



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:16 AM UTC

PDB ID : 5MWN / pdb_00005mwn
Title : Structure of the EAEC T6SS component TssK N-terminal domain in complex with llama nanobodies nbK18 and nbK27
Authors : Cambillau, C.; Nguyen, V.S.; Spinelli, S.; Legrand, P.
Deposited on : 2017-01-18
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

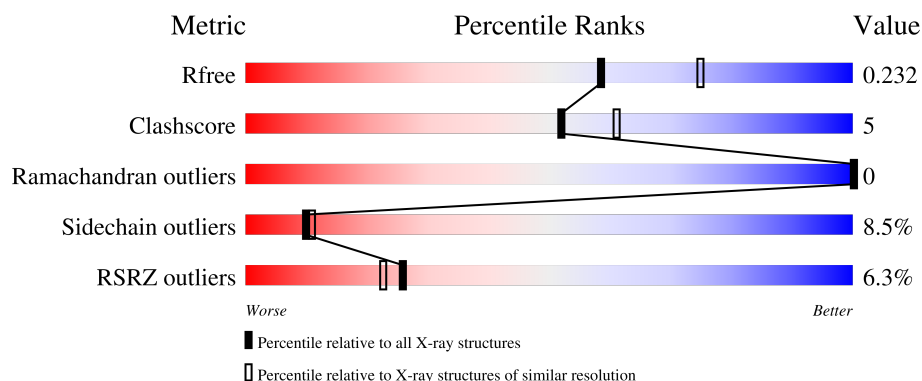
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	315	4% 82% 15% ..
1	B	315	5% 81% 17% .
1	C	315	7% 79% 16% ..
2	D	125	2% 87% 8% 5%
2	E	125	5% 90% 6% 5%

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Mol	Chain	Length	Quality of chain
2	F	125	2% 88% 8%
3	N	125	21% 82% 11% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11526 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	312	Total	C	N	O	S	0	0	0
			2432	1546	436	440	10			
1	B	315	Total	C	N	O	S	0	0	0
			2472	1566	443	452	11			
1	C	313	Total	C	N	O	S	0	0	0
			2425	1539	429	447	10			

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 llama nanobody raised against TssK, nbK18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	119	Total	C	N	O	S	0	0	0
			884	556	151	173	4			
2	E	119	Total	C	N	O	S	0	0	0
			879	555	150	170	4			
2	F	120	Total	C	N	O	S	0	0	0
			897	563	155	175	4			

- Molecule 3 is a protein called llama nanobody raised against TssK, nbK27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	117	Total	C	N	O	S	0	0	0
			833	521	145	162	5			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	0
			5	4	1		

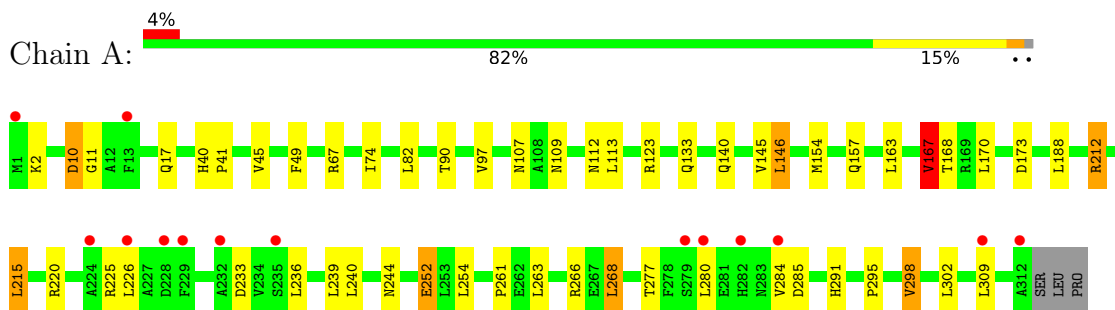
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	172	Total	O	0	0
			172	172		
5	C	151	Total	O	0	0
			151	151		
5	D	62	Total	O	0	0
			62	62		
5	E	52	Total	O	0	0
			52	52		
5	F	68	Total	O	0	0
			68	68		
5	N	21	Total	O	0	0
			21	21		

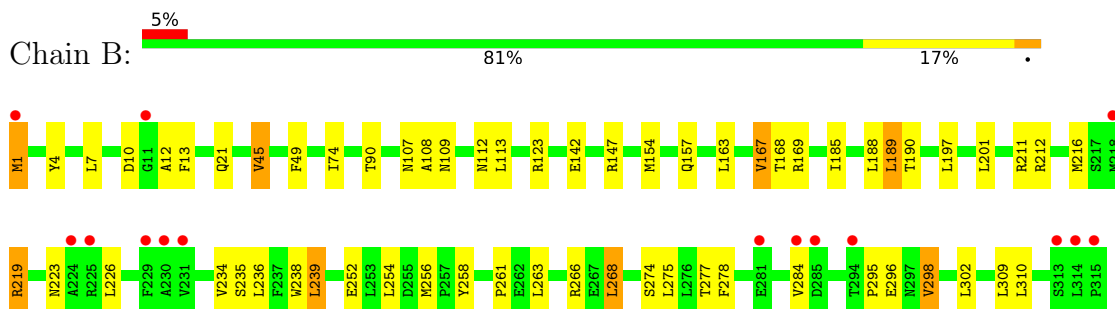
3 Residue-property plots [i](#)

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.

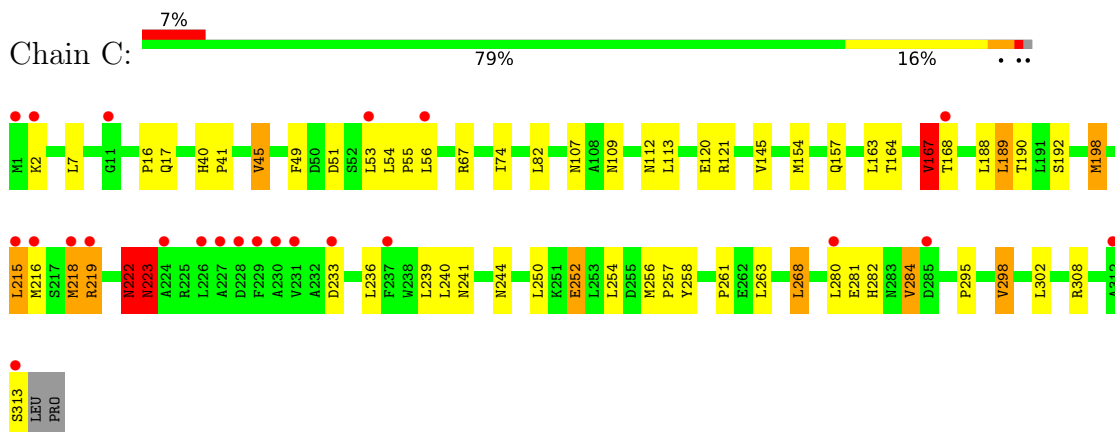
- Molecule 1: Type VI secretion protein



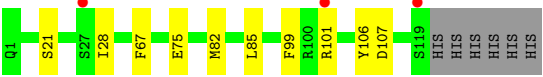
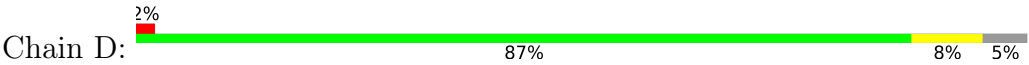
- Molecule 1: Type VI secretion protein



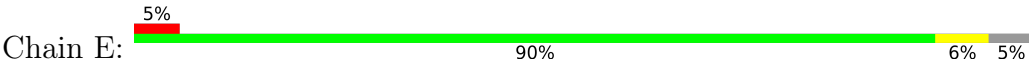
- Molecule 1: Type VI secretion protein



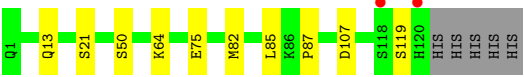
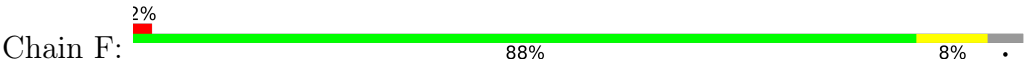
- Molecule 2: llama nanobody raised against TssK, nbK18



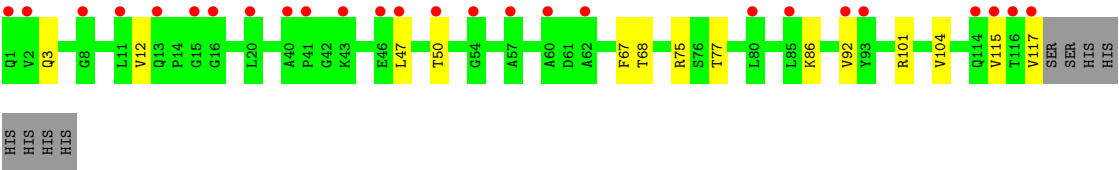
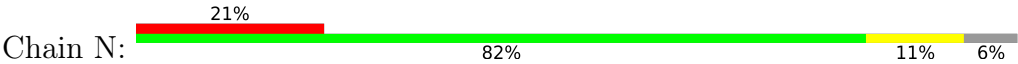
● Molecule 2: llama nanobody raised against TssK, nbK18



● Molecule 2: llama nanobody raised against TssK, nbK18



● Molecule 3: llama nanobody raised against TssK, nbK27



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.31Å 150.28Å 90.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 2.20 45.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.03-2.20) 98.3 (45.03-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.199 , 0.220 0.210 , 0.232	Depositor DCC
R_{free} test set	5039 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11526	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.72	0/2489	1.22	6/3402 (0.2%)
1	B	0.71	0/2531	1.24	7/3459 (0.2%)
1	C	0.75	1/2481 (0.0%)	1.27	9/3393 (0.3%)
2	D	0.63	0/900	0.99	1/1219 (0.1%)
2	E	0.67	0/895	1.05	0/1214
2	F	0.69	0/914	1.01	0/1238
3	N	0.70	0/849	1.10	1/1158 (0.1%)
All	All	0.71	1/11059 (0.0%)	1.18	24/15083 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	198	MET	SD-CE	-9.16	1.56	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	ASN	N-CA-C	-11.04	90.63	108.41
1	A	167	VAL	CB-CA-C	6.65	116.88	110.63
1	A	45	VAL	N-CA-C	-6.60	105.40	111.67
1	C	45	VAL	N-CA-C	-6.60	105.40	111.67
1	B	45	VAL	N-CA-C	-6.50	105.49	111.67
1	C	167	VAL	CB-CA-C	6.38	116.63	110.63
1	A	2	LYS	N-CA-C	6.19	118.82	111.71
2	D	67	PHE	CA-CB-CG	6.14	119.94	113.80
1	B	189	LEU	N-CA-C	-6.02	106.26	113.97
1	C	223	ASN	N-CA-C	5.94	118.61	110.24
1	C	2	LYS	N-CA-C	5.82	117.32	110.97
1	B	13	PHE	CA-CB-CG	5.80	119.61	113.80
1	B	163	LEU	N-CA-C	-5.78	99.83	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	189	LEU	N-CA-C	-5.59	106.81	113.97
3	N	67	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	163	LEU	N-CA-C	-5.40	100.49	109.46
1	C	163	LEU	N-CA-C	-5.38	100.54	109.46
1	B	10	ASP	N-CA-C	5.33	116.77	111.07
1	A	173	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	223	ASN	CA-CB-CG	5.25	117.85	112.60
1	B	12	ALA	N-CA-C	5.21	117.79	110.23
1	A	10	ASP	N-CA-C	5.13	116.87	111.28
1	C	233	ASP	CA-C-N	5.10	126.99	120.56
1	C	233	ASP	C-N-CA	5.10	126.99	120.56

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	2432	0	2400	31	0
1	B	2472	0	2434	38	0
1	C	2425	0	2370	46	0
2	D	884	0	850	7	0
2	E	879	0	842	1	0
2	F	897	0	861	5	0
3	N	833	0	767	3	0
4	C	5	0	0	0	0
5	A	173	0	0	2	0
5	B	172	0	0	0	0
5	C	151	0	0	2	0
5	D	62	0	0	0	0
5	E	52	0	0	0	0
5	F	68	0	0	0	0
5	N	21	0	0	0	0
All	All	11526	0	10524	109	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 5.

All (109) 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:A:244:ASN:HD22	1:B:277:THR:HG22	1.03	1.15
1:C:218:MET:O	1:C:222:ASN:ND2	1.77	1.14
1:B:185:ILE:HG22	1:B:296:GLU:HG3	1.36	1.07
1:B:1:MET:HG3	2:D:106:TYR:HE1	1.22	1.01
1:B:107:ASN:H	1:B:112:ASN:HD21	1.04	0.97
1:A:277:THR:O	1:C:219:ARG:NH2	1.97	0.97
1:A:107:ASN:H	1:A:112:ASN:HD21	1.09	0.93
1:B:185:ILE:HD11	1:B:188:LEU:HD11	1.49	0.92
1:A:277:THR:HG22	1:C:244:ASN:HD22	1.34	0.90
1:C:198:MET:HE1	1:C:257:PRO:HB2	1.52	0.89
1:A:244:ASN:ND2	1:B:277:THR:HG22	1.89	0.87
1:C:107:ASN:H	1:C:112:ASN:HD21	1.15	0.87
1:A:277:THR:HG21	1:C:241:ASN:HA	1.60	0.83
1:B:154:MET:H	1:B:157:GLN:HE21	1.32	0.77
1:B:109:ASN:HD22	2:D:107:ASP:H	1.30	0.75
1:C:223:ASN:ND2	1:C:223:ASN:H	1.83	0.74
1:A:154:MET:H	1:A:157:GLN:HE21	1.35	0.73
1:C:154:MET:H	1:C:157:GLN:HE21	1.33	0.72
1:B:1:MET:HG3	2:D:106:TYR:CE1	2.14	0.72
1:C:109:ASN:HD22	2:F:107:ASP:H	1.35	0.72
1:B:212:ARG:HE	1:C:284:VAL:HG13	1.55	0.71
1:C:198:MET:HE1	1:C:257:PRO:CB	2.20	0.71
1:B:185:ILE:CG2	1:B:296:GLU:HG3	2.21	0.68
1:C:222:ASN:ND2	1:C:222:ASN:H	1.95	0.65
1:C:219:ARG:CG	1:C:219:ARG:HH11	2.09	0.65
1:C:223:ASN:H	1:C:223:ASN:HD22	1.43	0.64
1:B:1:MET:CG	2:D:106:TYR:HE1	2.06	0.63
1:B:109:ASN:ND2	2:D:107:ASP:H	1.97	0.61
1:A:133:GLN:HE22	1:A:140:GLN:HE21	1.50	0.60
1:A:49:PHE:HZ	1:A:167:VAL:HG13	1.67	0.59
1:B:295:PRO:HA	1:B:298:VAL:HG13	1.84	0.59
2:D:82:MET:HE2	2:D:85:LEU:HD21	1.83	0.59
1:A:146:LEU:HB2	1:B:7:LEU:HG	1.85	0.59
1:B:1:MET:HE2	1:B:108:ALA:HB1	1.84	0.59
1:C:268:LEU:HB3	1:C:302:LEU:HD21	1.85	0.59
1:A:109:ASN:HD22	2:E:107:ASP:H	1.51	0.59
1:C:49:PHE:HZ	1:C:167:VAL:HG13	1.68	0.59
1:A:295:PRO:HA	1:A:298:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HA	1:B:190:THR:HG22	1.87	0.57
1:A:215:LEU:HD13	1:A:236:LEU:HD12	1.86	0.57
1:C:109:ASN:ND2	2:F:107:ASP:H	2.02	0.56
1:C:219:ARG:HG3	1:C:219:ARG:NH1	2.21	0.56
1:C:45:VAL:HA	1:C:190:THR:HG22	1.88	0.56
1:A:284:VAL:HG21	1:C:244:ASN:OD1	2.05	0.55
1:B:49:PHE:HZ	1:B:167:VAL:HG13	1.70	0.55
1:C:295:PRO:HA	1:C:298:VAL:HG13	1.88	0.55
2:F:82:MET:HE2	2:F:85:LEU:HD21	1.89	0.54
1:B:256:MET:HE2	1:C:40:HIS:CE1	2.42	0.54
1:C:219:ARG:HH11	1:C:219:ARG:HG3	1.72	0.54
3:N:12:VAL:O	3:N:117:VAL:HA	2.08	0.54
1:A:107:ASN:H	1:A:112:ASN:ND2	1.92	0.54
1:C:222:ASN:H	1:C:222:ASN:HD22	1.56	0.53
1:C:282:HIS:HE1	1:C:308:ARG:HH21	1.56	0.53
1:A:212:ARG:HH22	1:A:244:ASN:HA	1.73	0.53
1:C:215:LEU:HD11	1:C:239:LEU:HD23	1.93	0.51
3:N:47:LEU:HD11	3:N:50:THR:HB	1.92	0.50
1:B:190:THR:OG1	1:B:258:TYR:HA	2.11	0.50
1:B:212:ARG:NE	1:C:284:VAL:HG13	2.25	0.49
1:B:107:ASN:N	1:B:112:ASN:HD21	1.89	0.49
1:B:211:ARG:HD3	1:B:310:LEU:O	2.13	0.49
1:C:219:ARG:HH11	1:C:219:ARG:CB	2.26	0.49
1:A:215:LEU:HD11	1:A:239:LEU:HD23	1.95	0.48
2:D:99:PHE:CE2	2:D:101:ARG:HB2	2.48	0.48
1:B:216:MET:HA	1:B:219:ARG:HD2	1.95	0.48
1:C:219:ARG:CG	1:C:219:ARG:NH1	2.72	0.48
1:C:49:PHE:CZ	1:C:167:VAL:HG13	2.49	0.48
5:A:417:HOH:O	1:B:266:ARG:HD3	2.12	0.48
1:A:220:ARG:NH2	1:A:233:ASP:OD1	2.45	0.47
1:A:49:PHE:CZ	1:A:167:VAL:HG13	2.48	0.47
1:A:212:ARG:NH2	1:A:244:ASN:HA	2.28	0.47
1:B:49:PHE:CZ	1:B:167:VAL:HG13	2.49	0.47
1:A:188:LEU:HB2	1:A:261:PRO:HG3	1.96	0.47
1:C:222:ASN:ND2	1:C:222:ASN:N	2.60	0.47
1:C:120:GLU:HB2	2:F:50:SER:HB2	1.97	0.46
1:C:188:LEU:HB2	1:C:261:PRO:HG3	1.97	0.46
1:A:266:ARG:HD3	5:C:506:HOH:O	2.15	0.46
1:B:185:ILE:HG23	1:B:295:PRO:HG2	1.98	0.46
1:C:190:THR:OG1	1:C:258:TYR:HA	2.16	0.46
1:A:11:GLY:O	3:N:101:ARG:HD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:TYR:H	1:B:21:GLN:NE2	2.15	0.45
1:B:185:ILE:HG12	1:B:295:PRO:HG2	1.98	0.45
1:B:216:MET:O	1:B:219:ARG:HD2	2.17	0.45
1:B:188:LEU:HB2	1:B:261:PRO:HG3	1.99	0.45
1:A:97:VAL:HG12	1:A:170:LEU:HB2	1.98	0.45
1:B:268:LEU:HB3	1:B:302:LEU:HD21	2.00	0.44
1:C:252:GLU:HG3	5:C:506:HOH:O	2.16	0.44
1:B:185:ILE:CD1	1:B:197:LEU:HD22	2.48	0.44
1:C:192:SER:HA	1:C:198:MET:HE2	2.01	0.43
1:C:198:MET:CE	1:C:257:PRO:HB2	2.37	0.43
1:A:252:GLU:HG3	5:A:417:HOH:O	2.19	0.43
1:A:215:LEU:HB3	1:A:240:LEU:HD13	2.00	0.43
1:A:10:ASP:HA	1:C:16:PRO:HG3	2.02	0.42
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.93	0.42
1:A:291:HIS:H	1:A:298:VAL:HG11	1.85	0.42
1:C:215:LEU:HD13	1:C:236:LEU:HD12	2.01	0.42
1:A:41:PRO:O	1:A:67:ARG:HD3	2.19	0.42
1:A:268:LEU:HB3	1:A:302:LEU:HD21	2.01	0.41
2:F:87:PRO:HG3	2:F:119:SER:HB2	2.01	0.41
1:B:235:SER:O	1:B:239:LEU:HB2	2.21	0.41
1:C:41:PRO:O	1:C:67:ARG:HD3	2.20	0.41
1:B:238:TRP:HB2	1:B:278:PHE:HZ	1.86	0.41
1:A:40:HIS:HE1	1:C:256:MET:HE3	1.86	0.41
1:B:169:ARG:HH22	1:B:296:GLU:CD	2.28	0.41
1:C:240:LEU:HD12	1:C:240:LEU:HA	1.98	0.41
1:B:189:LEU:HD23	1:B:189:LEU:HA	1.92	0.40
1:C:282:HIS:HE1	1:C:308:ARG:NH2	2.18	0.40
1:C:54:LEU:N	1:C:55:PRO:CD	2.84	0.40
1:B:107:ASN:H	1:B:112:ASN:ND2	1.89	0.40
1:C:51:ASP:O	1:C:54:LEU:HB2	2.21	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	A	310/315 (98%)	304 (98%)	6 (2%)	0	100	100
1	B	313/315 (99%)	307 (98%)	6 (2%)	0	100	100
1	C	311/315 (99%)	305 (98%)	6 (2%)	0	100	100
2	D	117/125 (94%)	117 (100%)	0	0	100	100
2	E	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
2	F	118/125 (94%)	118 (100%)	0	0	100	100
3	N	115/125 (92%)	111 (96%)	4 (4%)	0	100	100
All	All	1401/1445 (97%)	1378 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	256/274 (93%)	234 (91%)	22 (9%)	10	10
1	B	265/274 (97%)	241 (91%)	24 (9%)	9	9
1	C	255/274 (93%)	227 (89%)	28 (11%)	6	6
2	D	90/101 (89%)	87 (97%)	3 (3%)	33	45
2	E	87/101 (86%)	81 (93%)	6 (7%)	14	16
2	F	92/101 (91%)	88 (96%)	4 (4%)	26	35
3	N	78/100 (78%)	70 (90%)	8 (10%)	7	7
All	All	1123/1225 (92%)	1028 (92%)	95 (8%)	10	11

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	74	ILE

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	90	THR
1	A	113	LEU
1	A	123	ARG
1	A	145	VAL
1	A	146	LEU
1	A	167	VAL
1	A	168	THR
1	A	212	ARG
1	A	215	LEU
1	A	225	ARG
1	A	226	LEU
1	A	252	GLU
1	A	254	LEU
1	A	263	LEU
1	A	268	LEU
1	A	280	LEU
1	A	285	ASP
1	A	298	VAL
1	A	309	LEU
1	B	1	MET
1	B	74	ILE
1	B	90	THR
1	B	113	LEU
1	B	123	ARG
1	B	142	GLU
1	B	147	ARG
1	B	167	VAL
1	B	168	THR
1	B	201	LEU
1	B	219	ARG
1	B	226	LEU
1	B	234	VAL
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	274	SER
1	B	275	LEU
1	B	284	VAL

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	309	LEU
1	C	7	LEU
1	C	17	GLN
1	C	53	LEU
1	C	56	LEU
1	C	74	ILE
1	C	82	LEU
1	C	113	LEU
1	C	121	ARG
1	C	145	VAL
1	C	164	THR
1	C	167	VAL
1	C	168	THR
1	C	215	LEU
1	C	216	MET
1	C	218	MET
1	C	219	ARG
1	C	222	ASN
1	C	223	ASN
1	C	250	LEU
1	C	252	GLU
1	C	254	LEU
1	C	263	LEU
1	C	268	LEU
1	C	280	LEU
1	C	281	GLU
1	C	284	VAL
1	C	298	VAL
1	C	313	SER
2	D	21	SER
2	D	28	ILE
2	D	75	GLU
2	E	12	VAL
2	E	21	SER
2	E	27	SER
2	E	33	VAL
2	E	45	ARG
2	E	101	ARG
2	F	13	GLN
2	F	21	SER
2	F	64	LYS

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Mol	Chain	Res	Type
2	F	75	GLU
3	N	3	GLN
3	N	68	THR
3	N	75	ARG
3	N	77	THR
3	N	86	LYS
3	N	92	VAL
3	N	104	VAL
3	N	115	VAL

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

Mol	Chain	Res	Type
1	A	40	HIS
1	A	60	ASN
1	A	109	ASN
1	A	112	ASN
1	A	133	GLN
1	A	157	GLN
1	A	177	GLN
1	B	21	GLN
1	B	60	ASN
1	B	109	ASN
1	B	112	ASN
1	B	157	GLN
1	B	177	GLN
1	B	213	GLN
1	B	307	ASN
1	C	40	HIS
1	C	109	ASN
1	C	112	ASN
1	C	157	GLN
1	C	177	GLN
1	C	222	ASN
1	C	223	ASN
1	C	244	ASN
1	C	282	HIS
1	C	307	ASN
2	D	73	ASN
2	D	83	ASN
2	E	83	ASN
2	F	83	ASN

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Mol	Chain	Res	Type
3	N	39	GLN
3	N	107	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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	C	401	-	4,4,4	2.07	1 (25%)	6,6,6	0.54	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	PO4	P-O1	2.37	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	312/315 (99%)	0.39	14 (4%) 38 35	41, 57, 104, 152	0
1	B	315/315 (100%)	0.37	15 (4%) 35 32	42, 57, 95, 133	0
1	C	313/315 (99%)	0.45	23 (7%) 21 18	39, 58, 134, 198	0
2	D	119/125 (95%)	0.23	3 (2%) 58 55	45, 60, 78, 106	0
2	E	119/125 (95%)	0.57	6 (5%) 34 31	47, 63, 84, 113	0
2	F	120/125 (96%)	0.09	2 (1%) 69 66	42, 54, 79, 148	0
3	N	117/125 (93%)	1.49	26 (22%) 2 1	64, 113, 133, 146	0
All	All	1415/1445 (97%)	0.47	89 (6%) 26 23	39, 59, 119, 198	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	119	SER	6.3
3	N	117	VAL	5.9
1	C	237	PHE	4.7
1	A	1	MET	4.5
1	C	1	MET	4.2
1	B	314	LEU	4.1
3	N	2	VAL	4.1
3	N	11	LEU	4.1
3	N	47	LEU	4.0
1	C	233	ASP	3.9
2	E	74	ALA	3.9
1	C	229	PHE	3.8
1	C	215	LEU	3.8
1	A	226	LEU	3.8
1	C	313	SER	3.7
3	N	92	VAL	3.6
1	B	1	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	284	VAL	3.5
1	C	231	VAL	3.5
1	B	313	SER	3.4
2	E	42	GLY	3.3
1	C	53	LEU	3.3
1	C	230	ALA	3.2
3	N	15	GLY	3.2
1	C	228	ASP	3.2
1	A	228	ASP	3.1
1	B	224	ALA	3.1
1	A	279	SER	3.1
1	A	282	HIS	3.0
1	A	312	ALA	3.0
2	D	119	SER	3.0
1	A	232	ALA	2.9
1	C	224	ALA	2.9
3	N	62	ALA	2.9
3	N	85	LEU	2.9
3	N	40	ALA	2.8
1	B	284	VAL	2.8
1	B	230	ALA	2.8
1	C	227	ALA	2.8
3	N	8	GLY	2.7
1	B	294	THR	2.7
1	C	11	GLY	2.7
3	N	114	GLN	2.6
3	N	60	ALA	2.6
2	F	120	HIS	2.6
1	B	11	GLY	2.6
1	B	315	PRO	2.6
3	N	41	PRO	2.6
1	A	235	SER	2.6
3	N	16	GLY	2.5
1	B	225	ARG	2.5
3	N	57	ALA	2.5
1	A	280	LEU	2.5
1	C	168	THR	2.4
1	C	2	LYS	2.4
1	C	285	ASP	2.4
3	N	1	GLN	2.4
1	A	224	ALA	2.4
2	F	118	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	N	115	VAL	2.4
3	N	20	LEU	2.4
1	A	13	PHE	2.3
1	B	281	GLU	2.3
1	C	219	ARG	2.3
1	B	285	ASP	2.3
3	N	116	THR	2.3
2	E	73	ASN	2.3
3	N	50	THR	2.3
2	E	75	GLU	2.3
3	N	46	GLU	2.3
1	A	229	PHE	2.2
1	C	312	ALA	2.2
1	B	231	VAL	2.2
3	N	80	LEU	2.2
2	D	27	SER	2.2
1	B	218	MET	2.2
3	N	13	GLN	2.2
1	A	309	LEU	2.1
1	C	226	LEU	2.1
1	C	216	MET	2.1
1	C	218	MET	2.1
1	B	229	PHE	2.1
3	N	93	TYR	2.1
1	C	280	LEU	2.1
1	C	56	LEU	2.1
2	D	101	ARG	2.1
3	N	54	GLY	2.1
3	N	43	LYS	2.0
2	E	113	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	C	401	5/5	0.81	0.16	98,99,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.