1:C:22:LEU:HD23	1:C:109:THR:HB	2.01	0.41
2:D:156:TRP:HB2	2:D:201:ARG:HB3	2.02	0.41
2:D:6:MET:HE2	2:D:90:CYS:HB3	2.02	0.41
2:B:20:LEU:HB2	2:B:75:LEU:HB3	2.03	0.41
2:F:195:ASN:HB3	2:F:198:ASN:ND2	2.35	0.41
2:D:117:THR:HA	2:D:118:PRO:HD3	1.92	0.41
2:B:126:PRO:HG3	2:B:137:ALA:HB1	2.03	0.40
1:A:122:PRO:HB3	1:A:143:PHE:HA	2.02	0.40
1:A:4:GLN:HB2	1:A:104:ILE:HG21	2.03	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	187/194 (96%)	177 (95%)	9 (5%)	1 (0%)	29	68
1	C	187/194 (96%)	178 (95%)	9 (5%)	0	100	100
1	E	187/194 (96%)	179 (96%)	8 (4%)	0	100	100
2	B	231/235 (98%)	225 (97%)	6 (3%)	0	100	100
2	D	231/235 (98%)	225 (97%)	5 (2%)	1 (0%)	34	72
2	F	231/235 (98%)	225 (97%)	5 (2%)	1 (0%)	34	72
All	All	1254/1287 (97%)	1209 (96%)	42 (3%)	3 (0%)	47	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	41	GLY
1	A	171	ASP
2	F	40	LEU

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	167/172 (97%)	166 (99%)	1 (1%)	86	95
1	C	167/172 (97%)	166 (99%)	1 (1%)	86	95
1	E	167/172 (97%)	166 (99%)	1 (1%)	86	95
2	B	206/208 (99%)	204 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	206/208 (99%)	204 (99%)	2 (1%)	76 91
2	F	206/208 (99%)	204 (99%)	2 (1%)	76 91
All	All	1119/1140 (98%)	1110 (99%)	9 (1%)	81 93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LYS
2	B	40	LEU
2	B	188	VAL
1	C	3	GLN
2	D	40	LEU
2	D	188	VAL
1	E	74	LEU
2	F	40	LEU
2	F	188	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (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

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	189/194 (97%)	-0.46	3 (1%) 72 44	56, 86, 147, 172	2 (1%)
1	C	189/194 (97%)	-0.38	3 (1%) 72 44	59, 88, 146, 166	8 (4%)
1	E	189/194 (97%)	0.87	36 (19%) 1 0	60, 86, 122, 140	189 (100%)
2	B	233/235 (99%)	-0.50	1 (0%) 92 79	53, 86, 125, 152	1 (0%)
2	D	233/235 (99%)	-0.50	0 100 100	53, 87, 128, 147	0
2	F	233/235 (99%)	0.71	23 (9%) 7 2	65, 90, 119, 137	233 (100%)
All	All	1266/1287 (98%)	-0.05	66 (5%) 27 10	53, 87, 131, 172	433 (34%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	SER	8.3
1	E	170	MET	7.0
1	E	184	THR	6.7
1	E	172	SER	6.4
2	F	219	SER	5.4
2	F	52	ASP	5.4
1	A	186	PHE	5.2
2	F	96	HIS	5.1
2	F	235	ALA	5.0
1	E	153	MET	5.0
1	E	133	GLN	4.8
2	F	38	PRO	4.7
2	F	177	ASN	4.6
1	E	152	THR	4.5
1	E	171	ASP	4.4
1	E	42	GLY	4.0
1	E	116	ASN	3.9
2	F	218	GLY	3.8
1	E	99	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	136	THR	3.8
2	F	217	GLU	3.7
1	E	151	LYS	3.7
2	F	82	THR	3.7
2	F	76	ILE	3.6
2	F	160	LYS	3.5
1	E	27	GLU	3.5
1	A	153	MET	3.5
1	E	28	ASN	3.4
1	E	132	SER	3.4
1	E	148	ASN	3.4
2	F	40	LEU	3.4
1	C	170	MET	3.4
1	E	150	PRO	3.2
1	E	186	PHE	3.1
2	F	108	THR	3.1
1	E	169	ALA	3.1
1	E	115	PRO	3.0
1	C	184	THR	3.0
2	F	150	HIS	3.0
1	E	135	SER	3.0
1	E	155	SER	3.0
2	B	214	LYS	3.0
1	E	131	ARG	2.9
1	E	118	GLN	2.7
1	E	107	LEU	2.7
2	F	124	PHE	2.7
1	C	153	MET	2.6
1	E	149	VAL	2.5
2	F	9	TYR	2.4
1	E	190	ASP	2.3
1	E	134	ASP	2.3
1	E	66	PHE	2.3
2	F	10	LEU	2.2
1	E	54	VAL	2.2
1	E	29	SER	2.2
1	E	119	ASN	2.2
2	F	106	ARG	2.2
1	E	58	LYS	2.2
2	F	171	GLN	2.1
1	E	70	ARG	2.1
1	A	152	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	85	THR	2.1
2	F	220	PRO	2.1
2	F	100	PHE	2.0
2	F	234	ARG	2.0
1	E	187	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.