



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2022 – 07:48 PM EDT

PDB ID : 8D5P
Title : Mouse TCR TG6
Authors : Wang, Y.; Dai, S.
Deposited on : 2022-06-05
Resolution : 2.75 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	:	2.29
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)	:	2.29

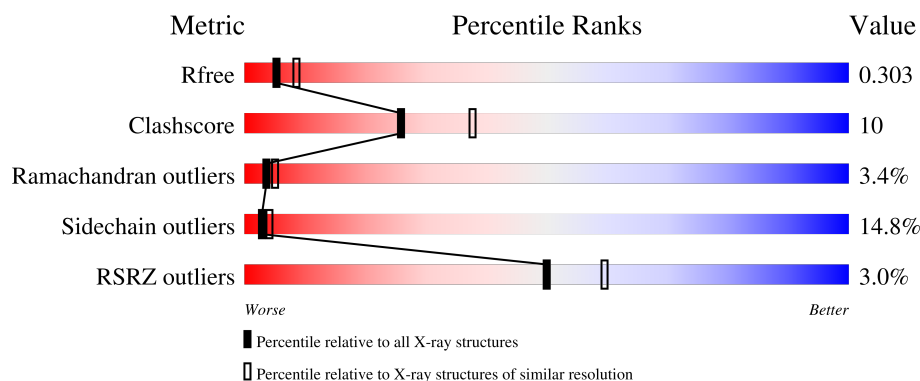
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	209	 3% 71% 22% 5%
1	C	209	 3% 64% 25% 7%
2	B	244	 4% 73% 20% 5%
2	D	244	 2% 72% 22% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7152 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 TCR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1621	1011	268	335	7			
1	C	204	Total	C	N	O	S	0	0	0
			1597	998	263	329	7			

- Molecule 2 is a protein called TCR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1960	1238	349	365	8			
2	D	243	Total	C	N	O	S	0	0	0
			1960	1238	349	365	8			

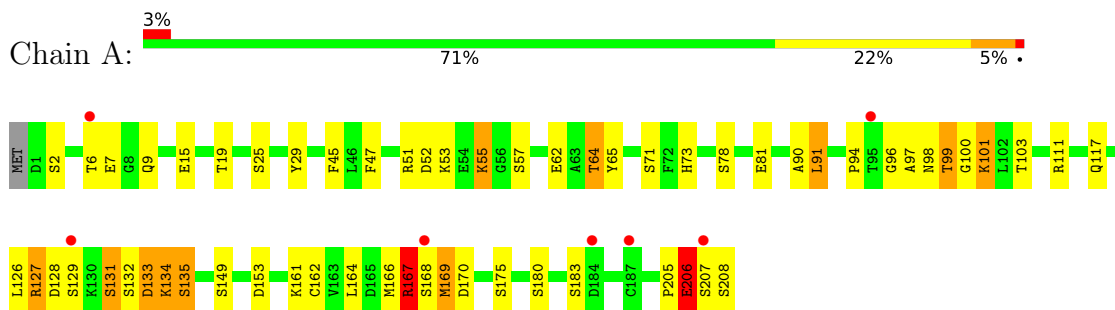
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	1	Total	O	0	0
			1	1		
3	C	3	Total	O	0	0
			3	3		
3	D	6	Total	O	0	0
			6	6		

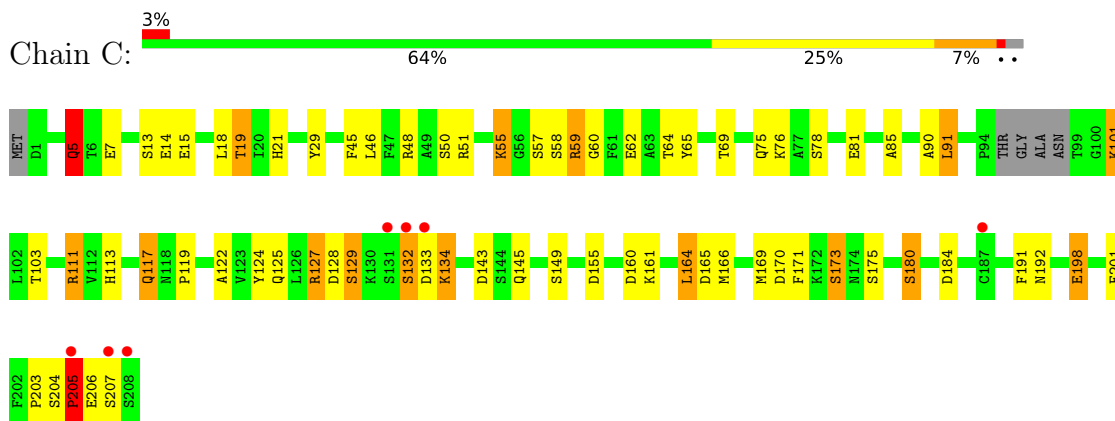
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

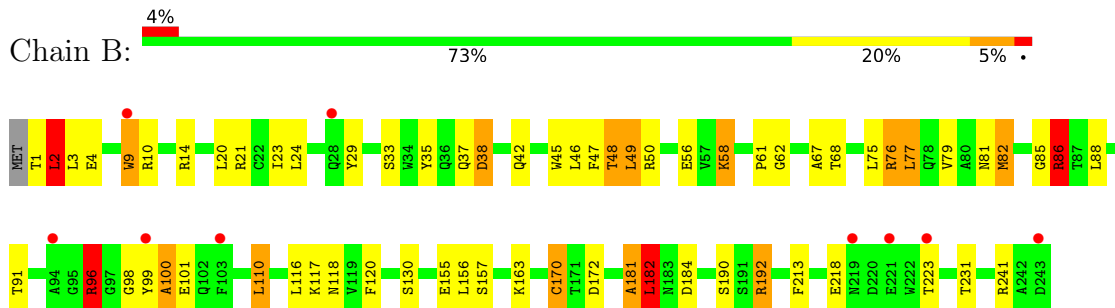
• Molecule 1: TCR-alpha



• Molecule 1: TCR-alpha

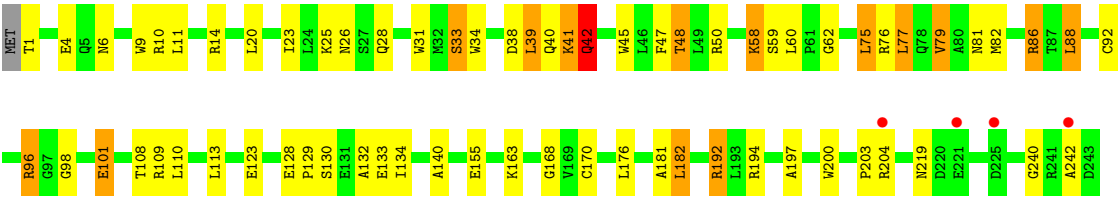


• Molecule 2: TCR-beta



• Molecule 2: TCR-beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.16Å 196.33Å 63.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 2.75 45.20 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.24-2.75) 98.0 (45.20-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.224 , 0.301 0.227 , 0.303	Depositor DCC
R_{free} test set	1426 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7152	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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

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	0.79	0/1661	1.04	0/2253
1	C	0.81	1/1636 (0.1%)	1.06	0/2217
2	B	0.73	0/2013	1.02	3/2741 (0.1%)
2	D	0.77	3/2013 (0.1%)	1.06	5/2741 (0.2%)
All	All	0.78	4/7323 (0.1%)	1.05	8/9952 (0.1%)

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	5
2	B	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	123	GLU	CD-OE1	7.19	1.33	1.25
2	D	155	GLU	CD-OE1	6.48	1.32	1.25
1	C	81	GLU	CD-OE1	5.71	1.31	1.25
2	D	133	GLU	CD-OE1	5.11	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	ASP	CB-CA-C	-7.07	96.27	110.40
2	D	86	ARG	CG-CD-NE	-6.46	98.23	111.80
2	D	86	ARG	CB-CA-C	-6.18	98.03	110.40
2	B	86	ARG	CB-CA-C	-5.78	98.85	110.40
2	B	86	ARG	CG-CD-NE	-5.66	99.91	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	38	ASP	CB-CA-C	5.30	121.01	110.40
2	D	42	GLN	CB-CA-C	-5.21	99.99	110.40
2	D	42	GLN	N-CA-CB	5.08	119.73	110.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	SER	Peptide
1	A	133	ASP	Peptide
1	A	97	ALA	Peptide
2	B	1	THR	Peptide
1	C	129	SER	Peptide
1	C	132	SER	Peptide
1	C	133	ASP	Peptide
1	C	204	SER	Peptide
1	C	5	GLN	Peptide

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	1621	0	1501	40	0
1	C	1597	0	1479	38	0
2	B	1960	0	1894	45	0
2	D	1960	0	1894	45	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	1	0
3	D	6	0	0	0	0
All	All	7152	0	6768	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 10.

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)
1:A:96:GLY:HA2	2:B:96:ARG:CG	1.63	1.28
1:A:96:GLY:HA2	2:B:96:ARG:HG2	1.17	1.06
2:D:33:SER:OG	2:D:48:THR:HG22	1.61	0.97
2:B:33:SER:OG	2:B:48:THR:HG22	1.62	0.97
1:A:96:GLY:CA	2:B:96:ARG:HG2	1.95	0.96
2:B:33:SER:OG	2:B:48:THR:CG2	2.19	0.89
2:D:4:GLU:OE2	2:D:25:LYS:CE	2.28	0.82
2:D:33:SER:OG	2:D:48:THR:CG2	2.28	0.81
1:A:127:ARG:HG3	1:A:128:ASP:H	1.45	0.81
1:C:205:PRO:HG3	2:D:132:ALA:HB2	1.63	0.80
1:C:125:GLN:OE1	1:C:127:ARG:NH1	2.16	0.78
2:D:62:GLY:O	2:D:82:MET:HA	1.83	0.78
1:A:96:GLY:HA2	2:B:96:ARG:CD	2.13	0.78
1:C:155:ASP:O	1:C:180:SER:OG	2.02	0.78
1:A:96:GLY:HA2	2:B:96:ARG:HG3	1.72	0.71
2:D:203:PRO:HD3	2:D:242:ALA:HB2	1.74	0.70
1:A:94:PRO:O	2:B:99:TYR:HB2	1.92	0.69
1:C:13:SER:HG	1:C:113:HIS:HE2	1.39	0.69
2:B:20:LEU:O	2:B:76:ARG:HG3	1.93	0.68
2:B:62:GLY:O	2:B:82:MET:HA	1.94	0.67
1:A:91:LEU:C	1:A:91:LEU:HD12	2.16	0.66
1:A:98:ASN:O	1:A:100:GLY:N	2.26	0.66
1:C:45:PHE:CZ	2:D:101:GLU:HG2	2.31	0.65
2:D:4:GLU:OE2	2:D:25:LYS:NZ	2.29	0.65
1:A:133:ASP:OD1	1:A:133:ASP:N	2.31	0.63
1:A:96:GLY:CA	2:B:96:ARG:CG	2.57	0.61
1:A:71:SER:HB2	1:A:73:HIS:CE1	2.35	0.61
1:A:166:MET:C	1:A:167:ARG:O	2.36	0.61
2:D:4:GLU:OE2	2:D:25:LYS:HE3	1.99	0.61
1:C:128:ASP:OD1	1:C:129:SER:N	2.34	0.60
1:A:55:LYS:HG3	1:A:64:THR:HB	1.84	0.60
1:A:132:SER:HB3	1:A:134:LYS:HB2	1.84	0.59
1:C:111:ARG:HH11	1:C:111:ARG:HG3	1.68	0.58
1:A:127:ARG:HG3	1:A:128:ASP:N	2.16	0.58
2:B:46:LEU:O	2:B:58:LYS:NZ	2.35	0.58
1:A:96:GLY:CA	2:B:96:ARG:CD	2.81	0.58
2:D:41:LYS:O	2:D:42:GLN:CB	2.51	0.57
1:A:164:LEU:HB3	2:B:170:CYS:HB3	1.87	0.57
1:C:13:SER:HG	1:C:113:HIS:CD2	2.22	0.57
1:C:91:LEU:C	1:C:91:LEU:HD12	2.25	0.57
2:B:33:SER:OG	2:B:48:THR:HG23	2.04	0.56
2:D:34:TRP:CE2	2:D:75:LEU:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:O	1:A:167:ARG:O	2.23	0.56
2:D:1:THR:OG1	2:D:1:THR:O	2.23	0.55
2:D:41:LYS:O	2:D:42:GLN:HB2	2.07	0.55
1:A:15:GLU:HA	1:A:78:SER:OG	2.07	0.54
1:A:132:SER:HB3	1:A:134:LYS:CB	2.36	0.54
2:D:11:LEU:HD23	2:D:113:LEU:HD11	1.89	0.54
1:C:117:GLN:HA	1:C:117:GLN:OE1	2.07	0.54
2:D:58:LYS:HD3	2:D:60:LEU:HD21	1.89	0.54
2:D:129:PRO:HD2	2:D:200:TRP:CZ2	2.43	0.52
1:A:126:LEU:HD12	1:A:126:LEU:N	2.24	0.52
2:B:156:LEU:HD23	2:B:157:SER:N	2.25	0.52
2:B:2:LEU:HD23	2:B:2:LEU:C	2.30	0.51
2:D:33:SER:HB3	2:D:47:PHE:O	2.11	0.51
1:A:132:SER:HB3	1:A:134:LYS:HE2	1.93	0.50
1:A:98:ASN:C	1:A:100:GLY:N	2.65	0.50
1:A:52:ASP:OD2	1:A:53:LYS:HE3	2.12	0.50
2:B:99:TYR:O	2:B:100:ALA:O	2.29	0.50
2:D:31:TRP:O	2:D:92:CYS:HA	2.11	0.49
2:D:203:PRO:HG3	2:D:242:ALA:CB	2.42	0.49
1:C:101:LYS:HB2	2:D:45:TRP:CD2	2.48	0.49
2:B:86:ARG:NH1	2:B:86:ARG:CG	2.76	0.49
1:C:5:GLN:HA	1:C:21:HIS:O	2.13	0.48
1:A:99:THR:HG23	1:A:101:LYS:HG2	1.95	0.48
2:B:85:GLY:C	2:B:86:ARG:HG3	2.33	0.48
2:B:98:GLY:O	2:B:100:ALA:O	2.32	0.48
2:B:82:MET:HE1	2:B:110:LEU:HB3	1.96	0.48
1:C:48:ARG:NH2	2:D:98:GLY:O	2.45	0.48
1:A:99:THR:CG2	1:A:101:LYS:HG2	2.43	0.48
1:C:122:ALA:HB1	1:C:124:TYR:CZ	2.49	0.47
2:D:77:LEU:CD1	2:D:88:LEU:HD22	2.43	0.47
1:C:129:SER:HB3	2:D:128:GLU:HG3	1.96	0.47
2:D:26:ASN:OD1	2:D:28:GLN:HB3	2.14	0.47
2:D:39:LEU:HD12	2:D:39:LEU:HA	1.80	0.47
2:B:82:MET:CE	2:B:110:LEU:HB3	2.44	0.47
1:C:58:SER:C	1:C:59:ARG:HG2	2.35	0.47
1:A:167:ARG:O	1:A:169:MET:N	2.47	0.47
2:D:192:ARG:N	2:D:192:ARG:HD3	2.29	0.47
2:D:203:PRO:CD	2:D:242:ALA:HB2	2.43	0.47
2:D:20:LEU:HD22	2:D:108:THR:HG21	1.96	0.47
1:A:45:PHE:CZ	1:A:47:PHE:HA	2.51	0.46
1:C:164:LEU:HD13	1:C:164:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:TRP:CG	2:B:10:ARG:N	2.84	0.46
2:B:4:GLU:O	2:B:4:GLU:HG3	2.16	0.46
1:C:19:THR:HB	1:C:75:GLN:HG2	1.98	0.46
1:C:134:LYS:HA	1:C:134:LYS:HD2	1.68	0.46
2:D:31:TRP:CZ3	2:D:96:ARG:HG2	2.51	0.46
1:A:90:ALA:HA	1:A:103:THR:O	2.16	0.46
2:D:176:LEU:C	2:D:176:LEU:HD12	2.36	0.46
1:A:166:MET:O	1:A:169:MET:O	2.34	0.46
1:C:45:PHE:CE1	2:D:101:GLU:HG2	2.51	0.46
2:D:40:GLN:C	2:D:41:LYS:O	2.51	0.46
1:C:129:SER:HB2	2:D:128:GLU:OE1	2.16	0.45
1:C:205:PRO:HG3	2:D:132:ALA:CB	2.42	0.45
1:A:55:LYS:HE2	1:A:62:GLU:CD	2.36	0.45
2:D:31:TRP:CZ3	2:D:50:ARG:HB2	2.51	0.45
2:D:77:LEU:HD11	2:D:88:LEU:HD22	1.99	0.45
1:C:13:SER:OG	1:C:113:HIS:NE2	2.34	0.45
2:B:181:ALA:O	2:B:182:LEU:HB2	2.17	0.45
1:C:111:ARG:HG3	1:C:111:ARG:NH1	2.32	0.45
1:A:96:GLY:N	2:B:96:ARG:HG2	2.31	0.45
1:A:127:ARG:CG	1:A:128:ASP:N	2.79	0.44
1:C:90:ALA:HA	1:C:103:THR:O	2.17	0.44
2:B:77:LEU:CD1	2:B:88:LEU:HD22	2.47	0.44
1:A:96:GLY:CA	2:B:96:ARG:HD3	2.47	0.44
2:B:118:ASN:O	2:B:120:PHE:HD1	2.00	0.44
2:B:4:GLU:O	2:B:4:GLU:CG	2.66	0.44
2:B:37:GLN:HA	2:B:42:GLN:O	2.18	0.44
1:C:55:LYS:HE2	1:C:62:GLU:OE1	2.18	0.44
1:C:15:GLU:HA	1:C:78:SER:OG	2.18	0.43
2:B:172:ASP:OD2	2:B:190:SER:HB3	2.18	0.43
2:D:134:ILE:HG23	2:D:197:ALA:HB1	2.00	0.43
2:D:129:PRO:CG	2:D:140:ALA:HB1	2.49	0.43
2:B:49:LEU:HD11	2:B:56:GLU:CG	2.49	0.43
2:B:33:SER:HA	2:B:47:PHE:O	2.19	0.43
1:C:164:LEU:CD2	2:D:168:GLY:C	2.87	0.43
1:C:171:PHE:HE2	2:D:194:ARG:HH11	1.66	0.43
1:C:117:GLN:O	1:C:119:PRO:HD3	2.19	0.42
1:C:206:GLU:H	1:C:206:GLU:HG2	1.48	0.42
1:A:2:SER:OG	1:A:25:SER:HB3	2.20	0.42
1:A:132:SER:CB	1:A:134:LYS:HE2	2.49	0.42
2:B:49:LEU:HD11	2:B:56:GLU:HG3	2.01	0.42
2:D:129:PRO:HG2	2:D:140:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:CYS:HB3	2:B:192:ARG:NH2	2.34	0.42
2:B:99:TYR:C	2:B:100:ALA:O	2.58	0.42
2:B:47:PHE:CD2	2:B:67:ALA:HB2	2.55	0.41
1:C:18:LEU:O	1:C:75:GLN:HA	2.20	0.41
1:C:191:PHE:O	1:C:192:ASN:C	2.59	0.41
2:D:59:SER:C	2:D:60:LEU:HD22	2.40	0.41
1:A:9:GLN:HE21	1:A:111:ARG:HH22	1.68	0.41
1:A:206:GLU:OE1	1:A:206:GLU:N	2.46	0.41
1:C:60:GLY:O	1:C:76:LYS:HG3	2.21	0.41
1:C:143:ASP:HB2	3:C:302:HOH:O	2.20	0.41
1:C:171:PHE:CE2	1:C:173:SER:HB3	2.55	0.41
1:C:198:GLU:H	1:C:198:GLU:HG2	1.73	0.41
2:B:35:TYR:CE2	2:B:45:TRP:HB2	2.56	0.41
2:B:182:LEU:HD12	2:B:184:ASP:OD1	2.22	0.41
1:C:201:PHE:CZ	1:C:203:PRO:HB3	2.56	0.40
2:B:2:LEU:O	2:B:2:LEU:HG	2.21	0.40
2:B:86:ARG:CG	2:B:86:ARG:HH11	2.34	0.40
2:B:213:PHE:O	2:B:231:THR:HA	2.21	0.40
2:D:34:TRP:NE1	2:D:75:LEU:HD13	2.37	0.40
2:B:3:LEU:HD23	2:B:24:LEU:HA	2.03	0.40
2:D:79:VAL:HG22	2:D:79:VAL:O	2.21	0.40
2:D:81:ASN:O	2:D:82:MET:HB3	2.22	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	206/209 (99%)	178 (86%)	21 (10%)	7 (3%)	3	5
1	C	200/209 (96%)	183 (92%)	12 (6%)	5 (2%)	5	9
2	B	241/244 (99%)	217 (90%)	12 (5%)	12 (5%)	2	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	241/244 (99%)	219 (91%)	16 (7%)	6 (2%)	5	9
All	All	888/906 (98%)	797 (90%)	61 (7%)	30 (3%)	3	5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	129	SER
1	A	167	ARG
2	B	96	ARG
2	B	100	ALA
2	B	182	LEU
1	C	169	MET
1	C	207	SER
2	D	182	LEU
1	A	131	SER
1	A	206	GLU
2	B	2	LEU
2	B	218	GLU
2	D	14	ARG
2	D	42	GLN
2	D	240	GLY
1	A	135	SER
2	B	14	ARG
2	B	38	ASP
1	C	85	ALA
1	C	132	SER
2	D	41	LYS
1	A	205	PRO
2	B	81	ASN
2	B	181	ALA
2	D	181	ALA
2	B	82	MET
2	B	116	LEU
2	B	61	PRO
1	C	205	PRO

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	182/183 (100%)	153 (84%)	29 (16%)	2	3
1	C	180/183 (98%)	146 (81%)	34 (19%)	1	2
2	B	212/213 (100%)	184 (87%)	28 (13%)	4	6
2	D	212/213 (100%)	187 (88%)	25 (12%)	5	8
All	All	786/792 (99%)	670 (85%)	116 (15%)	3	4

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	7	GLU
1	A	19	THR
1	A	29	TYR
1	A	51	ARG
1	A	55	LYS
1	A	57	SER
1	A	64	THR
1	A	65	TYR
1	A	81	GLU
1	A	91	LEU
1	A	101	LYS
1	A	117	GLN
1	A	127	ARG
1	A	134	LYS
1	A	135	SER
1	A	149	SER
1	A	153	ASP
1	A	161	LYS
1	A	167	ARG
1	A	168	SER
1	A	169	MET
1	A	170	ASP
1	A	175	SER
1	A	180	SER
1	A	183	SER
1	A	206	GLU
1	A	207	SER

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Mol	Chain	Res	Type
1	A	208	SER
2	B	2	LEU
2	B	9	TRP
2	B	21	ARG
2	B	23	ILE
2	B	29	TYR
2	B	48	THR
2	B	49	LEU
2	B	50	ARG
2	B	58	LYS
2	B	68	THR
2	B	75	LEU
2	B	76	ARG
2	B	77	LEU
2	B	79	VAL
2	B	86	ARG
2	B	91	THR
2	B	96	ARG
2	B	101	GLU
2	B	110	LEU
2	B	117	LYS
2	B	130	SER
2	B	155	GLU
2	B	163	LYS
2	B	170	CYS
2	B	182	LEU
2	B	192	ARG
2	B	223	THR
2	B	241	ARG
1	C	5	GLN
1	C	7	GLU
1	C	14	GLU
1	C	19	THR
1	C	29	TYR
1	C	46	LEU
1	C	50	SER
1	C	51	ARG
1	C	55	LYS
1	C	57	SER
1	C	59	ARG
1	C	64	THR
1	C	65	TYR

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Mol	Chain	Res	Type
1	C	69	THR
1	C	91	LEU
1	C	101	LYS
1	C	111	ARG
1	C	117	GLN
1	C	127	ARG
1	C	134	LYS
1	C	145	GLN
1	C	149	SER
1	C	160	ASP
1	C	161	LYS
1	C	164	LEU
1	C	165	ASP
1	C	166	MET
1	C	170	ASP
1	C	173	SER
1	C	175	SER
1	C	180	SER
1	C	184	ASP
1	C	198	GLU
1	C	205	PRO
2	D	6	ASN
2	D	9	TRP
2	D	10	ARG
2	D	23	ILE
2	D	33	SER
2	D	39	LEU
2	D	48	THR
2	D	58	LYS
2	D	75	LEU
2	D	76	ARG
2	D	77	LEU
2	D	79	VAL
2	D	86	ARG
2	D	88	LEU
2	D	96	ARG
2	D	101	GLU
2	D	109	ARG
2	D	110	LEU
2	D	130	SER
2	D	163	LYS
2	D	170	CYS

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Mol	Chain	Res	Type
2	D	182	LEU
2	D	192	ARG
2	D	204	ARG
2	D	219	ASN

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

Mol	Chain	Res	Type
1	A	21	HIS
1	A	37	GLN
2	B	37	GLN
1	C	75	GLN
2	D	118	ASN

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 monosaccharides 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

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	208/209 (99%)	0.18	7 (3%) 45 53	9, 34, 77, 94	0
1	C	204/209 (97%)	0.17	7 (3%) 45 53	11, 30, 73, 102	0
2	B	243/244 (99%)	0.13	9 (3%) 41 49	16, 35, 72, 92	0
2	D	243/244 (99%)	0.11	4 (1%) 72 79	13, 35, 68, 98	0
All	All	898/906 (99%)	0.15	27 (3%) 50 59	9, 34, 73, 102	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	208	SER	8.4
1	C	207	SER	5.9
1	C	131	SER	4.7
1	C	132	SER	4.2
2	D	242	ALA	3.5
2	D	204	ARG	3.5
1	C	133	ASP	3.5
2	D	221	GLU	3.4
1	C	187	CYS	3.3
2	B	221	GLU	3.0
1	A	184	ASP	2.9
1	A	168	SER	2.9
1	C	205	PRO	2.8
2	B	243	ASP	2.7
1	A	6	THR	2.6
2	B	219	ASN	2.6
1	A	187	CYS	2.6
2	B	223	THR	2.4
1	A	207	SER	2.3
1	A	95	THR	2.2
2	D	225	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	28	GLN	2.2
2	B	94	ALA	2.1
2	B	9	TRP	2.1
2	B	103	PHE	2.1
2	B	99	TYR	2.1
1	A	129	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 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.