Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:28 pm BST

PDB ID	:	5M30
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 following versions of software and data (see references ⓘ) were used in the production of this report:

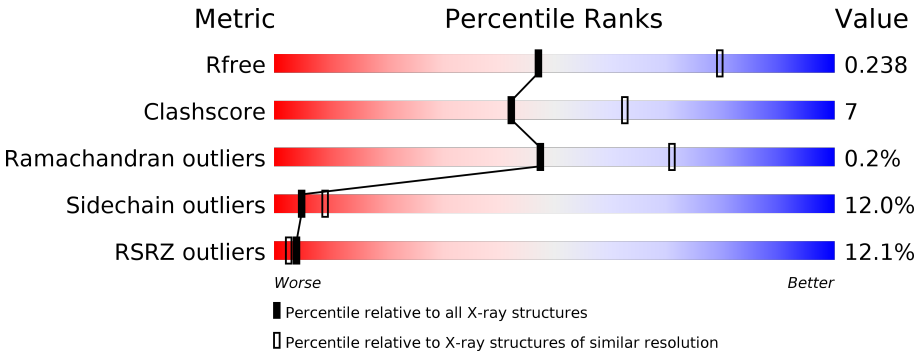
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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 <=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	3% 48% 13% • 36%
1	B	445	28% 70% 18% • 9%
1	C	445	4% 48% 13% • 37%
2	D	125	% 85% 9% • 5%
2	E	125	2% 90% 8% •
2	F	125	2% 85% 13% •

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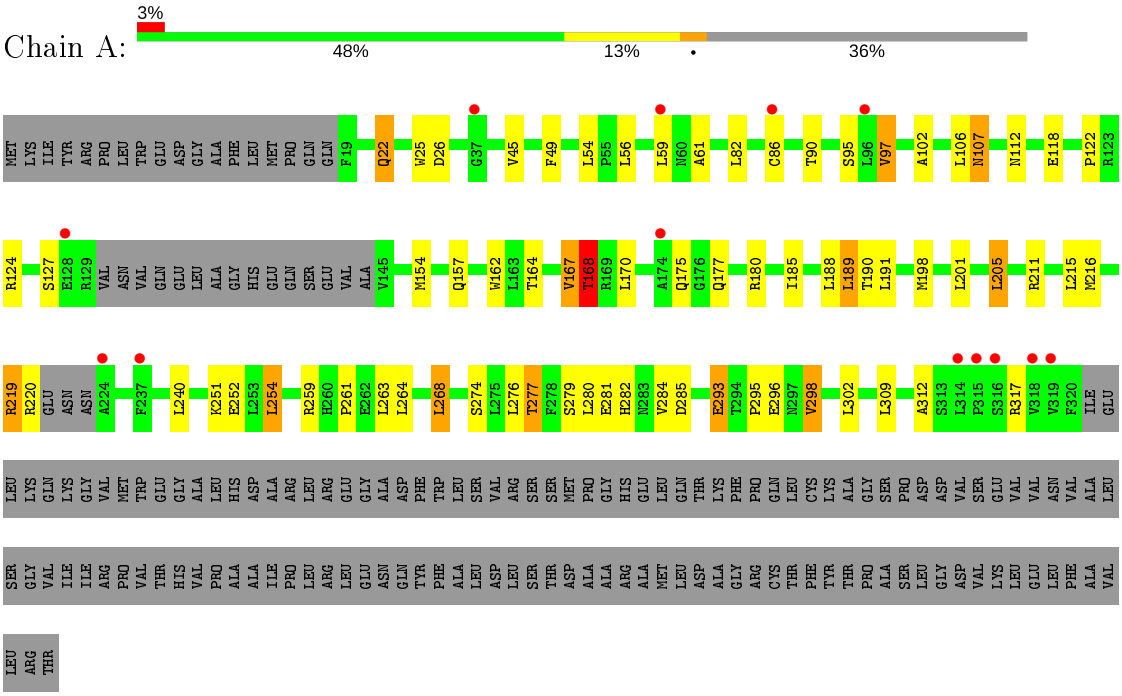
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	32	Total O 32 32	0	0
3	D	24	Total O 24 24	0	0
3	E	18	Total O 18 18	0	0
3	F	29	Total O 29 29	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

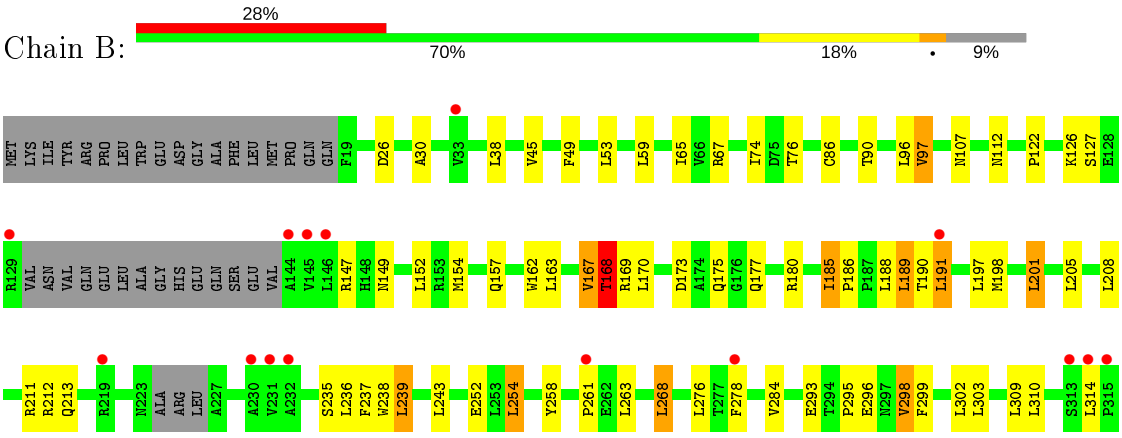
- Molecule 1: Type VI secretion protein

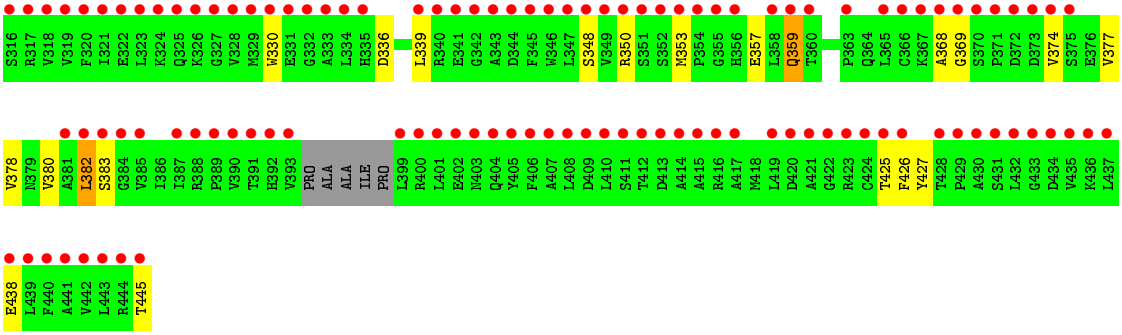
Chain A:



- Molecule 1: Type VI secretion protein

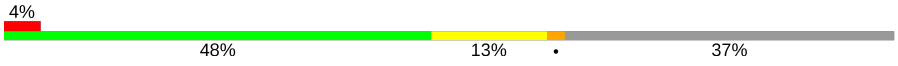
Chain B:

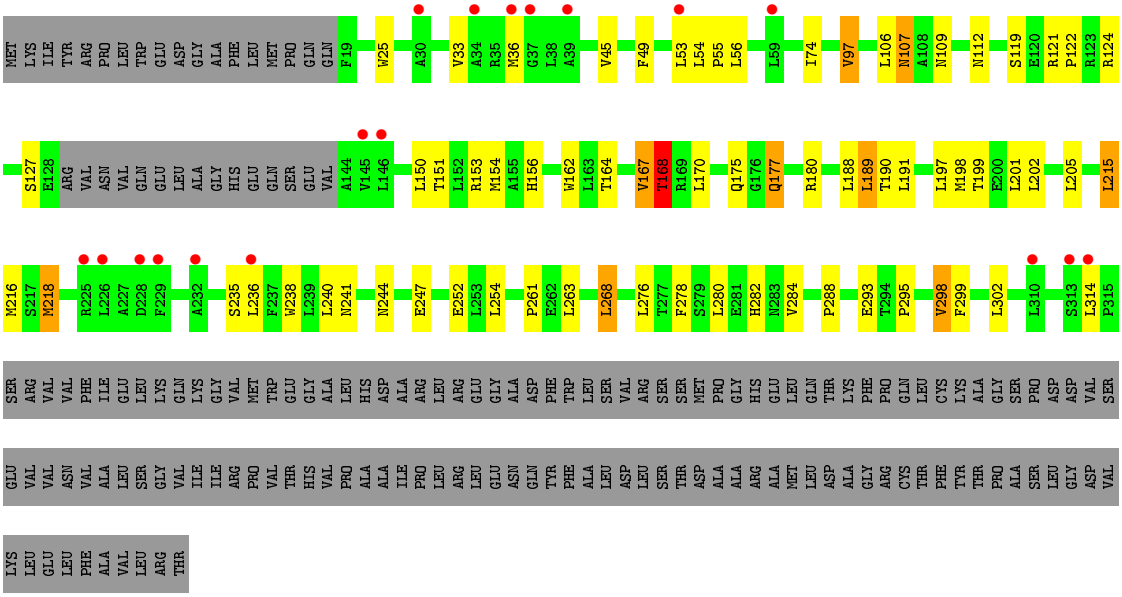




- Molecule 1: Type VI secretion protein

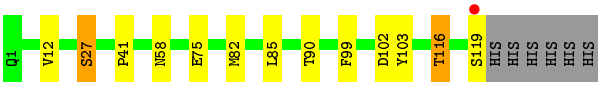
Chain C:





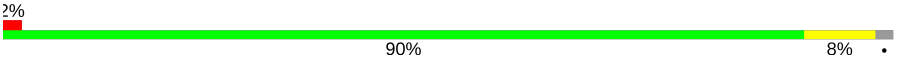
- Molecule 2: Anti-vesicular stomatitis virus N VHH

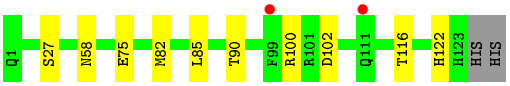
Chain D:



- Molecule 2: Anti-vesicular stomatitis virus N VHH

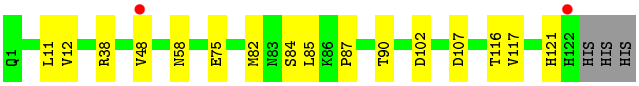
Chain E:





- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain F:


Q1
L11
V12
R38
V48
N58
E75
M82
N83
S84
L85
K86
P87
T90
D102
D107
T116
V117
H121
H122
HIS
HIS
HIS

4 Data and refinement statistics (i)

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) 86.2 (48.92-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.207 , 0.226 0.218 , 0.238	Depositor DCC
R_{free} test set	2978 reflections (4.99%)	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)	0.30 , 78.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/2233	0.74	1/3056 (0.0%)
1	B	0.50	0/3164	0.73	1/4320 (0.0%)
1	C	0.51	0/2177	0.76	1/2985 (0.0%)
2	D	0.47	0/903	0.73	0/1224
2	E	0.45	0/930	0.68	0/1261
2	F	0.45	0/934	0.73	0/1265
All	All	0.49	0/10341	0.73	3/14111 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	THR	N-CA-CB	5.36	120.49	110.30
1	C	168	THR	N-CA-CB	5.26	120.30	110.30
1	A	168	THR	N-CA-CB	5.14	120.06	110.30

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	35	0
1	B	3096	0	3030	61	0
1	C	2129	0	2067	40	0
2	D	887	0	849	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	137	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 (137) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:295:PRO:HA	1:B:298:VAL:HG13	1.88	0.55
1:B:191:LEU:HD22	1:B:198:MET:HE3	1.89	0.54
1:B:154:MET:N	1:B:157:GLN:HE21	2.01	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
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
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
2:F:82:MET:HE2	2:F:85:LEU:HD21	1.93	0.50
1:C:54:LEU:N	1:C:55:PRO:CD	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:82:MET:HE2	2:D:85:LEU:HD21	1.94	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
2:E:82:MET:HE2	2:E:85:LEU:HD21	1.95	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: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:B:30:ALA:HB1	1:C:33:VAL:HG21	1.97	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
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: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: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:B:191:LEU:HD13	1:B:198:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:HG3	1:A:162:TRP:CZ2	2.52	0.44
2:D:27:SER:O	2:D:99:PHE:HE1	2.00	0.44
1:B:198:MET:CE	1:B:198:MET:HA	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:359:GLN:H	1:B:359:GLN:HG2	1.52	0.43
1:B:59:LEU:HB3	1:B:86:CYS:HB3	2.00	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:C:293:GLU:CD	1:C:293:GLU:H	2.22	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:B:67:ARG:HD3	1:B:189:LEU:HD11	2.02	0.41
1:A:277:THR:HG22	1:C:244:ASN:HD22	1.86	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
1:B:369:GLY:C	1:B:382:LEU:HD11	2.41	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:HA	1:A:189:LEU:HD23	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	279/445 (63%)	266 (95%)	12 (4%)	1 (0%)	34 57
1	B	397/445 (89%)	381 (96%)	16 (4%)	0	100 100
1	C	278/445 (62%)	270 (97%)	8 (3%)	0	100 100
2	D	117/125 (94%)	113 (97%)	3 (3%)	1 (1%)	17 35
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	1312/1710 (77%)	1267 (97%)	43 (3%)	2 (0%)	47 71

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	189 (83%)	38 (17%)	2 3
1	B	325/382 (85%)	288 (89%)	37 (11%)	5 10
1	C	220/382 (58%)	189 (86%)	31 (14%)	3 6
2	D	90/101 (89%)	84 (93%)	6 (7%)	16 33
2	E	91/101 (90%)	85 (93%)	6 (7%)	16 33
2	F	93/101 (92%)	86 (92%)	7 (8%)	13 27
All	All	1046/1449 (72%)	921 (88%)	125 (12%)	5 9

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	25	TRP
1	A	54	LEU
1	A	56	LEU
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	124	ARG
1	A	127	SER
1	A	164	THR
1	A	167	VAL
1	A	168	THR
1	A	175	GLN
1	A	177	GLN
1	A	189	LEU
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	285	ASP
1	A	293	GLU
1	A	298	VAL
1	A	309	LEU
1	A	317	ARG
1	B	53	LEU
1	B	74	ILE
1	B	76	THR
1	B	90	THR
1	B	97	VAL

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Mol	Chain	Res	Type
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	201	LEU
1	B	205	LEU
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	293	GLU
1	B	298	VAL
1	B	309	LEU
1	B	314	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	425	THR
1	B	445	THR
1	C	53	LEU
1	C	56	LEU
1	C	97	VAL
1	C	107	ASN
1	C	119	SER
1	C	121	ARG
1	C	127	SER
1	C	164	THR
1	C	167	VAL
1	C	168	THR

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Mol	Chain	Res	Type
1	C	175	GLN
1	C	177	GLN
1	C	189	LEU
1	C	191	LEU
1	C	198	MET
1	C	201	LEU
1	C	205	LEU
1	C	215	LEU
1	C	216	MET
1	C	218	MET
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	298	VAL
1	C	314	LEU
2	D	12	VAL
2	D	27	SER
2	D	58	ASN
2	D	75	GLU
2	D	116	THR
2	D	119	SER
2	E	27	SER
2	E	58	ASN
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	58	ASN
2	F	75	GLU
2	F	84	SER
2	F	102	ASP
2	F	121	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	112	ASN
1	A	157	GLN
1	A	175	GLN
1	A	177	GLN
1	A	307	ASN
1	B	109	ASN
1	B	112	ASN
1	B	149	ASN
1	B	157	GLN
1	C	107	ASN
1	C	109	ASN
1	C	112	ASN
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	E	83	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 carbohydrates 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, 95^{th} 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%)	0.36	13 (4%) 32 26	64, 100, 172, 282	0
1	B	405/445 (91%)	1.47	125 (30%) 0 0	57, 102, 224, 278	1 (0%)
1	C	282/445 (63%)	0.40	18 (6%) 19 14	63, 96, 198, 234	0
2	D	119/125 (95%)	-0.10	1 (0%) 86 84	65, 85, 117, 128	0
2	E	123/125 (98%)	0.04	2 (1%) 72 68	65, 98, 135, 191	0
2	F	122/125 (97%)	0.09	2 (1%) 72 68	70, 87, 116, 216	0
All	All	1335/1710 (78%)	0.61	161 (12%) 4 2	57, 94, 199, 282	1 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	445	THR	9.6
1	B	399	LEU	9.2
1	B	383	SER	9.2
1	B	408	LEU	8.9
1	B	389	PRO	7.6
1	B	416	ARG	7.0
1	B	426	PHE	6.8
1	B	432	LEU	6.7
1	B	382	LEU	6.7
1	B	441	ALA	6.7
1	B	443	LEU	6.6
1	B	393	VAL	6.3
1	B	374	VAL	6.1
1	B	390	VAL	6.1
1	B	434	ASP	5.9
1	B	371	PRO	5.8
1	B	369	GLY	5.8
1	B	442	VAL	5.8
1	B	334	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	335	HIS	5.7
1	B	437	LEU	5.7
1	B	232	ALA	5.7
1	B	412	THR	5.7
1	B	350	ARG	5.5
1	B	423	ARG	5.4
1	B	429	PRO	5.4
1	B	145	VAL	5.1
1	B	424	CYS	5.1
1	C	314	LEU	5.1
1	B	354	PRO	5.1
1	B	318	VAL	5.1
1	B	315	PRO	5.0
1	B	363	PRO	5.0
1	B	370	SER	4.9
1	B	144	ALA	4.9
1	B	406	PHE	4.9
1	B	439	LEU	4.9
1	B	421	ALA	4.9
1	B	425	THR	4.9
1	B	417	ALA	4.8
1	B	409	ASP	4.8
1	B	324	LYS	4.8
1	C	313	SER	4.8
1	B	381	ALA	4.7
1	B	430	ALA	4.6
1	B	420	ASP	4.5
1	B	440	PHE	4.4
1	B	346	TRP	4.3
1	B	402	GLU	4.2
1	B	431	SER	4.1
1	B	339	LEU	4.1
1	B	319	VAL	4.1
1	A	319	VAL	4.1
1	B	129	ARG	4.0
1	B	230	ALA	4.0
1	B	349	VAL	4.0
1	B	401	LEU	3.9
1	B	411	SER	3.9
1	B	368	ALA	3.9
1	B	384	GLY	3.9
1	C	232	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	388	ARG	3.9
1	B	428	THR	3.8
1	B	404	GLN	3.7
1	B	405	TYR	3.7
1	C	146	LEU	3.7
1	B	414	ALA	3.6
1	B	345	PHE	3.6
1	B	353	MET	3.6
1	B	327	GLY	3.6
1	B	317	ARG	3.5
1	B	231	VAL	3.5
1	B	351	SER	3.5
1	B	330	TRP	3.5
1	A	316	SER	3.5
1	B	358	LEU	3.5
1	B	352	SER	3.4
1	B	444	ARG	3.4
1	B	322	GLU	3.4
1	B	320	PHE	3.3
1	B	392	HIS	3.3
1	B	403	ASN	3.3
1	B	391	THR	3.3
1	B	323	LEU	3.3
1	B	332	GLY	3.3
1	A	315	PRO	3.2
1	B	348	SER	3.2
1	B	375	SER	3.2
1	B	410	LEU	3.2
1	B	419	LEU	3.2
1	B	316	SER	3.2
1	A	314	LEU	3.2
1	B	435	VAL	3.1
1	B	365	LEU	3.1
1	C	228	ASP	3.1
1	B	385	VAL	3.0
2	D	119	SER	3.0
1	B	422	GLY	3.0
1	A	174	ALA	3.0
1	B	343	ALA	2.9
1	C	34	ALA	2.9
1	B	373	ASP	2.9
1	B	415	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	356	HIS	2.8
1	C	225	ARG	2.8
2	E	99	PHE	2.8
1	A	318	VAL	2.8
1	B	328	VAL	2.8
1	B	400	ARG	2.8
1	B	367	LYS	2.7
1	C	53	LEU	2.7
2	F	48	VAL	2.7
2	F	122	HIS	2.7
1	B	333	ALA	2.7
2	E	111	GLN	2.7
1	C	236	LEU	2.7
1	B	436	LYS	2.7
1	B	413	ASP	2.6
1	B	342	GLY	2.6
1	A	86	CYS	2.6
1	C	37	GLY	2.6
1	C	39	ALA	2.6
1	B	340	ARG	2.6
1	B	407	ALA	2.6
1	A	128	GLU	2.5
1	B	321	ILE	2.5
1	B	344	ASP	2.5
1	A	96	LEU	2.5
1	B	372	ASP	2.5
1	B	314	LEU	2.5
1	C	226	LEU	2.4
1	B	313	SER	2.4
1	B	146	LEU	2.4
1	B	326	LYS	2.4
1	B	325	GLN	2.4
1	A	224	ALA	2.3
1	C	59	LEU	2.3
1	B	355	GLY	2.3
1	B	191	LEU	2.3
1	C	145	VAL	2.3
1	B	261	PRO	2.3
1	C	310	LEU	2.3
1	B	341	GLU	2.3
1	C	229	PHE	2.2
1	B	438	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLU	2.2
1	B	33	VAL	2.2
1	B	347	LEU	2.2
1	B	359	GLN	2.1
1	C	36	MET	2.1
1	A	37	GLY	2.1
1	B	329	MET	2.1
1	A	237	PHE	2.1
1	B	366	CYS	2.1
1	B	278	PHE	2.1
1	B	433	GLY	2.1
1	A	59	LEU	2.0
1	B	387	ILE	2.0
1	C	30	ALA	2.0
1	B	360	THR	2.0
1	B	219	ARG	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 carbohydrates 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.