



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:28 PM UTC

PDB ID : 8SXP / pdb_00008sxp
Title : Crystal structure of long neurotoxin from the venom of the king cobra (3FTx-L15) in complex with Fab of broadly neutralizing antibody 95Mat5
Authors : Nguyen, T.K.Y.
Deposited on : 2023-05-23
Resolution : 2.90 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

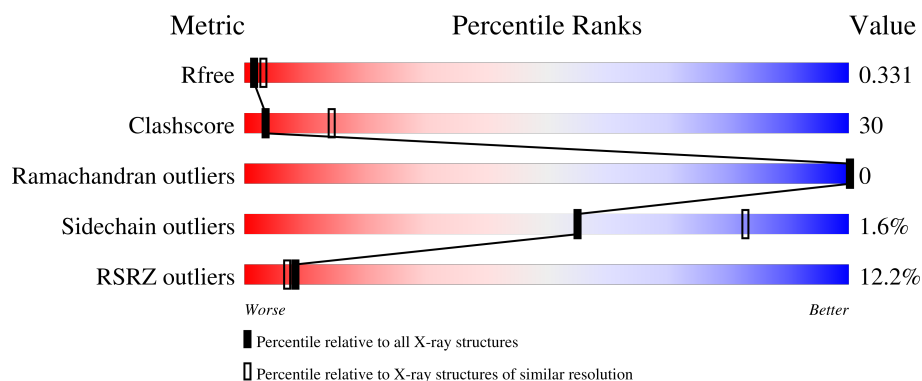
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	L	212	11% 63% 34% .
2	C	68	13% 43% 50% 6% .
3	H	228	13% 65% 32% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3830 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 95Mat5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1629	1018	271	335	5			

- Molecule 2 is a protein called Long neurotoxin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	S	0	0	0
			503	307	85	101	10			

- Molecule 3 is a protein called 95Mat5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	227	Total	C	N	O	S	0	0	0
			1695	1076	278	335	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.86Å 42.44Å 103.36Å 90.00° 103.70° 90.00°	Depositor
Resolution (Å)	45.49 – 2.90 45.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.1 (45.49-2.90) 82.2 (45.49-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.261 , 0.320 0.294 , 0.331	Depositor DCC
R_{free} test set	535 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3830	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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	L	0.91	0/1664	1.35	9/2259 (0.4%)
2	C	0.93	1/514 (0.2%)	2.05	12/699 (1.7%)
3	H	0.96	1/1739 (0.1%)	1.31	6/2371 (0.3%)
All	All	0.94	2/3917 (0.1%)	1.44	27/5329 (0.5%)

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
3	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	147	PRO	N-CD	10.03	1.61	1.47
2	C	20	ILE	C-N	-6.27	1.25	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	21	CYS	CB-CA-C	-30.57	71.81	110.94
1	L	8	PRO	CB-CA-C	-17.24	85.38	112.27
2	C	31	CYS	N-CA-C	-13.85	81.30	110.80
1	L	9	SER	N-CA-CB	-13.24	90.81	110.01
3	H	146	PHE	N-CA-C	9.34	130.45	109.81
2	C	31	CYS	N-CA-CB	8.04	124.09	110.49
1	L	185	ASP	N-CA-C	-7.99	102.55	111.82
1	L	184	ALA	N-CA-C	7.79	119.41	111.07
3	H	147	PRO	N-CA-C	-7.77	96.46	112.47
2	C	21	CYS	N-CA-C	-7.71	94.08	107.49
2	C	7	PRO	CB-CA-C	-6.98	100.05	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	13	THR	CB-CA-C	6.68	118.02	109.80
2	C	63	CYS	CB-CA-C	5.72	120.32	111.28
2	C	44	ALA	N-CA-C	-5.69	106.21	114.12
3	H	147	PRO	CA-N-CD	-5.52	104.28	112.00
2	C	13	THR	N-CA-C	-5.47	102.54	110.64
1	L	189	HIS	CA-C-O	-5.46	115.39	121.51
2	C	21	CYS	CA-CB-SG	-5.42	101.94	114.40
3	H	135	THR	N-CA-C	-5.38	100.13	108.31
3	H	62	LYS	N-CA-C	-5.28	102.57	110.23
2	C	35	GLY	CA-C-O	-5.26	118.53	122.37
1	L	30	SER	CB-CA-C	-5.22	109.03	116.34
3	H	178	LEU	CA-C-O	-5.21	115.52	121.40
1	L	76	SER	CB-CA-C	-5.19	110.61	116.63
1	L	9	SER	N-CA-C	-5.13	105.58	111.07
2	C	7	PRO	N-CA-C	5.09	122.97	112.47
1	L	61	ARG	N-CA-C	-5.05	105.22	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	98	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1629	0	1580	73	0
2	C	503	0	478	67	0
3	H	1695	0	1657	97	0
4	C	1	0	0	1	0
4	H	2	0	0	2	0
All	All	3830	0	3715	225	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 30.

All (225) 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:C:25:THR:CB	2:C:36:LYS:HD2	1.62	1.27
3:H:184:VAL:HG12	3:H:185:PRO:CD	1.66	1.25
2:C:6:THR:CG2	2:C:40:LEU:H	1.51	1.23
3:H:184:VAL:CG1	3:H:185:PRO:CD	2.22	1.17
3:H:184:VAL:CG1	3:H:185:PRO:HD2	1.75	1.15
3:H:159:LEU:HD23	3:H:163:VAL:CG2	1.80	1.11
3:H:145:TYR:CD1	3:H:145:TYR:O	2.03	1.10
2:C:6:THR:OG1	2:C:7:PRO:HD3	1.54	1.07
2:C:25:THR:HB	2:C:36:LYS:CD	1.85	1.06
1:L:135:LEU:HD22	3:H:181:VAL:HG11	1.35	1.05
3:H:184:VAL:HG12	3:H:185:PRO:HD2	1.08	1.04
3:H:18:VAL:HG23	3:H:82(c):LEU:HD11	1.05	1.01
3:H:159:LEU:CD2	3:H:163:VAL:CG2	2.37	1.01
3:H:159:LEU:HD21	3:H:182:VAL:HG11	1.43	1.01
2:C:25:THR:HG21	2:C:36:LYS:CE	1.91	1.00
3:H:18:VAL:CG2	3:H:82(c):LEU:HD11	1.92	1.00
3:H:159:LEU:HD21	3:H:182:VAL:CG1	1.91	0.99
3:H:18:VAL:HG23	3:H:82(c):LEU:CD1	1.91	0.98
3:H:159:LEU:CD2	3:H:163:VAL:HG22	1.93	0.98
2:C:21:CYS:SG	2:C:58:CYS:HB3	2.05	0.97
2:C:41:GLY:H	2:C:64:ASN:HD21	1.09	0.97
2:C:6:THR:CG2	2:C:40:LEU:N	2.28	0.96
2:C:25:THR:CG2	2:C:36:LYS:HD2	1.95	0.95
2:C:25:THR:HB	2:C:36:LYS:HD2	0.93	0.92
2:C:6:THR:HG23	2:C:40:LEU:H	1.32	0.92
1:L:163:VAL:HG22	1:L:175:LEU:HD13	1.49	0.92
2:C:36:LYS:HE3	3:H:100(a):GLU:OE2	1.70	0.90
2:C:6:THR:HG21	2:C:39:ASP:HA	1.49	0.90
2:C:6:THR:HG22	2:C:40:LEU:H	1.37	0.87
3:H:184:VAL:HG13	3:H:185:PRO:HD3	1.56	0.86
3:H:184:VAL:HG13	3:H:185:PRO:CD	2.04	0.86
2:C:41:GLY:H	2:C:64:ASN:ND2	1.74	0.85
2:C:25:THR:HG21	2:C:36:LYS:NZ	1.92	0.84
2:C:6:THR:HG23	2:C:40:LEU:N	1.92	0.84
2:C:25:THR:HG22	2:C:36:LYS:HZ2	1.43	0.84
2:C:6:THR:OG1	2:C:7:PRO:CD	2.25	0.83
2:C:25:THR:CG2	2:C:36:LYS:NZ	2.42	0.83
3:H:12:LYS:HG3	3:H:18:VAL:HG22	1.61	0.82
1:L:145:LYS:HB2	1:L:197:THR:OG1	1.81	0.80
1:L:8:PRO:O	1:L:102:THR:HB	1.83	0.79
3:H:184:VAL:CG1	3:H:185:PRO:HD3	2.10	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:LYS:HG2	3:H:100(a):GLU:CD	2.08	0.78
3:H:184:VAL:HG11	3:H:194:TYR:OH	1.83	0.78
3:H:159:LEU:HD23	3:H:163:VAL:HG23	1.67	0.76
1:L:163:VAL:CG2	1:L:175:LEU:HD13	2.17	0.74
1:L:135:LEU:CD2	3:H:181:VAL:HG11	2.15	0.74
2:C:25:THR:CG2	2:C:36:LYS:CD	2.65	0.74
2:C:25:THR:CG2	2:C:36:LYS:CE	2.66	0.73
1:L:140:TYR:HB3	1:L:141:PRO:HD3	1.70	0.73
3:H:159:LEU:CD2	3:H:182:VAL:HG11	2.18	0.73
2:C:25:THR:HG21	2:C:36:LYS:HE2	1.70	0.72
3:H:159:LEU:HD11	3:H:182:VAL:HG11	1.69	0.72
2:C:25:THR:CG2	2:C:36:LYS:HZ2	2.01	0.71
3:H:159:LEU:HD21	3:H:182:VAL:HG13	1.73	0.71
3:H:136:ALA:HB3	3:H:184:VAL:O	1.90	0.71
2:C:21:CYS:HB3	2:C:64:ASN:CG	2.16	0.71
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.73	0.70
2:C:36:LYS:HG2	3:H:100(a):GLU:OE1	1.91	0.70
3:H:54:PHE:CZ	3:H:100(d):PRO:HG2	2.26	0.70
3:H:145:TYR:CD1	3:H:145:TYR:C	2.70	0.69
2:C:46:CYS:HG	2:C:57:CYS:CB	2.08	0.68
1:L:118:PHE:CD1	3:H:124:LEU:HB3	2.29	0.67
1:L:184:ALA:O	1:L:188:LYS:HG3	1.94	0.67
3:H:146:PHE:HB3	3:H:147:PRO:HD3	1.76	0.67
3:H:145:TYR:O	3:H:145:TYR:CG	2.43	0.67
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.31	0.65
3:H:7:SER:OG	3:H:20:VAL:HG13	1.97	0.64
1:L:7:SER:HB3	1:L:22:THR:OG1	1.97	0.64
3:H:147:PRO:HB2	3:H:202:PRO:HG2	1.79	0.64
1:L:19:VAL:HG23	1:L:78:LEU:HD11	1.79	0.64
2:C:40:LEU:HD13	2:C:64:ASN:O	1.96	0.64
2:C:55:ILE:HB	4:C:101:HOH:O	1.97	0.63
3:H:51:TYR:HE1	3:H:52(a):PRO:HA	1.64	0.63
3:H:159:LEU:HD23	3:H:163:VAL:HG21	1.77	0.63
3:H:184:VAL:HG12	3:H:185:PRO:N	2.13	0.63
3:H:18:VAL:HG21	3:H:109:VAL:HG11	1.80	0.63
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.81	0.63
2:C:6:THR:HG21	2:C:39:ASP:CA	2.25	0.63
1:L:63:SER:OG	1:L:74:THR:HB	1.98	0.63
2:C:63:CYS:C	2:C:65:PRO:HD3	2.23	0.63
2:C:6:THR:HG23	2:C:40:LEU:O	1.98	0.63
2:C:21:CYS:HA	2:C:41:GLY:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:136:ALA:HB3	3:H:184:VAL:C	2.25	0.62
1:L:78:LEU:HD22	1:L:104:LEU:HD21	1.82	0.62
3:H:195:ILE:HG12	3:H:210:LYS:HA	1.80	0.62
1:L:83:PHE:HA	1:L:104:LEU:HD23	1.80	0.62
1:L:190:LYS:HA	1:L:212:GLY:HA2	1.81	0.62
1:L:114:SER:OG	1:L:137:ASN:HB3	2.00	0.61
2:C:22:TYR:HD2	2:C:24:LYS:HG3	1.67	0.60
2:C:6:THR:CG2	2:C:39:ASP:HA	2.28	0.59
3:H:159:LEU:HD21	3:H:163:VAL:HG22	1.80	0.59
1:L:94:THR:OG1	1:L:95:PRO:HD3	2.02	0.59
2:C:50:LYS:HB2	2:C:53:VAL:HG23	1.84	0.59
2:C:24:LYS:HA	2:C:55:ILE:HG12	1.85	0.59
3:H:2:VAL:HG11	3:H:94:ARG:HD2	1.83	0.59
3:H:121:VAL:HG22	3:H:198:VAL:HG21	1.85	0.58
2:C:21:CYS:O	2:C:57:CYS:HA	2.03	0.57
1:L:19:VAL:CG2	1:L:78:LEU:HD11	2.34	0.57
1:L:184:ALA:O	1:L:188:LYS:CG	2.53	0.56
1:L:6:GLN:HG2	1:L:88:CYS:SG	2.46	0.56
3:H:185:PRO:HB2	3:H:188:SER:HB3	1.88	0.56
3:H:159:LEU:CD1	3:H:182:VAL:HG11	2.36	0.56
2:C:22:TYR:O	2:C:40:LEU:HA	2.06	0.55
2:C:25:THR:CB	2:C:36:LYS:CD	2.58	0.55
1:L:145:LYS:CB	1:L:197:THR:OG1	2.54	0.55
3:H:87:THR:HG23	3:H:110:THR:HA	1.89	0.54
1:L:48:ILE:HG23	1:L:53:SER:O	2.07	0.54
2:C:38:ILE:HD11	3:H:100(a):GLU:HG3	1.87	0.54
1:L:4:MET:SD	1:L:90:GLN:HB3	2.48	0.54
1:L:94:THR:OG1	1:L:95:PRO:CD	2.56	0.54
3:H:213:PRO:O	3:H:214:LYS:C	2.51	0.54
3:H:184:VAL:HG11	3:H:194:TYR:CZ	2.42	0.53
1:L:2:ILE:HD11	1:L:92:TYR:HD2	1.73	0.53
1:L:8:PRO:HG2	1:L:21:ILE:HG23	1.90	0.53
2:C:45:THR:O	2:C:46:CYS:C	2.52	0.53
2:C:63:CYS:SG	2:C:63:CYS:O	2.67	0.53
2:C:41:GLY:N	2:C:64:ASN:HD21	1.93	0.53
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.91	0.52
1:L:158:ASN:O	1:L:179:LEU:HD12	2.09	0.52
1:L:14:SER:O	1:L:17:ASP:HB2	2.09	0.52
1:L:186:TYR:HA	1:L:192:TYR:OH	2.09	0.52
2:C:50:LYS:H	2:C:53:VAL:HB	1.75	0.52
3:H:145:TYR:O	3:H:145:TYR:HD1	1.84	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:PHE:CE2	1:L:211:ARG:HB2	2.44	0.52
3:H:95:ILE:HG23	3:H:100(g):SER:O	2.08	0.52
1:L:2:ILE:CD1	1:L:92:TYR:HD2	2.22	0.52
1:L:108:ARG:HG2	1:L:109:THR:H	1.75	0.52
2:C:38:ILE:HD11	3:H:100(a):GLU:HA	1.91	0.52
1:L:48:ILE:HD13	1:L:64:GLY:HA3	1.91	0.52
1:L:115:VAL:CG2	1:L:196:VAL:HG21	2.40	0.52
3:H:63:PHE:HB3	3:H:67:VAL:CG2	2.39	0.52
1:L:8:PRO:HD3	1:L:22:THR:OG1	2.09	0.51
2:C:1:THR:HG22	2:C:19:ASP:OD1	2.10	0.51
3:H:134:GLY:O	3:H:135:THR:C	2.52	0.51
3:H:146:PHE:CB	3:H:147:PRO:HD3	2.40	0.51
1:L:48:ILE:HD13	1:L:64:GLY:N	2.25	0.50
1:L:63:SER:HG	1:L:74:THR:HB	1.75	0.50
3:H:51:TYR:CE1	3:H:52(a):PRO:HA	2.45	0.50
3:H:142:VAL:HG11	3:H:150:VAL:HG11	1.92	0.50
1:L:14:SER:O	1:L:78:LEU:HD12	2.12	0.50
3:H:148:GLU:O	3:H:149:PRO:C	2.55	0.50
3:H:165:THR:CG2	3:H:178:LEU:HD21	2.41	0.50
3:H:195:ILE:HD11	3:H:210:LYS:HG2	1.93	0.50
3:H:60:ALA:O	3:H:64:GLN:HG3	2.11	0.50
1:L:62:PHE:CE1	1:L:75:ILE:HG23	2.47	0.49
1:L:141:PRO:HD2	1:L:198:HIS:CE1	2.48	0.49
3:H:54:PHE:CE2	3:H:100(d):PRO:HG2	2.47	0.49
1:L:11:LEU:CD2	1:L:19:VAL:HG13	2.43	0.49
1:L:135:LEU:HD22	3:H:181:VAL:CG1	2.24	0.49
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.48	0.48
2:C:6:THR:O	2:C:9:ALA:N	2.47	0.48
2:C:22:TYR:CD2	2:C:24:LYS:HG3	2.46	0.48
3:H:54:PHE:HZ	3:H:100(d):PRO:HG2	1.77	0.48
1:L:48:ILE:HD13	1:L:64:GLY:CA	2.44	0.48
1:L:150:VAL:HG22	1:L:192:TYR:CD1	2.49	0.48
2:C:12:GLN:O	2:C:13:THR:C	2.57	0.48
1:L:185:ASP:N	1:L:185:ASP:OD1	2.47	0.48
3:H:32:TYR:CD2	3:H:94:ARG:HD3	2.49	0.48
3:H:114:ALA:HB3	3:H:146:PHE:CE1	2.49	0.48
1:L:83:PHE:CD2	1:L:104:LEU:HG	2.48	0.48
2:C:25:THR:HG21	2:C:36:LYS:CD	2.32	0.48
3:H:145:TYR:HE1	3:H:148:GLU:HA	1.79	0.48
1:L:4:MET:HE3	1:L:33:LEU:CD1	2.45	0.47
3:H:52(a):PRO:O	3:H:53:ILE:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:CYS:HG	2:C:57:CYS:HB2	1.78	0.47
3:H:128:SER:O	3:H:129:LYS:C	2.57	0.47
3:H:201:LYS:N	3:H:202:PRO:CD	2.78	0.47
3:H:2:VAL:HG11	3:H:94:ARG:CD	2.44	0.47
3:H:35:SER:HA	3:H:50:GLY:HA2	1.96	0.47
3:H:145:TYR:CE1	3:H:176:TYR:HB2	2.49	0.47
3:H:147:PRO:HB2	3:H:202:PRO:CG	2.45	0.47
3:H:152:VAL:HG22	3:H:198:VAL:HG22	1.97	0.47
2:C:20:ILE:HG23	2:C:57:CYS:HB3	1.96	0.46
2:C:21:CYS:SG	2:C:64:ASN:HB2	2.55	0.46
3:H:52:ILE:HD11	3:H:100(f):GLU:HG3	1.96	0.46
3:H:37:VAL:HG22	3:H:47:TRP:HA	1.96	0.46
3:H:63:PHE:HB3	3:H:67:VAL:HG23	1.97	0.46
1:L:2:ILE:HD11	1:L:92:TYR:CD2	2.50	0.46
2:C:3:CYS:HB2	2:C:14:CYS:SG	2.55	0.46
1:L:170:ASP:HB3	1:L:172:THR:HG23	1.97	0.46
3:H:148:GLU:HB3	3:H:149:PRO:HD3	1.98	0.46
1:L:137:ASN:ND2	3:H:183:THR:HG21	2.31	0.46
3:H:41:PRO:O	3:H:43:GLN:HG3	2.16	0.45
3:H:43:GLN:CD	4:H:301:HOH:O	2.59	0.45
2:C:1:THR:C	2:C:14:CYS:HB2	2.42	0.45
2:C:23:THR:HG22	2:C:64:ASN:OD1	2.17	0.45
1:L:33:LEU:HD11	1:L:88:CYS:HB2	1.98	0.45
1:L:119:PRO:HB3	1:L:209:PHE:CE2	2.52	0.45
2:C:67:PRO:O	2:C:68:THR:C	2.59	0.44
3:H:124:LEU:HD12	3:H:181:VAL:HG22	1.99	0.44
1:L:195:GLU:HA	1:L:206:THR:HG22	1.99	0.44
1:L:30:SER:OG	1:L:31:SER:N	2.51	0.44
2:C:38:ILE:CD1	3:H:100(a):GLU:HA	2.47	0.44
3:H:146:PHE:CD1	3:H:146:PHE:O	2.70	0.44
3:H:136:ALA:O	3:H:183:THR:HA	2.18	0.43
1:L:140:TYR:CB	1:L:141:PRO:HD3	2.45	0.43
3:H:132:SER:C	3:H:134:GLY:H	2.26	0.43
3:H:80:MET:HE3	3:H:80:MET:HB3	1.79	0.43
3:H:125:ALA:HB1	3:H:126:PRO:HD2	2.01	0.43
2:C:22:TYR:HB3	2:C:47:PRO:HG2	2.02	0.42
3:H:61:GLN:O	3:H:64:GLN:HB2	2.19	0.42
1:L:82:ASP:O	1:L:104:LEU:HD23	2.19	0.42
3:H:43:GLN:HB3	4:H:301:HOH:O	2.20	0.42
3:H:165:THR:HG22	3:H:178:LEU:HD21	2.00	0.42
1:L:20:THR:HA	1:L:73:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HG2	1:L:109:THR:N	2.34	0.42
1:L:8:PRO:HB2	1:L:102:THR:HB	2.02	0.41
1:L:11:LEU:HD21	1:L:19:VAL:HG13	2.01	0.41
1:L:90:GLN:NE2	1:L:97:THR:OG1	2.54	0.41
2:C:22:TYR:HE1	2:C:42:CYS:O	2.04	0.41
1:L:4:MET:SD	1:L:90:GLN:HG2	2.61	0.41
1:L:6:GLN:HG3	1:L:99:GLY:HA3	2.02	0.41
1:L:9:SER:O	1:L:102:THR:HA	2.20	0.41
3:H:18:VAL:CG2	3:H:82(c):LEU:CD1	2.72	0.41
1:L:94:THR:N	1:L:95:PRO:HD2	2.36	0.41
2:C:22:TYR:CD2	2:C:24:LYS:HE3	2.55	0.41
3:H:200:HIS:C	3:H:202:PRO:HD2	2.46	0.41
1:L:163:VAL:HG22	1:L:175:LEU:CD1	2.36	0.41
1:L:115:VAL:HG21	1:L:196:VAL:HG21	2.04	0.40
2:C:58:CYS:SG	2:C:59:SER:N	2.94	0.40
2:C:3:CYS:HG	2:C:21:CYS:HG	1.65	0.40
2:C:40:LEU:HB3	2:C:64:ASN:CG	2.46	0.40
1:L:80:PRO:HA	1:L:83:PHE:CD1	2.57	0.40
1:L:175:LEU:HD12	1:L:176:SER:H	1.85	0.40
2:C:28:ASP:OD2	3:H:100:TYR:OH	2.26	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	210/212 (99%)	196 (93%)	14 (7%)	0	100	100
2	C	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
3	H	225/228 (99%)	207 (92%)	18 (8%)	0	100	100
All	All	501/508 (99%)	462 (92%)	39 (8%)	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	L	188/188 (100%)	185 (98%)	3 (2%)	55	83
2	C	60/60 (100%)	59 (98%)	1 (2%)	53	82
3	H	189/190 (100%)	186 (98%)	3 (2%)	55	83
All	All	437/438 (100%)	430 (98%)	7 (2%)	55	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	185	ASP
1	L	210	ASN
1	L	211	ARG
2	C	63	CYS
3	H	29	PHE
3	H	97	LEU
3	H	147	PRO

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

Mol	Chain	Res	Type
1	L	137	ASN
1	L	210	ASN
2	C	64	ASN
3	H	58	ASN
3	H	164	HIS

5.3.3 RNA ⓘ

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	L	212/212 (100%)	0.96	24 (11%) 10 9	30, 81, 129, 164	0
2	C	68/68 (100%)	1.20	9 (13%) 7 6	30, 119, 144, 147	0
3	H	227/228 (99%)	0.99	29 (12%) 7 6	30, 82, 155, 220	0
All	All	507/508 (99%)	1.01	62 (12%) 8 7	30, 86, 143, 220	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	92	TYR	5.0
2	C	21	CYS	3.9
3	H	211	VAL	3.7
3	H	187	SER	3.5
3	H	135	THR	3.5
1	L	11	LEU	3.5
3	H	136	ALA	3.3
2	C	66	PHE	3.3
3	H	97	LEU	3.2
2	C	63	CYS	3.2
3	H	148	GLU	3.2
1	L	21	ILE	3.1
1	L	148	TRP	3.1
3	H	29	PHE	3.1
1	L	115	VAL	3.1
1	L	8	PRO	3.1
1	L	209	PHE	3.0
3	H	125	ALA	3.0
1	L	146	VAL	3.0
1	L	135	LEU	2.9
2	C	67	PRO	2.9
3	H	152	VAL	2.8
3	H	94	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	105	GLN	2.7
3	H	138	LEU	2.7
3	H	158	ALA	2.6
2	C	65	PRO	2.6
1	L	191	VAL	2.6
3	H	194	TYR	2.6
3	H	32	TYR	2.5
2	C	3	CYS	2.5
1	L	4	MET	2.4
3	H	120	SER	2.4
3	H	193	THR	2.4
1	L	120	PRO	2.4
2	C	30	PHE	2.4
3	H	159	LEU	2.4
1	L	192	TYR	2.3
3	H	198	VAL	2.3
1	L	7	SER	2.3
3	H	30	SER	2.2
1	L	104	LEU	2.2
1	L	93	SER	2.2
3	H	102	TYR	2.2
3	H	54	PHE	2.2
1	L	19	VAL	2.2
1	L	170	ASP	2.2
3	H	146	PHE	2.2
3	H	184	VAL	2.1
1	L	140	TYR	2.1
1	L	106	ILE	2.1
3	H	126	PRO	2.1
1	L	181	LEU	2.1
3	H	45	LEU	2.1
1	L	177	SER	2.1
3	H	175	LEU	2.1
1	L	212	GLY	2.1
3	H	154	TRP	2.1
2	C	46	CYS	2.0
1	L	197	THR	2.0
2	C	7	PRO	2.0
3	H	181	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.