



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:57 AM UTC

PDB ID : 5M30 / pdb_00005m30
Title : Structure of TssK from T6SS EAEC in complex with nanobody nb18
Authors : Nguyen, V.S.; Cambillau, C.; Spinelli, C.; Desmyter, A.; Legrand, P.; Cascales, E.
Deposited on : 2016-10-13
Resolution : 2.60 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:

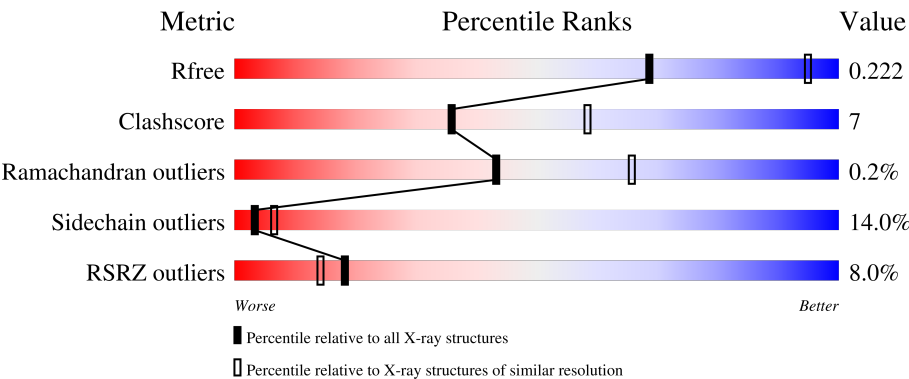
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	445	5% 46% 13% • • 36%
1	B	445	11% 66% 21% • • 9%
1	C	445	4% 47% 13% • • 37%
2	D	125	3% 82% 11% • 5%
2	E	125	6% 89% 10% •

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Mol	Chain	Length	Quality of chain
2	F	125	3% 82% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10331 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 Type VI secretion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	1	0
			2183	1389	391	395	8			
1	B	405	Total	C	N	O	S	0	0	0
			3096	1969	546	567	14			
1	C	282	Total	C	N	O	S	0	0	0
			2129	1357	371	392	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LEU	ALA	conflict	UNP A0A0P7QEP7
B	202	LEU	ALA	conflict	UNP A0A0P7QEP7
C	202	LEU	ALA	conflict	UNP A0A0P7QEP7

- Molecule 2 is a protein called Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	119	Total	C	N	O	S	0	0	0
			887	556	152	175	4			
2	E	123	Total	C	N	O	S	0	0	0
			912	571	158	179	4			
2	F	122	Total	C	N	O	S	0	0	0
			916	574	160	178	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	70	Total	O	0	0
			70	70		

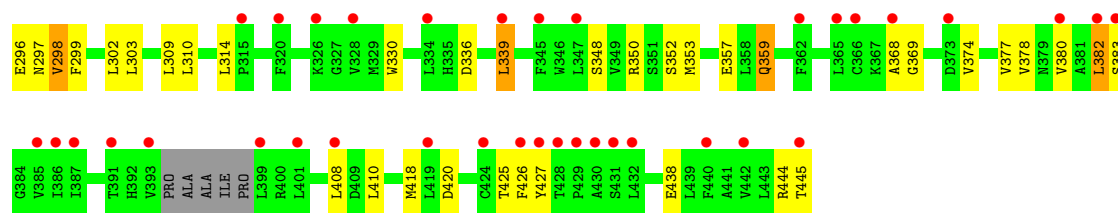
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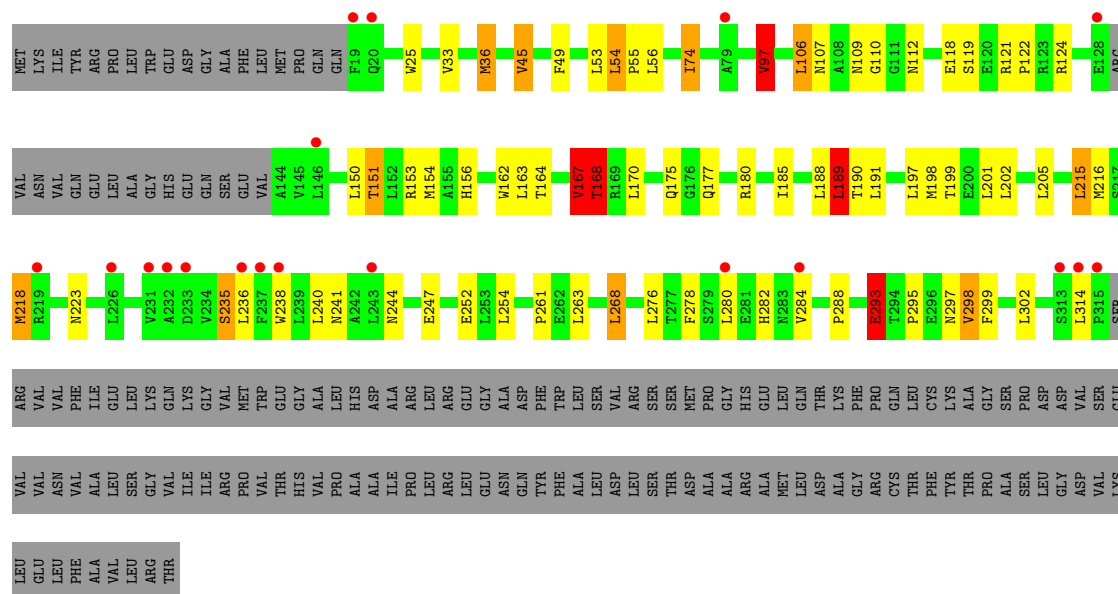
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	24	Total 24	O 24	0	0
3	E	18	Total 18	O 18	0	0
3	F	29	Total 29	O 29	0	0

- Molecule 1: Type VI secretion protein

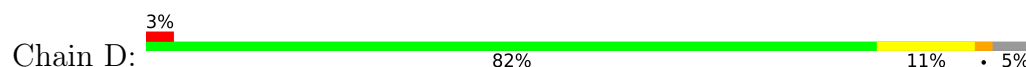




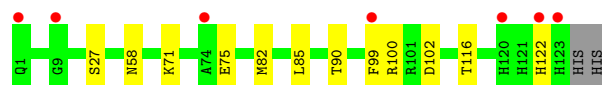
- Molecule 1: Type VI secretion protein



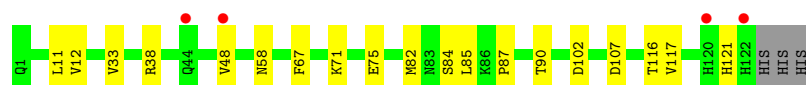
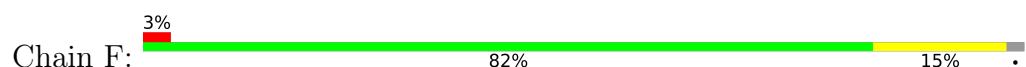
- Molecule 2: Anti-vesicular stomatitis virus N VHH



- Molecule 2: Anti-vesicular stomatitis virus N VHH



- Molecule 2: Anti-vesicular stomatitis virus N VHH



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.24Å 153.67Å 154.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.60 48.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.5 (48.92-2.60) 85.3 (48.92-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.207 , 0.226 (Not available) , 0.222	Depositor DCC
R_{free} test set	2978 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	88.2	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.86	1/2233 (0.0%)	1.39	15/3056 (0.5%)
1	B	0.87	1/3164 (0.0%)	1.35	17/4320 (0.4%)
1	C	0.88	3/2177 (0.1%)	1.42	15/2985 (0.5%)
2	D	0.77	0/903	1.10	0/1224
2	E	0.77	0/930	1.12	1/1261 (0.1%)
2	F	0.75	0/934	1.15	1/1265 (0.1%)
All	All	0.84	5/10341 (0.0%)	1.32	49/14111 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	185	ILE	CA-C	6.08	1.57	1.52
1	A	36	MET	SD-CE	-5.93	1.64	1.79
1	B	185	ILE	CG1-CD1	-5.23	1.31	1.51
1	C	36	MET	SD-CE	-5.19	1.66	1.79
1	C	167	VAL	CA-C	5.04	1.59	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	VAL	CB-CA-C	8.02	118.17	110.63
1	C	167	VAL	CB-CA-C	7.58	117.75	110.63
1	A	45	VAL	N-CA-C	-7.11	106.14	111.90
1	B	19	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	189	LEU	N-CA-C	-6.88	105.04	113.50
1	A	189	LEU	N-CA-C	-6.49	105.52	113.50
1	C	45	VAL	N-CA-C	-6.37	106.74	111.90
1	A	26	ASP	N-CA-C	-6.35	104.44	111.36
1	B	189	LEU	N-CA-C	-6.35	105.66	113.41
1	C	297	ASN	CA-CB-CG	6.13	118.73	112.60
1	C	235	SER	CA-C-N	6.13	128.41	120.44
1	C	235	SER	C-N-CA	6.13	128.41	120.44
1	A	163	LEU	N-CA-C	-5.98	99.91	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ASN	CA-CB-CG	5.78	118.38	112.60
2	E	99	PHE	CA-CB-CG	5.71	119.51	113.80
1	A	283	ASN	CA-CB-CG	5.64	118.24	112.60
1	C	163	LEU	N-CA-C	-5.60	100.11	109.24
1	A	26	ASP	CA-C-N	5.59	128.12	120.46
1	A	26	ASP	C-N-CA	5.59	128.12	120.46
1	A	185	ILE	CB-CA-C	5.56	115.78	110.16
1	B	45	VAL	N-CA-C	-5.56	107.39	111.90
1	B	163	LEU	N-CA-C	-5.47	100.38	109.46
1	B	352	SER	CA-C-N	5.47	128.00	120.67
1	B	352	SER	C-N-CA	5.47	128.00	120.67
1	B	173	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	97	VAL	CB-CA-C	5.46	117.55	110.12
1	C	110	GLY	CA-C-N	5.39	127.08	122.29
1	C	110	GLY	C-N-CA	5.39	127.08	122.29
1	B	420	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	168	THR	N-CA-CB	5.31	120.49	111.57
1	C	293	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	285	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	444	ARG	CA-C-N	5.23	131.12	121.70
1	B	444	ARG	C-N-CA	5.23	131.12	121.70
1	C	168	THR	N-CA-CB	5.20	120.30	111.57
1	C	97	VAL	CB-CA-C	5.18	117.17	110.12
1	C	110	GLY	N-CA-C	5.18	119.67	112.57
1	B	110	GLY	N-CA-C	5.15	119.62	112.57
1	A	167	VAL	CA-C-N	5.12	131.61	122.09
1	A	167	VAL	C-N-CA	5.12	131.61	122.09
1	A	292	HIS	N-CA-C	5.11	116.53	111.07
1	C	167	VAL	CA-C-N	5.09	131.56	122.09
1	C	167	VAL	C-N-CA	5.09	131.56	122.09
1	B	292	HIS	CA-C-N	5.07	128.01	120.31
1	B	292	HIS	C-N-CA	5.07	128.01	120.31
1	A	114	ASP	CA-CB-CG	5.06	117.66	112.60
2	F	67	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	168	THR	N-CA-CB	5.05	120.06	111.57
1	A	97	VAL	CB-CA-C	5.04	116.97	110.12

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	2183	0	2129	37	0
1	B	3096	0	3030	65	0
1	C	2129	0	2067	41	0
2	D	887	0	849	6	0
2	E	912	0	857	2	0
2	F	916	0	876	5	0
3	A	35	0	0	0	0
3	B	70	0	0	0	0
3	C	32	0	0	0	0
3	D	24	0	0	0	0
3	E	18	0	0	0	0
3	F	29	0	0	0	0
All	All	10331	0	9808	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (145) 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:C:49:PHE:HZ	1:C:167:VAL:HG13	1.36	0.90
1:B:49:PHE:HZ	1:B:167:VAL:HG13	1.39	0.88
1:B:238:TRP:HB2	1:B:278:PHE:HZ	1.40	0.87
1:B:154:MET:H	1:B:157:GLN:HE21	1.24	0.85
1:A:185:ILE:HG12	1:A:296:GLU:HG3	1.59	0.81
1:B:107:ASN:H	1:B:112:ASN:HD21	1.29	0.79
1:A:154:MET:H	1:A:157:GLN:HE21	1.31	0.78
1:A:22:GLN:O	1:A:26:ASP:HB2	1.83	0.77
1:B:368:ALA:HB3	1:B:382:LEU:HD21	1.69	0.75
1:B:185:ILE:HG23	1:B:296:GLU:HG3	1.70	0.74
1:C:107:ASN:H	1:C:112:ASN:HD21	1.37	0.72
1:C:168:THR:HG21	1:C:180:ARG:HD2	1.71	0.72
1:B:238:TRP:HB2	1:B:278:PHE:CZ	2.24	0.72
1:B:49:PHE:CZ	1:B:167:VAL:HG13	2.25	0.71
1:B:26:ASP:HB2	1:C:25:TRP:HH2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:THR:HG21	1:B:180:ARG:HD2	1.73	0.70
1:B:26:ASP:HB2	1:C:25:TRP:CH2	2.27	0.70
1:B:185:ILE:HD11	1:B:188:LEU:HD11	1.73	0.69
1:B:163:LEU:HD21	2:D:103:TYR:HB3	1.76	0.68
1:A:295:PRO:HA	1:A:298:VAL:HG13	1.76	0.68
1:A:61:ALA:O	1:A:82:LEU:HD23	1.94	0.67
1:B:336:ASP:HB3	1:B:339:LEU:HD23	1.76	0.66
1:B:238:TRP:CB	1:B:278:PHE:HZ	2.09	0.65
1:A:168:THR:HG21	1:A:180:ARG:HD2	1.78	0.65
1:A:277:THR:HG21	1:C:241:ASN:HA	1.80	0.64
1:A:259:ARG:HB2	1:A:259:ARG:HH11	1.62	0.63
1:C:55:PRO:HG3	1:C:177:GLN:HE22	1.64	0.63
1:A:201:LEU:HD11	1:A:264:LEU:HD21	1.82	0.62
1:B:107:ASN:H	1:B:112:ASN:ND2	1.98	0.61
1:B:198:MET:HA	1:B:198:MET:HE2	1.82	0.61
1:B:126:LYS:HB2	1:B:149:ASN:HD21	1.66	0.60
1:C:74:ILE:HG12	1:C:150:LEU:HD21	1.82	0.59
1:C:33:VAL:HA	1:C:36:MET:HE3	1.84	0.59
1:C:49:PHE:CZ	1:C:167:VAL:HG13	2.29	0.58
1:A:154:MET:N	1:A:157:GLN:HE21	2.01	0.58
1:A:201:LEU:HD22	1:A:254:LEU:HD11	1.85	0.58
1:A:33:VAL:HA	1:A:36:MET:HE3	1.86	0.57
1:A:107:ASN:H	1:A:112:ASN:HD21	1.51	0.57
1:C:199:THR:HA	1:C:202:LEU:HD12	1.86	0.57
1:B:33:VAL:HA	1:B:36:MET:HE3	1.87	0.57
1:B:235:SER:O	1:B:239:LEU:HB2	2.04	0.56
1:C:151:THR:HG22	1:C:153:ARG:HG3	1.87	0.55
1:B:49:PHE:HZ	1:B:167:VAL:CG1	2.16	0.55
1:B:191:LEU:HD22	1:B:198:MET:HE3	1.88	0.55
1:B:295:PRO:HA	1:B:298:VAL:HG13	1.88	0.55
2:D:82:MET:HE2	2:D:85:LEU:HD21	1.90	0.54
2:F:82:MET:HE2	2:F:85:LEU:HD21	1.90	0.54
1:B:154:MET:N	1:B:157:GLN:HE21	2.01	0.54
1:A:191:LEU:HD22	1:A:198:MET:HE3	1.90	0.54
1:A:122:PRO:HG3	1:A:162:TRP:CE2	2.42	0.54
1:A:45:VAL:HA	1:A:190:THR:HG22	1.90	0.53
1:B:197:LEU:HD11	1:B:299:PHE:HB3	1.90	0.53
1:B:122:PRO:HG3	1:B:162:TRP:CE2	2.43	0.53
1:B:154:MET:H	1:B:157:GLN:NE2	2.01	0.53
1:B:382:LEU:HD22	1:B:382:LEU:H	1.71	0.53
1:C:122:PRO:HG3	1:C:162:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ILE:HG13	1:B:295:PRO:HG2	1.91	0.53
1:A:185:ILE:HG13	1:A:295:PRO:HG2	1.90	0.53
1:C:218:MET:HB3	1:C:236:LEU:HD11	1.90	0.52
1:B:188:LEU:HB2	1:B:261:PRO:HG2	1.90	0.52
2:E:82:MET:HE2	2:E:85:LEU:HD21	1.90	0.52
1:A:276:LEU:HD11	1:A:284:VAL:HA	1.91	0.52
1:B:45:VAL:HG22	1:B:65:ILE:HB	1.92	0.52
1:C:55:PRO:HG3	1:C:177:GLN:NE2	2.25	0.52
1:B:97:VAL:HG12	1:B:170:LEU:HB2	1.92	0.52
1:A:205:LEU:HD21	1:A:251:LYS:HG3	1.92	0.51
1:C:107:ASN:H	1:C:112:ASN:ND2	2.05	0.51
1:C:97:VAL:HG12	1:C:170:LEU:HB2	1.93	0.51
1:C:106:LEU:HG	1:C:124:ARG:HD2	1.93	0.50
1:C:154:MET:HB3	1:C:156:HIS:HD2	1.77	0.50
1:C:240:LEU:HG	1:C:244:ASN:ND2	2.26	0.50
1:C:109:ASN:HD22	2:F:107:ASP:H	1.60	0.50
1:C:54:LEU:N	1:C:55:PRO:CD	2.75	0.50
1:B:330:TRP:HB2	1:B:426:PHE:HB2	1.93	0.50
1:A:97:VAL:HG12	1:A:170:LEU:HB2	1.94	0.50
1:A:216:MET:O	1:A:219:ARG:HG3	2.12	0.49
1:B:126:LYS:HB2	1:B:149:ASN:ND2	2.26	0.49
1:B:268:LEU:HB3	1:B:302:LEU:HD21	1.95	0.49
1:C:122:PRO:HG3	1:C:162:TRP:CZ2	2.47	0.49
1:C:293:GLU:H	1:C:293:GLU:CD	2.22	0.48
1:A:188:LEU:HB2	1:A:261:PRO:HG3	1.95	0.48
1:B:122:PRO:HG3	1:B:162:TRP:CZ2	2.49	0.48
1:B:212:ARG:CZ	1:C:284:VAL:HG11	2.43	0.48
1:B:377:VAL:HG23	1:B:427:TYR:CZ	2.49	0.48
1:C:288:PRO:HD2	1:C:302:LEU:HD13	1.95	0.48
1:B:190:THR:OG1	1:B:258:TYR:HA	2.14	0.48
1:B:378:VAL:HG12	1:B:427:TYR:HB3	1.95	0.47
1:B:30:ALA:HB1	1:C:33:VAL:HG21	1.97	0.47
1:B:173:ASP:HB2	1:B:177:GLN:H	1.79	0.47
1:B:185:ILE:HD11	1:B:188:LEU:CD1	2.44	0.47
1:A:274:SER:O	1:A:277:THR:HG23	2.15	0.47
1:C:107:ASN:N	1:C:112:ASN:HD21	2.10	0.47
1:A:59:LEU:HB3	1:A:86:CYS:HB3	1.96	0.47
1:C:295:PRO:HA	1:C:298:VAL:HG13	1.96	0.47
1:B:211:ARG:HD2	1:B:310:LEU:O	2.15	0.47
1:B:237:PHE:CZ	1:C:238:TRP:HB3	2.50	0.47
2:F:38:ARG:HG2	2:F:48:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:90:THR:HG23	2:E:116:THR:HA	1.96	0.46
2:D:90:THR:HG23	2:D:116:THR:HA	1.96	0.46
1:B:276:LEU:HD13	1:B:284:VAL:HA	1.97	0.46
1:A:49:PHE:HZ	1:A:167:VAL:HG13	1.81	0.46
1:B:368:ALA:HB3	1:B:382:LEU:CD2	2.40	0.46
1:B:369:GLY:C	1:B:382:LEU:HD11	2.41	0.45
1:C:215:LEU:HD12	1:C:240:LEU:HB2	1.96	0.45
2:D:102:ASP:HA	2:D:103:TYR:HA	1.70	0.45
1:A:154:MET:H	1:A:157:GLN:NE2	2.07	0.45
1:B:410:LEU:HD22	1:B:418:MET:HE1	1.98	0.45
1:B:38:LEU:HD11	1:C:36:MET:HB3	1.98	0.45
2:F:87:PRO:HA	2:F:117:VAL:HB	1.98	0.45
1:A:293:GLU:H	1:A:293:GLU:HG2	1.51	0.45
1:B:96:LEU:HD11	1:B:169:ARG:HD3	1.98	0.45
1:A:107:ASN:H	1:A:112:ASN:ND2	2.14	0.44
1:C:45:VAL:HA	1:C:190:THR:HG22	1.98	0.44
1:A:268:LEU:HB3	1:A:302:LEU:HD21	1.98	0.44
1:A:122:PRO:HG3	1:A:162:TRP:CZ2	2.52	0.44
1:B:191:LEU:HD13	1:B:198:MET:HE3	2.00	0.44
2:D:27:SER:O	2:D:99:PHE:HE1	2.00	0.44
1:B:198:MET:HA	1:B:198:MET:CE	2.48	0.43
1:C:188:LEU:HB2	1:C:261:PRO:HG3	1.99	0.43
1:B:185:ILE:HD12	1:B:186:PRO:HD2	2.00	0.43
1:B:59:LEU:HB3	1:B:86:CYS:HB3	2.00	0.43
1:B:359:GLN:H	1:B:359:GLN:HG2	1.52	0.43
1:B:212:ARG:NE	1:C:284:VAL:HG21	2.34	0.42
2:F:90:THR:HG23	2:F:116:THR:HA	2.00	0.42
1:B:169:ARG:HH22	1:B:296:GLU:CD	2.27	0.42
1:C:276:LEU:HD13	1:C:284:VAL:HA	2.00	0.42
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.93	0.42
1:B:201:LEU:HD22	1:B:303:LEU:HD11	2.01	0.41
1:B:369:GLY:HA2	1:B:378:VAL:HG21	2.02	0.41
1:B:201:LEU:HB3	1:B:254:LEU:HD21	2.03	0.41
1:B:208:LEU:HG	1:B:243:LEU:HD22	2.02	0.41
1:A:277:THR:HG22	1:C:244:ASN:HD22	1.86	0.41
1:B:67:ARG:HD3	1:B:189:LEU:HD11	2.02	0.41
1:A:201:LEU:HB3	1:A:254:LEU:HD11	2.02	0.41
1:C:197:LEU:HD11	1:C:299:PHE:HB3	2.03	0.41
1:C:268:LEU:HB3	1:C:302:LEU:HD21	2.03	0.41
1:A:45:VAL:HA	1:A:190:THR:CG2	2.51	0.41
1:B:368:ALA:CB	1:B:382:LEU:HD21	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:HE3	2:D:97:ALA:HB2	2.02	0.41
1:B:348:SER:HB3	1:B:438:GLU:HB2	2.02	0.41
1:C:215:LEU:HD12	1:C:240:LEU:HD13	2.02	0.41
1:A:211:ARG:O	1:A:215:LEU:HD23	2.21	0.40
1:A:102:ALA:HB1	1:A:162:TRP:CD1	2.56	0.40
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.89	0.40
1:A:264:LEU:O	1:A:268:LEU:HB2	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	245/445 (55%)	233 (95%)	11 (4%)	1 (0%)	30	51
1	B	350/445 (79%)	335 (96%)	15 (4%)	0	100	100
1	C	270/445 (61%)	262 (97%)	8 (3%)	0	100	100
2	D	117/125 (94%)	113 (97%)	3 (3%)	1 (1%)	14	30
2	E	121/125 (97%)	118 (98%)	3 (2%)	0	100	100
2	F	120/125 (96%)	119 (99%)	1 (1%)	0	100	100
All	All	1223/1710 (72%)	1180 (96%)	41 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	41	PRO
1	A	312	ALA

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	227/382 (59%)	184 (81%)	43 (19%)	1	2
1	B	325/382 (85%)	280 (86%)	45 (14%)	3	7
1	C	220/382 (58%)	185 (84%)	35 (16%)	2	4
2	D	90/101 (89%)	83 (92%)	7 (8%)	11	26
2	E	91/101 (90%)	84 (92%)	7 (8%)	12	27
2	F	93/101 (92%)	84 (90%)	9 (10%)	8	17
All	All	1046/1449 (72%)	900 (86%)	146 (14%)	3	6

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	TRP
1	A	27	VAL
1	A	54	LEU
1	A	56	LEU
1	A	74	ILE
1	A	90	THR
1	A	95	SER
1	A	97	VAL
1	A	106	LEU
1	A	107	ASN
1	A	118	GLU
1	A	123	ARG
1	A	124	ARG
1	A	164	THR
1	A	167	VAL
1	A	168	THR
1	A	173	ASP
1	A	175	GLN
1	A	177	GLN
1	A	185	ILE
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	191	LEU
1	A	198	MET
1	A	205	LEU
1	A	219	ARG
1	A	220	ARG
1	A	240	LEU
1	A	252	GLU
1	A	254	LEU
1	A	263	LEU
1	A	268	LEU
1	A	277	THR
1	A	279	SER
1	A	280	LEU
1	A	281	GLU
1	A	282	HIS
1	A	283	ASN
1	A	285	ASP
1	A	293	GLU
1	A	298	VAL
1	A	309	LEU
1	A	317	ARG
1	B	29	LEU
1	B	45	VAL
1	B	53	LEU
1	B	74	ILE
1	B	76	THR
1	B	90	THR
1	B	97	VAL
1	B	106	LEU
1	B	123	ARG
1	B	127	SER
1	B	147	ARG
1	B	152	LEU
1	B	167	VAL
1	B	168	THR
1	B	175	GLN
1	B	185	ILE
1	B	189	LEU
1	B	191	LEU
1	B	198	MET
1	B	201	LEU
1	B	205	LEU

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Mol	Chain	Res	Type
1	B	213	GLN
1	B	236	LEU
1	B	239	LEU
1	B	252	GLU
1	B	254	LEU
1	B	263	LEU
1	B	268	LEU
1	B	275	LEU
1	B	293	GLU
1	B	298	VAL
1	B	309	LEU
1	B	314	LEU
1	B	339	LEU
1	B	350	ARG
1	B	353	MET
1	B	357	GLU
1	B	359	GLN
1	B	374	VAL
1	B	380	VAL
1	B	382	LEU
1	B	383	SER
1	B	408	LEU
1	B	425	THR
1	B	445	THR
1	C	53	LEU
1	C	54	LEU
1	C	56	LEU
1	C	74	ILE
1	C	97	VAL
1	C	106	LEU
1	C	118	GLU
1	C	119	SER
1	C	121	ARG
1	C	151	THR
1	C	164	THR
1	C	167	VAL
1	C	168	THR
1	C	175	GLN
1	C	189	LEU
1	C	191	LEU
1	C	198	MET
1	C	201	LEU

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Mol	Chain	Res	Type
1	C	205	LEU
1	C	215	LEU
1	C	216	MET
1	C	218	MET
1	C	223	ASN
1	C	235	SER
1	C	247	GLU
1	C	252	GLU
1	C	254	LEU
1	C	263	LEU
1	C	268	LEU
1	C	278	PHE
1	C	280	LEU
1	C	282	HIS
1	C	293	GLU
1	C	298	VAL
1	C	314	LEU
2	D	12	VAL
2	D	27	SER
2	D	58	ASN
2	D	71	LYS
2	D	75	GLU
2	D	116	THR
2	D	119	SER
2	E	27	SER
2	E	58	ASN
2	E	71	LYS
2	E	75	GLU
2	E	100	ARG
2	E	102	ASP
2	E	122	HIS
2	F	11	LEU
2	F	12	VAL
2	F	33	VAL
2	F	58	ASN
2	F	71	LYS
2	F	75	GLU
2	F	84	SER
2	F	102	ASP
2	F	121	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	109	ASN
1	A	112	ASN
1	A	157	GLN
1	A	175	GLN
1	A	177	GLN
1	B	28	HIS
1	B	109	ASN
1	B	112	ASN
1	B	149	ASN
1	B	157	GLN
1	B	291	HIS
1	B	356	HIS
1	B	359	GLN
1	B	403	ASN
1	C	28	HIS
1	C	60	ASN
1	C	107	ASN
1	C	109	ASN
1	C	112	ASN
1	C	148	HIS
1	C	156	HIS
1	C	177	GLN
1	C	244	ASN
2	D	76	ASN
2	D	83	ASN
2	E	3	GLN
2	E	76	ASN
2	F	76	ASN
2	F	83	ASN

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	284/445 (63%)	0.67	24 (8%) 16 13	38, 100, 172, 282	1 (0%)
1	B	405/445 (91%)	0.73	49 (12%) 8 6	57, 102, 224, 278	1 (0%)
1	C	282/445 (63%)	0.53	19 (6%) 24 19	63, 96, 198, 234	0
2	D	119/125 (95%)	0.25	4 (3%) 48 42	65, 85, 117, 128	0
2	E	123/125 (98%)	0.45	7 (5%) 29 24	65, 98, 134, 191	0
2	F	122/125 (97%)	0.16	4 (3%) 49 43	70, 87, 116, 216	0
All	All	1335/1710 (78%)	0.55	107 (8%) 18 14	38, 94, 199, 282	2 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	430	ALA	5.3
1	B	227	ALA	5.1
1	C	219	ARG	4.6
2	D	119	SER	4.6
1	B	228	ASP	4.3
1	C	284	VAL	4.2
1	A	19	PHE	4.2
1	A	315	PRO	4.1
1	B	368	ALA	4.0
2	E	123	HIS	3.9
1	B	145	VAL	3.9
1	B	393	VAL	3.8
2	D	102	ASP	3.7
1	A	314	LEU	3.7
1	C	237	PHE	3.7
1	B	362	PHE	3.6
1	B	347	LEU	3.6
1	B	431	SER	3.6
1	A	86	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	220	ARG	3.6
1	B	230	ALA	3.5
1	B	440	PHE	3.4
2	F	122	HIS	3.4
1	A	320	PHE	3.4
1	C	280	LEU	3.4
1	C	313	SER	3.3
1	B	231	VAL	3.3
1	A	129	ARG	3.3
1	C	20	GLN	3.3
1	B	408	LEU	3.2
2	E	120	HIS	3.2
1	A	313	SER	3.2
1	C	315	PRO	3.1
1	B	19	PHE	3.0
1	C	19	PHE	3.0
1	C	146	LEU	3.0
1	B	426	PHE	3.0
1	C	226	LEU	3.0
1	B	386	ILE	3.0
1	A	25	TRP	2.9
1	A	282	HIS	2.9
1	B	387	ILE	2.9
1	B	419	LEU	2.9
1	A	236	LEU	2.9
1	B	25	TRP	2.8
1	B	391	THR	2.8
1	B	399	LEU	2.8
1	C	236	LEU	2.8
1	A	87	ASP	2.8
1	A	280	LEU	2.8
1	A	239	LEU	2.8
1	B	429	PRO	2.7
2	E	122	HIS	2.7
1	A	237	PHE	2.7
1	C	238	TRP	2.7
2	F	44	GLN	2.7
1	B	232	ALA	2.7
1	B	428	THR	2.7
1	A	283	ASN	2.7
1	C	128	GLU	2.6
1	B	401	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	224	ALA	2.6
1	B	345	PHE	2.6
1	B	20	GLN	2.6
2	D	44	GLN	2.6
1	B	339	LEU	2.6
1	A	238	TRP	2.6
1	A	58	ARG	2.6
1	A	145	VAL	2.6
2	E	99	PHE	2.6
1	B	442	VAL	2.5
1	B	373	ASP	2.5
1	B	365	LEU	2.5
1	B	382	LEU	2.5
1	B	326	LYS	2.5
2	F	120	HIS	2.5
1	B	380	VAL	2.5
1	B	385	VAL	2.5
1	B	219	ARG	2.4
1	B	334	LEU	2.4
1	B	424	CYS	2.4
1	B	383	SER	2.4
1	B	366	CYS	2.4
1	A	311	GLU	2.4
1	B	315	PRO	2.4
1	B	427	TYR	2.4
1	B	320	PHE	2.4
1	C	314	LEU	2.3
1	A	23	ALA	2.3
1	C	233	ASP	2.2
2	E	1	GLN	2.2
1	B	328	VAL	2.2
1	B	445	THR	2.2
1	A	89	SER	2.2
1	B	202	LEU	2.2
1	B	278	PHE	2.2
1	C	232	ALA	2.1
2	E	9	GLY	2.1
1	A	56	LEU	2.1
1	B	432	LEU	2.1
1	C	243	LEU	2.1
1	C	231	VAL	2.1
2	E	74	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	1	GLN	2.1
1	C	79	ALA	2.0
1	A	318	VAL	2.0
2	F	48	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.