



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:21 PM UTC

PDB ID : 6LUP / pdb_00006lup
Title : Crystal structure of shark MHC CLASS I for 2.3 angstrom
Authors : Wu, Y.; Xia, C.
Deposited on : 2020-01-30
Resolution : 2.30 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

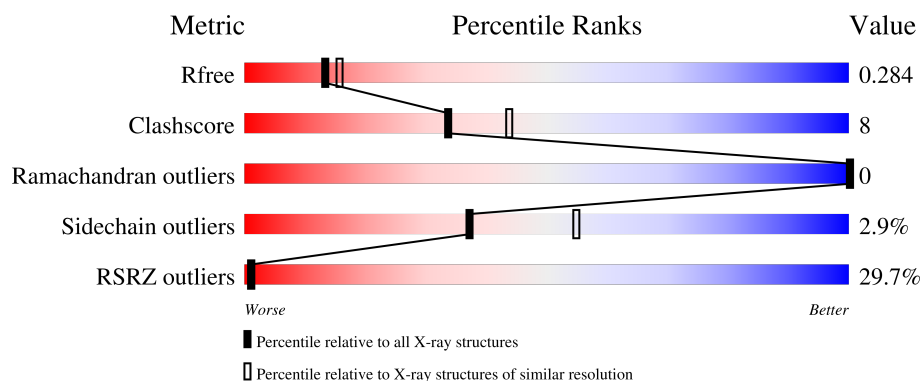
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	267	14% 85% 13%
1	D	267	27% 81% 17%
2	B	96	39% 78% 18%
2	E	96	78% 78% 21%
3	C	9	100%

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Mol	Chain	Length	Quality of chain
3	F	9	 89% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6192 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 MHC class I protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2162	1363	374	416	9			
1	D	267	Total	C	N	O	S	0	0	0
			2162	1363	374	416	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			776	492	127	154	3			
2	E	96	Total	C	N	O	S	0	0	0
			776	492	127	154	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	-	expression tag	UNP F4ZE04
B	3	THR	-	expression tag	UNP F4ZE04
B	4	SER	-	expression tag	UNP F4ZE04
B	96	ARG	-	expression tag	UNP F4ZE04
B	97	TYR	-	expression tag	UNP F4ZE04
E	2	ALA	-	expression tag	UNP F4ZE04
E	3	THR	-	expression tag	UNP F4ZE04
E	4	SER	-	expression tag	UNP F4ZE04
E	96	ARG	-	expression tag	UNP F4ZE04
E	97	TYR	-	expression tag	UNP F4ZE04

- Molecule 3 is a protein called PHE-ALA-ASN-PHE-PHE-ILE-ARG-GLY-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			78	54	13	11			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	0	0	0
			78	54	13	11			

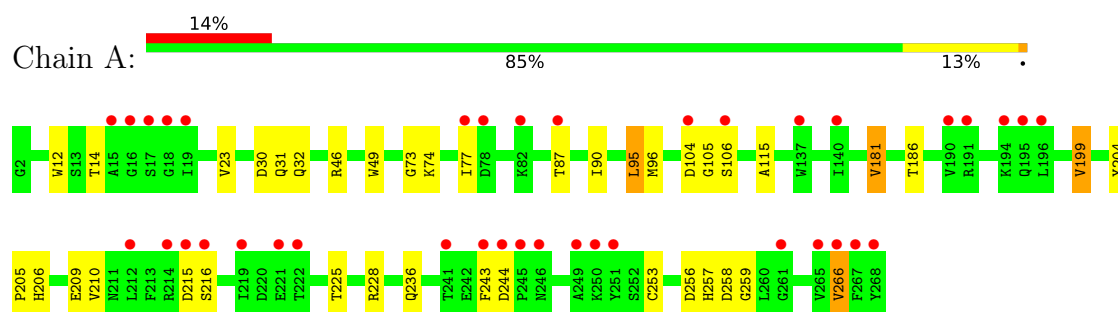
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	25	Total	O	0	0
			25	25		
4	C	6	Total	O	0	0
			6	6		
4	D	41	Total	O	0	0
			41	41		
4	E	20	Total	O	0	0
			20	20		
4	F	2	Total	O	0	0
			2	2		

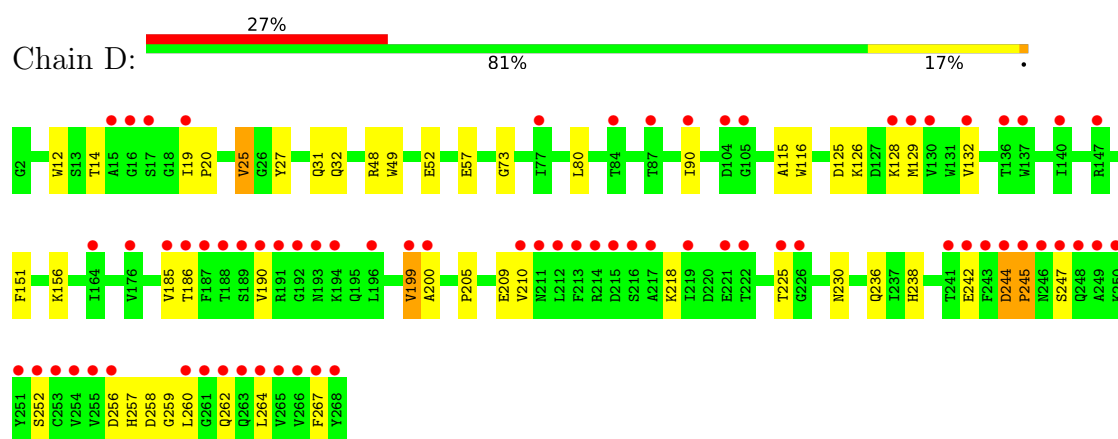
3 Residue-property plots [i](#)

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.

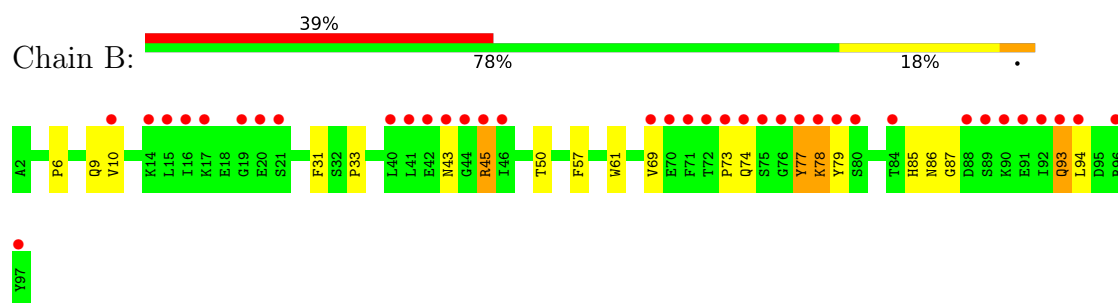
• Molecule 1: MHC class I protein



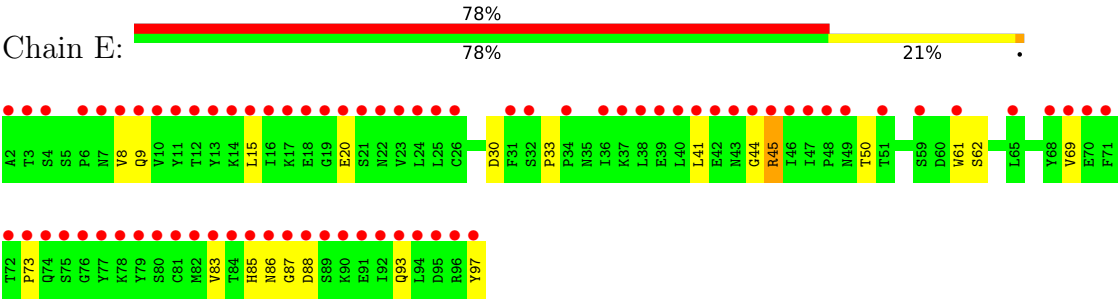
• Molecule 1: MHC class I protein



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin

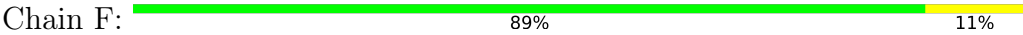


● Molecule 3: PHE-ALA-ASN-PHE-PHE-ILE-ARG-GLY-LEU



There are no outlier residues recorded for this chain.

● Molecule 3: PHE-ALA-ASN-PHE-PHE-ILE-ARG-GLY-LEU



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	125.86Å 125.86Å 132.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.62 – 2.30 45.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.62-2.30) 99.8 (45.62-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.255 , 0.283 0.255 , 0.284	Depositor DCC
R_{free} test set	2672 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6192	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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	0.41	0/2221	0.84	5/3012 (0.2%)
1	D	0.40	0/2221	0.77	3/3012 (0.1%)
2	B	0.37	0/794	0.73	1/1076 (0.1%)
2	E	0.33	0/794	0.67	0/1076
3	C	0.38	0/80	0.64	0/104
3	F	0.40	0/80	0.74	0/104
All	All	0.39	0/6190	0.78	9/8384 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CA-C-N	9.37	129.13	119.19
1	A	244	ASP	C-N-CA	9.37	129.13	119.19
1	A	243	PHE	N-CA-C	7.62	121.54	109.50
1	A	244	ASP	N-CA-C	5.78	118.64	109.40
1	A	87	THR	CA-CB-OG1	-5.43	101.45	109.60
1	D	244	ASP	CA-C-N	5.28	125.98	120.12
1	D	244	ASP	C-N-CA	5.28	125.98	120.12
1	D	245	PRO	N-CA-C	5.23	120.47	114.20
2	B	77	TYR	N-CA-C	5.02	117.71	110.28

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	2162	0	2036	29	0
1	D	2162	0	2036	35	0
2	B	776	0	750	21	0
2	E	776	0	750	16	0
3	C	78	0	78	0	0
3	F	78	0	78	1	0
4	A	66	0	0	1	0
4	B	25	0	0	0	0
4	C	6	0	0	0	0
4	D	41	0	0	0	0
4	E	20	0	0	0	0
4	F	2	0	0	0	0
All	All	6192	0	5728	91	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 (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:HG22	2:B:69:VAL:CG1	2.03	0.88
2:E:45:ARG:HG2	2:E:45:ARG:HH11	1.37	0.88
1:A:105:GLY:HA3	1:A:106:SER:HB2	1.58	0.84
2:B:45:ARG:HG2	2:B:45:ARG:HH11	1.44	0.80
1:D:225:THR:HG22	1:D:238:HIS:H	1.46	0.80
1:A:31:GLN:NE2	1:A:49:TRP:HE1	1.80	0.79
1:D:14:THR:HG21	1:D:90:ILE:HA	1.66	0.76
1:D:31:GLN:NE2	1:D:49:TRP:HE1	1.91	0.67
1:A:14:THR:HG21	1:A:90:ILE:HA	1.76	0.67
1:D:209:GLU:HB2	1:D:256:ASP:HB2	1.77	0.66
1:D:225:THR:OG1	2:E:9:GLN:NE2	2.30	0.64
1:D:225:THR:CG2	1:D:238:HIS:H	2.11	0.63
1:A:257:HIS:CD2	1:A:259:GLY:H	2.16	0.62
2:E:50:THR:HG22	2:E:69:VAL:HB	1.81	0.62
1:A:209:GLU:HB2	1:A:256:ASP:HB2	1.82	0.62
2:E:33:PRO:O	2:E:85:HIS:HE1	1.82	0.61
1:A:105:GLY:HA3	1:A:106:SER:CB	2.29	0.61
2:B:33:PRO:O	2:B:85:HIS:HE1	1.84	0.60
1:D:31:GLN:HE22	1:D:49:TRP:HE1	1.48	0.60
2:B:50:THR:HG22	2:B:69:VAL:HG13	1.83	0.59
1:A:30:ASP:OD2	1:A:206:HIS:HD2	1.84	0.59
2:B:74:GLN:HB2	2:B:77:TYR:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:VAL:HG23	2:B:94:LEU:HA	1.86	0.58
1:A:31:GLN:HE22	1:A:49:TRP:HE1	1.52	0.57
1:A:105:GLY:CA	1:A:106:SER:HB2	2.33	0.57
2:E:45:ARG:HG2	2:E:45:ARG:NH1	2.16	0.56
1:D:25:VAL:HG13	1:D:32:GLN:HG3	1.89	0.55
1:D:257:HIS:CD2	1:D:259:GLY:H	2.25	0.54
1:D:230:ASN:HD21	1:D:236:GLN:HE21	1.56	0.52
1:D:190:VAL:HB	2:E:97:TYR:HB2	1.92	0.52
2:B:45:ARG:HG2	2:B:45:ARG:NH1	2.19	0.52
1:A:258:ASP:HA	4:A:331:HOH:O	2.10	0.51
1:A:181:VAL:HG12	1:A:204:TYR:HB3	1.92	0.51
2:B:50:THR:HG22	2:B:69:VAL:HG11	1.91	0.51
2:E:45:ARG:HH11	2:E:45:ARG:CG	2.15	0.51
1:D:115:ALA:HB2	2:E:61:TRP:CE2	2.45	0.50
1:D:186:THR:HB	1:D:199:VAL:HG13	1.93	0.50
1:A:115:ALA:HB2	2:B:61:TRP:CE2	2.47	0.49
2:B:74:GLN:HB2	2:B:77:TYR:CD2	2.45	0.49
1:A:228:ARG:HE	1:A:236:GLN:HE21	1.59	0.49
1:A:104:ASP:O	1:A:106:SER:HB2	2.13	0.48
1:D:48:ARG:NH2	1:D:52:GLU:OE2	2.46	0.48
1:A:96:MET:HG3	2:B:57:PHE:HE1	1.79	0.48
2:B:45:ARG:HH11	2:B:45:ARG:CG	2.22	0.48
2:B:45:ARG:HH21	1:D:57:GLU:HG3	1.79	0.48
1:A:186:THR:HB	1:A:199:VAL:HG13	1.95	0.47
1:D:125:ASP:O	1:D:128:LYS:O	2.32	0.47
1:A:95:LEU:HD23	1:A:96:MET:N	2.30	0.47
1:A:225:THR:HB	2:B:9:GLN:HE22	1.80	0.47
1:D:185:VAL:HG11	1:D:264:LEU:CD1	2.45	0.47
1:D:205:PRO:O	1:D:257:HIS:HE1	1.98	0.46
1:A:96:MET:HG3	2:B:57:PHE:CE1	2.49	0.46
1:A:215:ASP:O	1:A:216:SER:HB2	2.16	0.46
2:B:73:PRO:HA	2:B:79:TYR:OH	2.15	0.46
1:A:74:LYS:O	1:A:77:ILE:HG12	2.15	0.46
1:D:129:MET:HE3	1:D:156:LYS:HD2	1.98	0.46
2:B:43:ASN:OD1	2:B:77:TYR:CD1	2.68	0.45
1:A:30:ASP:OD2	1:A:206:HIS:CD2	2.67	0.45
1:D:126:LYS:O	1:D:129:MET:HE2	2.16	0.45
1:A:205:PRO:O	1:A:257:HIS:HE1	2.00	0.45
1:D:25:VAL:CG1	1:D:27:TYR:CE1	2.99	0.45
2:B:78:LYS:HE2	2:B:93:GLN:NE2	2.32	0.45
1:D:186:THR:HG21	2:E:15:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:HA	1:D:245:PRO:HD3	1.53	0.45
2:E:20:GLU:O	2:E:73:PRO:HD2	2.16	0.45
2:E:8:VAL:HG21	2:E:83:VAL:HG21	1.99	0.44
1:D:257:HIS:CG	1:D:258:ASP:H	2.34	0.44
1:A:253:CYS:HB3	1:A:266:VAL:HG13	2.00	0.44
2:E:45:ARG:NH1	2:E:45:ARG:CG	2.78	0.44
1:A:228:ARG:HE	1:A:236:GLN:NE2	2.16	0.43
2:B:43:ASN:HD21	2:B:78:LYS:H	1.67	0.43
1:D:19:ILE:HG23	1:D:20:PRO:HD2	1.99	0.43
1:A:32:GLN:NE2	1:A:46:ARG:HG3	2.34	0.43
1:D:185:VAL:HG11	1:D:264:LEU:HD11	2.00	0.42
1:D:200:ALA:O	1:D:236:GLN:HA	2.19	0.42
2:E:41:LEU:HD23	2:E:44:GLY:HA2	2.00	0.42
1:D:252:SER:HB3	1:D:267:PHE:CE1	2.55	0.42
1:D:14:THR:CG2	1:D:90:ILE:HA	2.45	0.42
2:E:86:ASN:HB3	2:E:87:GLY:H	1.64	0.42
1:A:12:TRP:CE2	1:A:73:GLY:HA3	2.54	0.42
1:D:257:HIS:CG	1:D:258:ASP:N	2.88	0.42
1:A:31:GLN:HE21	1:A:49:TRP:HE1	1.61	0.42
1:A:12:TRP:CD2	1:A:73:GLY:HA3	2.56	0.41
2:E:30:ASP:HA	2:E:62:SER:HB2	2.03	0.41
1:D:260:LEU:C	1:D:262:GLN:H	2.28	0.41
1:D:12:TRP:CE2	1:D:73:GLY:HA3	2.55	0.41
2:B:6:PRO:HA	2:B:31:PHE:HB3	2.03	0.41
1:D:225:THR:HG1	2:E:9:GLN:HE22	1.65	0.41
2:B:86:ASN:HB3	2:B:87:GLY:H	1.59	0.40
1:D:80:LEU:HD13	1:D:116:TRP:HB2	2.03	0.40
1:D:151:PHE:CD1	3:F:7:ARG:HG2	2.57	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	265/267 (99%)	257 (97%)	8 (3%)	0	100	100
1	D	265/267 (99%)	257 (97%)	8 (3%)	0	100	100
2	B	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
2	E	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	732/744 (98%)	710 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	236/236 (100%)	230 (98%)	6 (2%)	42	60
1	D	236/236 (100%)	229 (97%)	7 (3%)	36	53
2	B	90/90 (100%)	87 (97%)	3 (3%)	33	50
2	E	90/90 (100%)	87 (97%)	3 (3%)	33	50
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
All	All	666/666 (100%)	647 (97%)	19 (3%)	37	55

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	95	LEU
1	A	181	VAL
1	A	199	VAL
1	A	210	VAL
1	A	266	VAL
2	B	45	ARG

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Mol	Chain	Res	Type
2	B	78	LYS
2	B	93	GLN
1	D	25	VAL
1	D	132	VAL
1	D	199	VAL
1	D	210	VAL
1	D	218	LYS
1	D	242	GLU
1	D	247	SER
2	E	45	ARG
2	E	88	ASP
2	E	93	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	76	ASN
1	A	108	ASN
1	A	113	GLN
1	A	143	ASN
1	A	173	ASN
1	A	175	ASN
1	A	206	HIS
1	A	230	ASN
1	A	236	GLN
1	A	248	GLN
1	A	257	HIS
2	B	9	GLN
2	B	43	ASN
2	B	52	GLN
2	B	74	GLN
2	B	85	HIS
2	B	93	GLN
1	D	31	GLN
1	D	32	GLN
1	D	76	ASN
1	D	113	GLN
1	D	143	ASN
1	D	173	ASN
1	D	195	GLN
1	D	230	ASN

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Mol	Chain	Res	Type
1	D	246	ASN
1	D	257	HIS
2	E	9	GLN
2	E	52	GLN
2	E	85	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	267/267 (100%)	0.79	38 (14%) 6 7	31, 51, 93, 107	0
1	D	267/267 (100%)	1.24	71 (26%) 1 2	31, 57, 112, 136	0
2	B	96/96 (100%)	1.64	37 (38%) 1 0	36, 58, 100, 104	0
2	E	96/96 (100%)	3.32	75 (78%) 0 0	49, 80, 133, 141	0
3	C	9/9 (100%)	-0.28	0 100 100	24, 28, 47, 52	0
3	F	9/9 (100%)	-0.25	0 100 100	26, 28, 49, 56	0
All	All	744/744 (100%)	1.36	221 (29%) 1 1	24, 58, 109, 141	0

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	44	GLY	7.8
2	E	16	ILE	7.4
2	E	79	TYR	6.6
2	E	41	LEU	6.4
2	E	97	TYR	6.2
1	D	268	TYR	6.1
2	E	94	LEU	5.7
2	E	43	ASN	5.6
2	E	77	TYR	5.6
2	E	24	LEU	5.5
2	E	78	LYS	5.5
2	E	19	GLY	5.4
2	E	46	ILE	5.4
2	E	89	SER	5.4
2	E	80	SER	5.4
2	B	77	TYR	5.3
1	D	249	ALA	5.3
2	E	76	GLY	5.3
2	E	15	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
2	E	74	GLN	5.0
2	E	17	LYS	4.9
1	D	265	VAL	4.9
1	D	87	THR	4.9
1	D	267	PHE	4.8
2	E	84	THR	4.7
2	E	71	PHE	4.7
1	A	17	SER	4.6
2	E	40	LEU	4.6
2	E	92	ILE	4.6
2	E	75	SER	4.6
2	E	3	THR	4.5
2	B	15	LEU	4.4
2	B	72	THR	4.4
1	A	268	TYR	4.4
2	B	76	GLY	4.4
1	D	250	LYS	4.4
2	E	21	SER	4.4
2	E	91	GLU	4.4
2	E	72	THR	4.4
2	E	73	PRO	4.3
2	E	96	ARG	4.3
2	E	93	GLN	4.3
2	B	97	TYR	4.3
1	D	251	TYR	4.2
1	D	253	CYS	4.2
2	E	45	ARG	4.2
1	D	264	LEU	4.1
1	D	261	GLY	4.0
1	A	249	ALA	4.0
2	E	42	GLU	4.0
2	B	16	ILE	4.0
2	E	47	ILE	4.0
2	E	83	VAL	3.9
2	B	78	LYS	3.9
2	E	8	VAL	3.9
2	B	19	GLY	3.8
1	A	87	THR	3.8
1	D	243	PHE	3.8
1	D	247	SER	3.8
1	D	266	VAL	3.8
1	D	215	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	20	GLU	3.7
2	E	82	MET	3.7
1	D	17	SER	3.7
1	D	254	VAL	3.7
2	E	10	VAL	3.7
1	D	219	ILE	3.7
2	E	23	VAL	3.7
1	A	251	TYR	3.7
1	D	244	ASP	3.6
2	B	79	TYR	3.6
2	B	20	GLU	3.6
2	E	90	LYS	3.6
1	D	199	VAL	3.6
1	D	263	GLN	3.5
2	B	21	SER	3.5
2	B	88	ASP	3.5
1	D	248	GLN	3.5
2	E	69	VAL	3.4
2	E	25	LEU	3.4
2	E	11	TYR	3.4
1	D	226	GLY	3.4
2	E	18	GLU	3.4
1	D	222	THR	3.3
2	E	48	PRO	3.3
1	D	252	SER	3.3
2	B	75	SER	3.3
2	E	14	LYS	3.3
2	E	26	CYS	3.3
2	B	71	PHE	3.3
2	E	65	LEU	3.2
2	B	93	GLN	3.2
1	D	200	ALA	3.2
1	D	245	PRO	3.2
1	D	186	THR	3.2
2	E	95	ASP	3.2
2	E	81	CYS	3.1
1	D	241	THR	3.1
1	D	216	SER	3.1
2	E	88	ASP	3.1
2	E	2	ALA	3.1
2	E	9	GLN	3.1
1	D	196	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	212	LEU	3.1
2	B	73	PRO	3.1
2	B	90	LYS	3.1
2	E	12	THR	3.1
1	D	225	THR	3.0
1	D	105	GLY	3.0
1	A	243	PHE	3.0
1	D	260	LEU	3.0
1	A	19	ILE	3.0
1	A	250	LYS	2.9
1	A	214	ARG	2.9
1	A	16	GLY	2.9
1	D	15	ALA	2.9
1	A	82	LYS	2.9
2	E	38	LEU	2.9
1	A	222	THR	2.9
2	E	22	ASN	2.9
2	B	92	ILE	2.8
2	E	49	ASN	2.8
2	B	41	LEU	2.8
2	B	17	LYS	2.8
2	E	7	ASN	2.8
2	E	4	SER	2.8
1	A	77	ILE	2.8
1	A	219	ILE	2.8
2	B	94	LEU	2.8
2	E	68	TYR	2.8
1	A	267	PHE	2.7
2	B	46	ILE	2.7
1	A	215	ASP	2.7
1	D	19	ILE	2.7
2	B	42	GLU	2.7
2	B	89	SER	2.7
2	E	13	TYR	2.7
1	D	104	ASP	2.7
2	B	43	ASN	2.7
1	D	128	LYS	2.6
1	D	187	PHE	2.6
1	A	18	GLY	2.6
2	E	36	ILE	2.6
2	E	31	PHE	2.6
1	D	213	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	10	VAL	2.6
1	A	241	THR	2.6
2	B	45	ARG	2.5
1	D	84	THR	2.5
2	B	44	GLY	2.5
1	A	190	VAL	2.5
1	D	77	ILE	2.5
1	D	137	TRP	2.5
1	A	265	VAL	2.5
1	D	130	VAL	2.5
1	D	262	GLN	2.5
1	A	15	ALA	2.5
1	D	246	ASN	2.5
1	A	245	PRO	2.5
2	B	14	LYS	2.5
2	B	74	GLN	2.5
1	D	255	VAL	2.4
2	E	86	ASN	2.4
2	E	87	GLY	2.4
1	D	189	SER	2.4
1	D	185	VAL	2.4
1	A	195	GLN	2.4
2	E	39	GLU	2.4
1	A	261	GLY	2.4
1	A	78	ASP	2.4
1	D	217	ALA	2.4
1	D	194	LYS	2.4
2	E	70	GLU	2.4
2	B	84	THR	2.3
1	A	106	SER	2.3
1	D	221	GLU	2.3
2	B	96	ARG	2.3
1	A	216	SER	2.3
1	D	190	VAL	2.3
1	A	104	ASP	2.3
1	D	211	ASN	2.3
1	D	132	VAL	2.3
2	B	69	VAL	2.3
1	A	191	ARG	2.2
1	D	192	GLY	2.2
1	D	136	THR	2.2
1	D	129	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	LYS	2.2
1	D	176	VAL	2.2
1	A	221	GLU	2.2
1	D	188	THR	2.2
2	B	80	SER	2.2
2	E	51	THR	2.2
1	A	212	LEU	2.2
1	D	90	ILE	2.2
1	D	191	ARG	2.2
2	B	40	LEU	2.2
2	E	34	PRO	2.2
1	D	147	ARG	2.1
1	D	210	VAL	2.1
2	B	91	GLU	2.1
2	E	6	PRO	2.1
1	D	140	ILE	2.1
1	A	246	ASN	2.1
1	D	242	GLU	2.1
1	D	256	ASP	2.1
2	E	85	HIS	2.1
2	E	37	LYS	2.1
2	B	70	GLU	2.1
1	A	266	VAL	2.1
1	A	137	TRP	2.1
2	E	32	SER	2.1
2	E	59	SER	2.1
1	A	196	LEU	2.1
1	A	140	ILE	2.1
1	A	244	ASP	2.1
1	D	164	ILE	2.1
1	D	193	ASN	2.1
1	D	16	GLY	2.1
2	E	61	TRP	2.1
1	D	214	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.