



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 PM UTC

PDB ID : 2XTE / pdb_00002xte
Title : Structure of the TBL1 tetramerisation domain
Authors : Oberoi, J.; Fairall, L.; Watson, P.J.; Greenwood, J.A.; Schwabe, J.W.R.
Deposited on : 2010-10-06
Resolution : 3.90 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

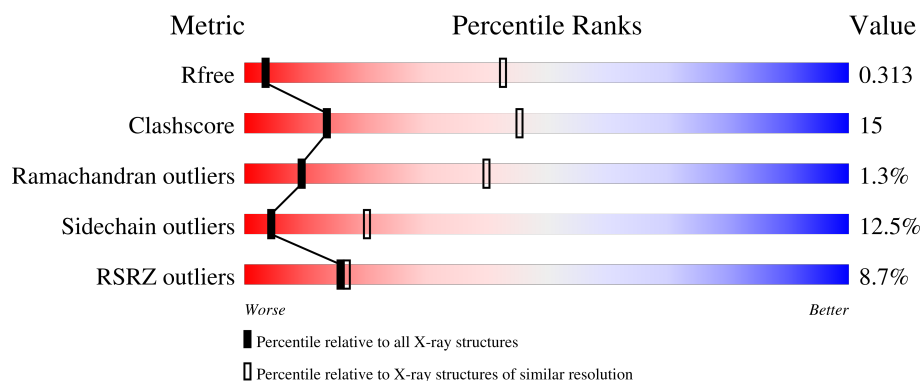
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



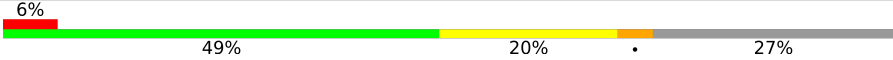
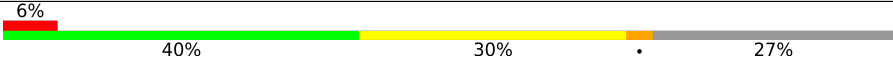
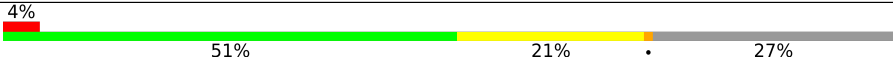
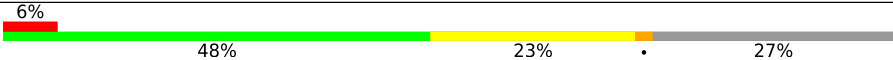
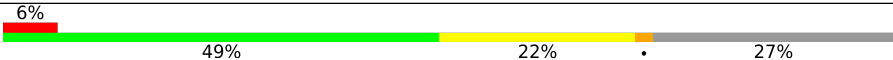
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	90	6% 49% 24% 27%
1	B	90	7% 44% 23% 6% 27%
1	C	90	8% 47% 26% . 27%
1	D	90	8% 43% 23% . . 27%
1	E	90	3% 47% 21% 6% 27%

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Mol	Chain	Length	Quality of chain
1	F	90	
1	G	90	
1	H	90	
1	I	90	
1	J	90	
1	K	90	
1	L	90	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6036 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.

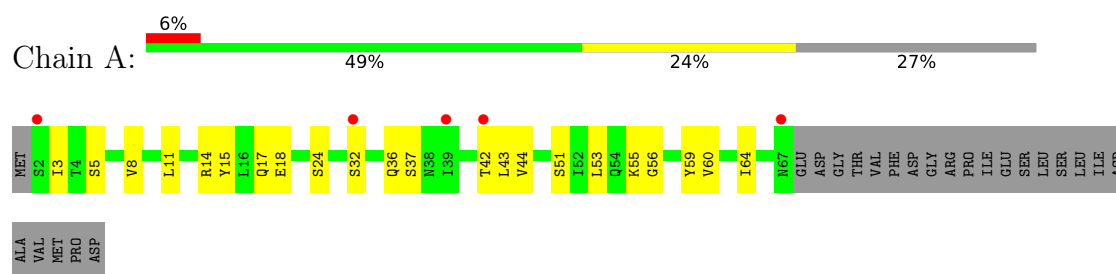
- Molecule 1 is a protein called F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	B	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	C	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	D	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	E	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	F	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	G	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	H	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	I	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	J	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	K	66	Total	C	N	O	0	0	0
			503	320	82	101			
1	L	66	Total	C	N	O	0	0	0
			503	320	82	101			

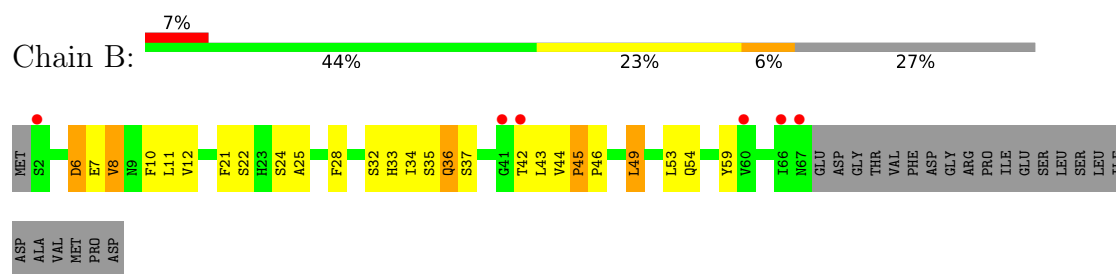
3 Residue-property plots [i](#)

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.

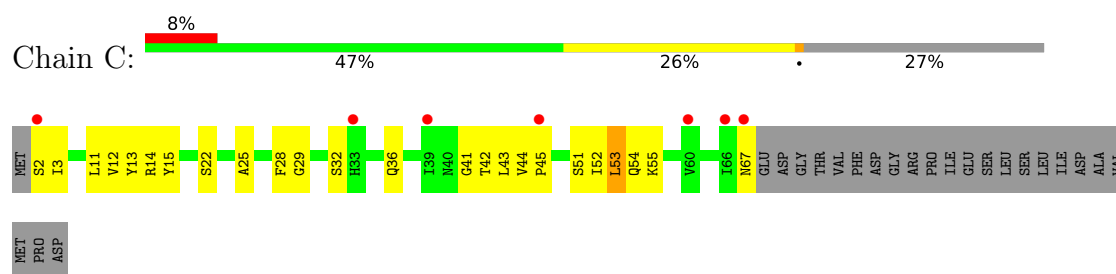
- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



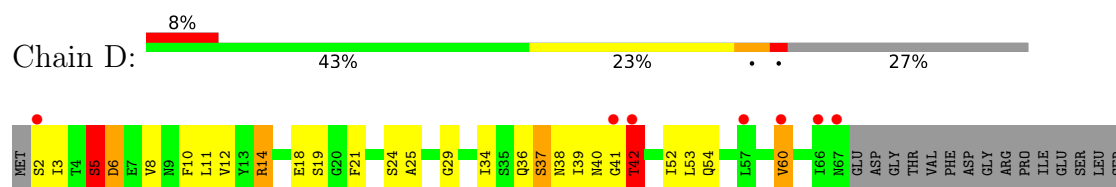
- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



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• Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 E7 V8 L11 R14 Q17 S22 F28 G29 S32 H33 I34 S36 Q36 S37 M40 G41 T42 L43 V44 P45 P46 A47 A48 L49 I50 L53 Q54 K55 Y59 V60 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE SER LEU SER LEU

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• Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 I3 V8 L11 Y12 Y13 R14 Y15 E18 I34 S35 Q36 I39 N40 G41 T42 L43 V44 A47 S51 I52 L53 Q54 K55 G56 Y59 V60 E63 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE SER LEU SER LEU ILE ASP ALA VAL

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• Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 S5 V8 N9 V12 Y13 R14 Y15 A25 G29 S32 H33 I34 S36 Q36 N38 I39 T42 L43 V44 P45 A48 S51 I52 L53 Q54 K55 G56 L57 Y59 V60 E61 A62 E63 I64 S65 I66 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE SER LEU SER LEU PRO

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• Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 I3 V8 N9 F10 L11 N9 V12 Y13 R14 Y15 S19 G20 F21 E31 S32 H33 I34 S36 Q36 I39 N40 G41 T42 L43 V44 P45 L49 I50 S51 I52 L53 Q54 K55 V60 I66 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE SER LEU SER LEU

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• Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 I3 T4 S5 D6 E7 V8 N9 F10 L11 Y12 Y13 R14 Y15 S22 H23 S24 A25 E31 S32 Q36 S37 N38 I39 T42 L43 V44 P45 S51 I52 L53 Q54 K55 G56 Y59 V60 S65 I66 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE SER LEU SER

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- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 F10 L11 V12 Y13 S19 G20 F21 S22 H23 S24 A25 E31 S32 S33 S37 N40 G41 T42 L43 V44 L53 Q54 K55 G56 V60 I66 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE GLU SER LEU SER ILE ASP ALA VAL MET PRO ASP

- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 T3 T4 S5 D6 E7 N8 N9 F10 L11 V12 Y13 R14 Y15 I34 S35 Q36 S37 N38 I39 V44 P45 A48 S51 I52 I53 Q54 K55 G56 L57 Y58 V60 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE GLU SER LEU SER ILE ASP VAL

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- Molecule 1: F-BOX-LIKE/WD REPEAT-CONTAINING PROTEIN TBL1X



MET S2 T3 T4 E7 V8 N9 F10 L11 V12 S19 F28 G29 I34 S35 Q36 N40 G41 T42 I43 V44 P45 A47 A48 L49 L53 G56 Y59 V60 I66 N67 GLU ASP GLY THR VAL PHE ASP GLY ARG PRO ILE GLU SER LEU SER ILE ASP ALA

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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.02Å 150.19Å 164.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.10 – 3.90 111.02 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (111.10-3.90) 99.8 (111.02-3.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.273 , 0.302 0.276 , 0.313	Depositor DCC
R_{free} test set	1023 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	97.8	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 94.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6036	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.63% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/513	0.99	0/700
1	B	0.68	0/513	0.98	3/700 (0.4%)
1	C	0.73	0/513	0.99	0/700
1	D	0.66	0/513	0.98	1/700 (0.1%)
1	E	0.69	0/513	0.99	1/700 (0.1%)
1	F	0.72	0/513	1.15	3/700 (0.4%)
1	G	0.74	0/513	1.10	1/700 (0.1%)
1	H	0.63	0/513	1.03	3/700 (0.4%)
1	I	0.67	0/513	1.08	4/700 (0.6%)
1	J	0.66	0/513	0.91	0/700
1	K	0.71	0/513	1.01	1/700 (0.1%)
1	L	0.66	0/513	1.06	3/700 (0.4%)
All	All	0.69	0/6156	1.02	20/8400 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	44	VAL	CA-C-N	9.03	126.16	119.66
1	F	44	VAL	C-N-CA	9.03	126.16	119.66
1	L	45	PRO	CA-C-N	7.64	129.39	119.84
1	L	45	PRO	C-N-CA	7.64	129.39	119.84
1	L	34	ILE	N-CA-C	6.83	117.59	110.62
1	H	45	PRO	CA-C-N	6.64	126.67	119.90
1	H	45	PRO	C-N-CA	6.64	126.67	119.90
1	D	42	THR	N-CA-C	-6.54	105.60	113.97
1	I	44	VAL	CA-C-N	5.99	126.55	120.38
1	I	44	VAL	C-N-CA	5.99	126.55	120.38
1	F	34	ILE	N-CA-C	5.98	116.64	110.36
1	B	45	PRO	CA-C-N	5.85	125.82	120.03
1	B	45	PRO	C-N-CA	5.85	125.82	120.03
1	I	65	SER	N-CA-C	5.66	119.36	112.23
1	H	42	THR	N-CA-C	-5.58	105.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	45	PRO	N-CA-C	5.44	117.33	110.70
1	G	65	SER	N-CA-C	5.39	118.95	112.38
1	E	34	ILE	N-CA-C	5.30	117.71	111.09
1	K	34	ILE	N-CA-C	5.23	115.96	110.62
1	B	34	ILE	N-CA-C	5.17	117.55	111.09

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	503	0	459	18	0
1	B	503	0	459	21	0
1	C	503	0	459	24	0
1	D	503	0	459	19	0
1	E	503	0	459	23	0
1	F	503	0	459	20	0
1	G	503	0	459	17	0
1	H	503	0	459	17	0
1	I	503	0	459	17	0
1	J	503	0	459	15	0
1	K	503	0	459	18	0
1	L	503	0	459	20	0
All	All	6036	0	5508	169	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 15.

All (169) 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:E:59:TYR:HD2	1:F:55:LYS:HE3	1.28	0.96
1:E:59:TYR:CD2	1:F:55:LYS:HE3	2.06	0.90
1:K:55:LYS:HZ3	1:L:60:VAL:HG22	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD12	1:B:53:LEU:HD12	1.64	0.79
1:L:40:ASN:HB3	1:L:43:LEU:HD12	1.68	0.76
1:C:32:SER:HA	1:D:21:PHE:HE1	1.52	0.72
1:E:55:LYS:HD3	1:F:59:TYR:HD2	1.54	0.72
1:B:43:LEU:O	1:B:45:PRO:HD3	1.89	0.72
1:A:43:LEU:HD22	1:C:55:LYS:HD2	1.73	0.71
1:A:53:LEU:CD1	1:B:53:LEU:CD1	2.71	0.69
1:I:59:TYR:CD2	1:J:55:LYS:HE2	2.27	0.69
1:K:55:LYS:HE3	1:L:59:TYR:HD2	1.58	0.68
1:C:3:ILE:HG22	1:D:54:GLN:NE2	2.09	0.68
1:I:3:ILE:HG22	1:J:54:GLN:NE2	2.09	0.66
1:G:55:LYS:NZ	1:H:60:VAL:HG22	2.10	0.66
1:E:53:LEU:HD12	1:F:53:LEU:HD12	1.79	0.65
1:E:60:VAL:HA	1:F:55:LYS:HZ3	1.61	0.64
1:I:56:GLY:O	1:I:60:VAL:HG23	1.97	0.64
1:G:9:ASN:OD1	1:H:15:TYR:OH	2.14	0.64
1:F:56:GLY:O	1:F:60:VAL:HG23	1.96	0.63
1:D:34:ILE:O	1:D:37:SER:HB2	1.98	0.63
1:L:10:PHE:CE2	1:L:44:VAL:HG21	2.34	0.62
1:E:59:TYR:HB2	1:F:59:TYR:HB2	1.82	0.61
1:A:53:LEU:CD1	1:B:53:LEU:HD12	2.30	0.61
1:K:55:LYS:NZ	1:L:60:VAL:HG22	2.13	0.60
1:I:3:ILE:HG22	1:J:54:GLN:HE21	1.67	0.60
1:E:53:LEU:HD21	1:F:11:LEU:HD23	1.83	0.59
1:L:11:LEU:HB3	1:L:49:LEU:HD13	1.84	0.59
1:I:6:ASP:O	1:I:9:ASN:HB2	2.03	0.59
1:A:43:LEU:HD13	1:C:55:LYS:HE3	1.83	0.59
1:D:10:PHE:CZ	1:D:41:GLY:HA3	2.38	0.58
1:F:3:ILE:HG23	1:F:3:ILE:O	2.04	0.58
1:I:55:LYS:NZ	1:J:60:VAL:HG22	2.17	0.58
1:L:8:VAL:O	1:L:12:VAL:HG23	2.04	0.58
1:A:42:THR:O	1:A:43:LEU:HD23	2.04	0.57
1:E:43:LEU:O	1:E:45:PRO:HD3	2.04	0.57
1:C:14:ARG:O	1:C:15:TYR:C	2.47	0.57
1:E:59:TYR:HD2	1:F:55:LYS:CE	2.11	0.57
1:F:8:VAL:O	1:F:12:VAL:HG23	2.05	0.57
1:A:32:SER:HA	1:B:21:PHE:HE1	1.70	0.56
1:C:32:SER:HA	1:D:21:PHE:CE1	2.37	0.56
1:K:53:LEU:HD13	1:L:53:LEU:HD12	1.88	0.56
1:J:40:ASN:HB3	1:J:43:LEU:HB2	1.88	0.55
1:F:14:ARG:HD2	1:F:18:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:O	1:B:12:VAL:HG23	2.07	0.54
1:B:7:GLU:HG2	1:E:43:LEU:HG	1.89	0.54
1:J:22:SER:HA	1:J:25:ALA:HB3	1.90	0.54
1:B:46:PRO:HG3	1:F:60:VAL:HG21	1.89	0.54
1:C:41:GLY:C	1:C:43:LEU:H	2.15	0.54
1:I:31:GLU:CD	1:J:23:HIS:HB2	2.33	0.54
1:A:3:ILE:HG22	1:B:54:GLN:NE2	2.24	0.53
1:B:11:LEU:HB3	1:B:49:LEU:HD12	1.91	0.53
1:I:32:SER:HA	1:J:21:PHE:HE1	1.73	0.52
1:I:42:THR:O	1:I:43:LEU:HD23	2.09	0.52
1:C:2:SER:N	1:C:3:ILE:HA	2.24	0.52
1:D:5:SER:O	1:D:8:VAL:N	2.40	0.52
1:C:53:LEU:HD13	1:D:53:LEU:HD12	1.89	0.52
1:C:55:LYS:NZ	1:D:60:VAL:HG22	2.24	0.52
1:K:3:ILE:O	1:K:3:ILE:HG23	2.08	0.52
1:E:47:ALA:O	1:E:48:ALA:C	2.52	0.52
1:F:40:ASN:CG	1:F:43:LEU:HD12	2.35	0.51
1:E:40:ASN:HB3	1:E:43:LEU:HB2	1.91	0.51
1:C:54:GLN:NE2	1:D:3:ILE:HG22	2.26	0.51
1:H:51:SER:O	1:H:55:LYS:HG3	2.10	0.51
1:D:5:SER:O	1:D:8:VAL:HG12	2.10	0.51
1:E:7:GLU:O	1:E:11:LEU:HB2	2.11	0.51
1:D:40:ASN:C	1:D:42:THR:H	2.18	0.50
1:G:42:THR:O	1:G:43:LEU:HD23	2.11	0.50
1:K:57:LEU:O	1:K:60:VAL:HB	2.11	0.50
1:L:40:ASN:O	1:L:43:LEU:HB2	2.11	0.50
1:A:55:LYS:HD2	1:C:43:LEU:HD22	1.93	0.50
1:E:59:TYR:HD1	1:F:59:TYR:HD1	1.59	0.50
1:G:55:LYS:HZ3	1:H:60:VAL:HG22	1.77	0.50
1:A:56:GLY:O	1:A:60:VAL:HG23	2.12	0.50
1:K:6:ASP:HB3	1:K:37:SER:OG	2.11	0.49
1:K:55:LYS:HE3	1:L:59:TYR:CD2	2.43	0.49
1:L:43:LEU:O	1:L:45:PRO:HD3	2.12	0.49
1:G:14:ARG:O	1:G:15:TYR:C	2.54	0.49
1:D:29:GLY:O	1:D:34:ILE:HG22	2.12	0.49
1:L:49:LEU:O	1:L:53:LEU:HB2	2.12	0.49
1:C:28:PHE:O	1:C:29:GLY:C	2.54	0.49
1:J:10:PHE:CE2	1:J:44:VAL:HG21	2.46	0.49
1:G:55:LYS:HZ1	1:H:60:VAL:HG22	1.77	0.48
1:C:42:THR:O	1:C:43:LEU:HD23	2.13	0.48
1:K:13:TYR:O	1:K:14:ARG:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:VAL:O	1:C:13:TYR:C	2.57	0.47
1:E:32:SER:O	1:E:33:HIS:C	2.56	0.47
1:H:11:LEU:HB3	1:H:49:LEU:HD13	1.96	0.47
1:K:53:LEU:HD13	1:L:53:LEU:CD1	2.44	0.47
1:J:12:VAL:O	1:J:13:TYR:C	2.58	0.47
1:D:14:ARG:HD2	1:D:18:GLU:OE1	2.13	0.47
1:H:3:ILE:O	1:H:3:ILE:HG23	2.15	0.47
1:H:41:GLY:HA2	1:H:44:VAL:HG23	1.95	0.47
1:I:8:VAL:O	1:I:12:VAL:HG23	2.15	0.46
1:G:25:ALA:O	1:G:29:GLY:N	2.43	0.46
1:A:59:TYR:HB2	1:B:59:TYR:HB2	1.97	0.46
1:E:55:LYS:HD3	1:F:59:TYR:CD2	2.41	0.46
1:F:41:GLY:C	1:F:43:LEU:H	2.24	0.46
1:C:41:GLY:C	1:C:43:LEU:N	2.74	0.46
1:C:55:LYS:HZ2	1:D:60:VAL:HG22	1.81	0.46
1:C:22:SER:O	1:C:25:ALA:HB3	2.16	0.46
1:B:24:SER:O	1:B:25:ALA:C	2.57	0.45
1:C:44:VAL:HG22	1:C:45:PRO:CD	2.46	0.45
1:C:53:LEU:HD13	1:D:53:LEU:CD1	2.47	0.45
1:F:47:ALA:O	1:F:51:SER:OG	2.32	0.45
1:G:53:LEU:HD13	1:H:53:LEU:HD13	1.99	0.45
1:B:32:SER:O	1:B:33:HIS:C	2.60	0.44
1:I:14:ARG:O	1:I:15:TYR:C	2.60	0.44
1:J:56:GLY:O	1:J:60:VAL:HG23	2.17	0.44
1:E:28:PHE:O	1:E:29:GLY:C	2.61	0.44
1:E:49:LEU:O	1:E:50:ILE:C	2.61	0.44
1:G:12:VAL:O	1:G:13:TYR:C	2.60	0.44
1:K:56:GLY:HA2	1:L:56:GLY:N	2.33	0.44
1:C:51:SER:O	1:C:52:ILE:C	2.61	0.44
1:I:11:LEU:HD23	1:J:53:LEU:HD21	1.99	0.44
1:C:53:LEU:HD12	1:D:52:ILE:CG2	2.48	0.44
1:D:2:SER:HA	1:D:3:ILE:HA	1.75	0.43
1:G:32:SER:OG	1:G:34:ILE:HB	2.18	0.43
1:H:12:VAL:O	1:H:13:TYR:C	2.61	0.43
1:C:44:VAL:HG22	1:C:45:PRO:HD2	1.99	0.43
1:F:53:LEU:O	1:F:54:GLN:C	2.62	0.43
1:G:53:LEU:CD1	1:H:53:LEU:HD13	2.47	0.43
1:A:14:ARG:O	1:A:15:TYR:C	2.62	0.43
1:H:2:SER:HA	1:H:3:ILE:HA	1.81	0.43
1:D:39:ILE:HG22	1:D:41:GLY:N	2.34	0.42
1:J:24:SER:O	1:J:25:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:OG	1:B:28:PHE:HA	2.19	0.42
1:H:44:VAL:HA	1:H:45:PRO:HD3	1.78	0.42
1:K:14:ARG:O	1:K:15:TYR:C	2.61	0.42
1:G:45:PRO:O	1:G:48:ALA:HB2	2.20	0.42
1:G:59:TYR:O	1:G:63:GLU:HG3	2.18	0.42
1:I:53:LEU:O	1:I:54:GLN:C	2.62	0.42
1:B:36:GLN:N	1:B:36:GLN:HE21	2.17	0.42
1:K:59:TYR:HB2	1:L:59:TYR:HB2	2.01	0.42
1:B:6:ASP:OD2	1:B:6:ASP:N	2.52	0.42
1:L:7:GLU:O	1:L:11:LEU:HD23	2.20	0.42
1:K:56:GLY:O	1:K:60:VAL:HG23	2.19	0.42
1:A:3:ILE:HG23	1:A:3:ILE:O	2.20	0.41
1:A:64:ILE:HG23	1:E:17:GLN:HB3	2.02	0.41
1:B:45:PRO:HA	1:B:46:PRO:HD3	1.70	0.41
1:G:32:SER:O	1:G:33:HIS:C	2.63	0.41
1:C:51:SER:O	1:C:54:GLN:N	2.53	0.41
1:G:32:SER:HA	1:H:21:PHE:CE1	2.55	0.41
1:L:40:ASN:O	1:L:44:VAL:HG23	2.20	0.41
1:H:53:LEU:HD12	1:H:53:LEU:HA	1.91	0.41
1:K:3:ILE:O	1:K:3:ILE:CG2	2.68	0.41
1:K:45:PRO:O	1:K:48:ALA:HB2	2.20	0.41
1:L:46:PRO:C	1:L:48:ALA:N	2.78	0.41
1:I:24:SER:OG	1:J:31:GLU:OE1	2.32	0.41
1:A:55:LYS:HE2	1:B:59:TYR:HD2	1.85	0.41
1:E:32:SER:O	1:E:34:ILE:N	2.54	0.41
1:L:28:PHE:O	1:L:29:GLY:C	2.62	0.41
1:L:45:PRO:O	1:L:48:ALA:HB2	2.21	0.41
1:A:17:GLN:O	1:A:18:GLU:C	2.64	0.41
1:K:9:ASN:O	1:K:10:PHE:C	2.64	0.41
1:D:24:SER:O	1:D:25:ALA:C	2.64	0.41
1:E:14:ARG:HD2	1:E:14:ARG:HA	1.75	0.41
1:H:31:GLU:C	1:H:33:HIS:H	2.29	0.41
1:I:22:SER:O	1:I:25:ALA:HB3	2.21	0.41
1:I:51:SER:O	1:I:52:ILE:C	2.61	0.41
1:G:44:VAL:HA	1:G:45:PRO:HD3	1.88	0.41
1:E:40:ASN:O	1:E:43:LEU:HB2	2.20	0.40
1:K:6:ASP:HB3	1:K:37:SER:HG	1.85	0.40
1:I:55:LYS:HZ3	1:J:60:VAL:HG22	1.84	0.40
1:A:59:TYR:HD1	1:B:59:TYR:HD1	1.69	0.40
1:F:14:ARG:O	1:F:15:TYR:C	2.64	0.40
1:G:53:LEU:HD13	1:H:53:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PHE:CE2	1:B:44:VAL:HG21	2.56	0.40
1:B:43:LEU:HD11	1:E:7:GLU:HG2	2.04	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	64/90 (71%)	56 (88%)	8 (12%)	0	100	100
1	B	64/90 (71%)	57 (89%)	7 (11%)	0	100	100
1	C	64/90 (71%)	50 (78%)	14 (22%)	0	100	100
1	D	64/90 (71%)	56 (88%)	6 (9%)	2 (3%)	3	25
1	E	64/90 (71%)	54 (84%)	7 (11%)	3 (5%)	2	19
1	F	64/90 (71%)	51 (80%)	13 (20%)	0	100	100
1	G	64/90 (71%)	54 (84%)	9 (14%)	1 (2%)	7	36
1	H	64/90 (71%)	55 (86%)	9 (14%)	0	100	100
1	I	64/90 (71%)	51 (80%)	12 (19%)	1 (2%)	7	36
1	J	64/90 (71%)	50 (78%)	13 (20%)	1 (2%)	7	36
1	K	64/90 (71%)	49 (77%)	14 (22%)	1 (2%)	7	36
1	L	64/90 (71%)	58 (91%)	5 (8%)	1 (2%)	7	36
All	All	768/1080 (71%)	641 (84%)	117 (15%)	10 (1%)	9	40

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	33	HIS
1	J	33	HIS

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Mol	Chain	Res	Type
1	D	5	SER
1	L	47	ALA
1	D	6	ASP
1	E	48	ALA
1	G	5	SER
1	I	5	SER
1	K	15	TYR
1	E	50	ILE

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	50/79 (63%)	43 (86%)	7 (14%)	3	17
1	B	50/79 (63%)	42 (84%)	8 (16%)	2	14
1	C	50/79 (63%)	46 (92%)	4 (8%)	11	35
1	D	50/79 (63%)	39 (78%)	11 (22%)	1	6
1	E	50/79 (63%)	45 (90%)	5 (10%)	7	27
1	F	50/79 (63%)	44 (88%)	6 (12%)	5	21
1	G	50/79 (63%)	41 (82%)	9 (18%)	2	12
1	H	50/79 (63%)	44 (88%)	6 (12%)	5	21
1	I	50/79 (63%)	44 (88%)	6 (12%)	5	21
1	J	50/79 (63%)	47 (94%)	3 (6%)	17	44
1	K	50/79 (63%)	43 (86%)	7 (14%)	3	17
1	L	50/79 (63%)	47 (94%)	3 (6%)	17	44
All	All	600/948 (63%)	525 (88%)	75 (12%)	4	20

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	8	VAL

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	36	GLN
1	A	37	SER
1	A	44	VAL
1	A	51	SER
1	B	6	ASP
1	B	8	VAL
1	B	22	SER
1	B	35	SER
1	B	36	GLN
1	B	37	SER
1	B	42	THR
1	B	49	LEU
1	C	11	LEU
1	C	36	GLN
1	C	53	LEU
1	C	67	ASN
1	D	5	SER
1	D	6	ASP
1	D	11	LEU
1	D	12	VAL
1	D	14	ARG
1	D	19	SER
1	D	36	GLN
1	D	37	SER
1	D	38	ASN
1	D	42	THR
1	D	60	VAL
1	E	8	VAL
1	E	22	SER
1	E	36	GLN
1	E	37	SER
1	E	53	LEU
1	F	11	LEU
1	F	35	SER
1	F	36	GLN
1	F	44	VAL
1	F	51	SER
1	F	54	GLN
1	G	5	SER
1	G	8	VAL
1	G	14	ARG

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Mol	Chain	Res	Type
1	G	36	GLN
1	G	37	SER
1	G	38	ASN
1	G	51	SER
1	G	53	LEU
1	G	57	LEU
1	H	8	VAL
1	H	12	VAL
1	H	19	SER
1	H	35	SER
1	H	36	GLN
1	H	53	LEU
1	I	11	LEU
1	I	36	GLN
1	I	37	SER
1	I	51	SER
1	I	65	SER
1	I	67	ASN
1	J	19	SER
1	J	22	SER
1	J	37	SER
1	K	5	SER
1	K	8	VAL
1	K	11	LEU
1	K	36	GLN
1	K	44	VAL
1	K	51	SER
1	K	53	LEU
1	L	4	THR
1	L	12	VAL
1	L	36	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	B	17	GLN
1	B	33	HIS
1	B	36	GLN
1	B	40	ASN
1	B	54	GLN
1	D	17	GLN

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Mol	Chain	Res	Type
1	D	36	GLN
1	D	67	ASN
1	E	17	GLN
1	E	54	GLN
1	F	54	GLN
1	F	58	GLN
1	G	54	GLN
1	H	17	GLN
1	H	36	GLN
1	H	67	ASN
1	I	54	GLN
1	I	67	ASN
1	J	17	GLN
1	J	54	GLN
1	J	58	GLN
1	J	67	ASN
1	K	54	GLN
1	L	36	GLN
1	L	54	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 oligosaccharides 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 ⓘ

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	66/90 (73%)	0.53	5 (7%)	20 19	59, 87, 158, 200	0
1	B	66/90 (73%)	0.43	6 (9%)	15 16	52, 86, 158, 200	0
1	C	66/90 (73%)	0.61	7 (10%)	11 14	55, 90, 154, 200	0
1	D	66/90 (73%)	0.65	7 (10%)	11 14	55, 88, 138, 174	0
1	E	66/90 (73%)	0.43	3 (4%)	38 28	60, 86, 158, 190	0
1	F	66/90 (73%)	0.47	5 (7%)	20 19	56, 92, 155, 191	0
1	G	66/90 (73%)	0.65	9 (13%)	7 10	60, 91, 167, 200	0
1	H	66/90 (73%)	0.72	8 (12%)	8 12	58, 88, 142, 198	0
1	I	66/90 (73%)	0.40	5 (7%)	20 19	58, 89, 152, 200	0
1	J	66/90 (73%)	0.32	4 (6%)	27 23	60, 93, 156, 184	0
1	K	66/90 (73%)	0.61	5 (7%)	20 19	56, 95, 162, 200	0
1	L	66/90 (73%)	0.58	5 (7%)	20 19	63, 90, 169, 200	0
All	All	792/1080 (73%)	0.53	69 (8%)	16 17	52, 90, 166, 200	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	67	ASN	5.2
1	F	67	ASN	4.7
1	E	42	THR	4.5
1	H	2	SER	4.3
1	F	39	ILE	4.0
1	L	42	THR	4.0
1	A	39	ILE	4.0
1	L	66	ILE	4.0
1	J	42	THR	4.0
1	D	2	SER	3.7
1	A	67	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	67	ASN	3.5
1	C	67	ASN	3.4
1	G	64	ILE	3.3
1	B	42	THR	3.3
1	E	60	VAL	3.3
1	K	2	SER	3.3
1	L	19	SER	3.3
1	D	67	ASN	3.2
1	C	39	ILE	3.2
1	H	13	TYR	3.1
1	H	42	THR	3.1
1	D	66	ILE	3.0
1	I	67	ASN	2.9
1	G	36	GLN	2.9
1	G	39	ILE	2.9
1	K	39	ILE	2.9
1	H	66	ILE	2.9
1	D	57	LEU	2.9
1	F	55	LYS	2.9
1	H	67	ASN	2.8
1	G	62	ALA	2.8
1	H	39	ILE	2.8
1	K	55	LYS	2.8
1	I	39	ILE	2.7
1	L	2	SER	2.7
1	D	60	VAL	2.6
1	G	63	GLU	2.6
1	D	41	GLY	2.5
1	C	45	PRO	2.5
1	B	67	ASN	2.4
1	J	66	ILE	2.4
1	C	60	VAL	2.4
1	A	2	SER	2.4
1	A	32	SER	2.4
1	I	43	LEU	2.3
1	C	2	SER	2.3
1	B	2	SER	2.3
1	L	10	PHE	2.3
1	J	2	SER	2.3
1	G	60	VAL	2.3
1	B	66	ILE	2.2
1	F	63	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	10	PHE	2.1
1	J	60	VAL	2.1
1	F	42	THR	2.1
1	B	41	GLY	2.1
1	A	42	THR	2.1
1	I	55	LYS	2.1
1	C	33	HIS	2.0
1	G	45	PRO	2.0
1	C	66	ILE	2.0
1	G	55	LYS	2.0
1	E	67	ASN	2.0
1	K	45	PRO	2.0
1	H	52	ILE	2.0
1	I	2	SER	2.0
1	D	42	THR	2.0
1	B	60	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.