



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:14 PM UTC

PDB ID : 6E1R / pdb_00006e1r
Title : Crystal structure of the Acinetobacter phage vB_ApiP_P1 tailspike protein
Authors : Plattner, M.; Shneider, M.M.; Oliveira, H.; Azeredo, J.; Leiman, P.G.
Deposited on : 2018-07-10
Resolution : 2.69 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

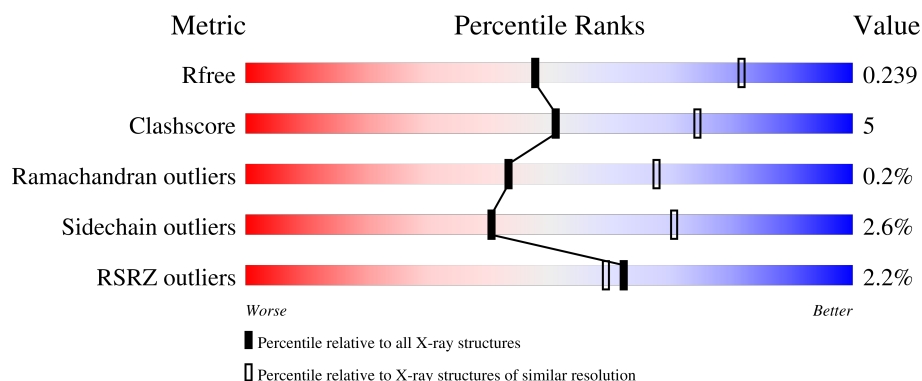
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	554	 84% 13% ..
1	B	554	 85% 12% ..
1	C	554	 86% 12% ..
1	D	554	 4% 84% 13% ..
1	E	554	 5% 83% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	554	3% 82% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25193 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 Tailspike protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	Se	0	0	0
			4053	2550	682	799	11	11			
1	B	543	Total	C	N	O	S	Se	0	0	0
			4045	2544	681	798	11	11			
1	C	544	Total	C	N	O	S	Se	0	0	0
			4053	2550	682	799	11	11			
1	D	544	Total	C	N	O	S	Se	0	0	0
			4053	2550	682	799	11	11			
1	E	544	Total	C	N	O	S	Se	0	0	0
			4053	2550	682	799	11	11			
1	F	544	Total	C	N	O	S	Se	0	0	0
			4053	2550	682	799	11	11			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

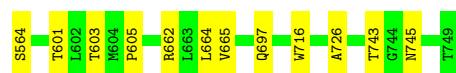
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

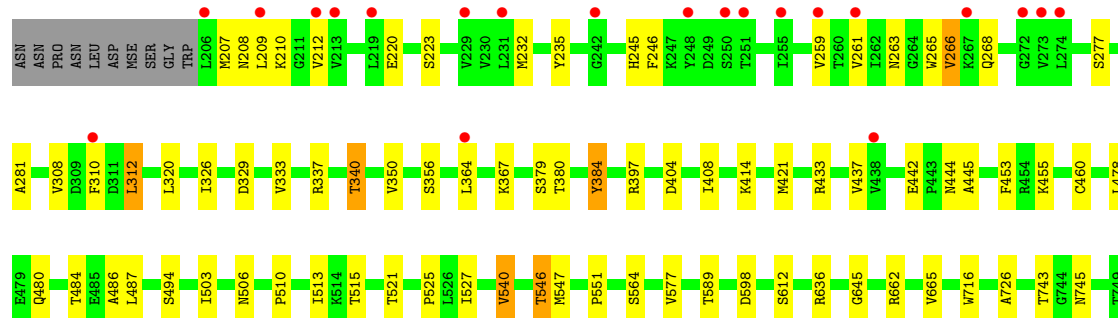
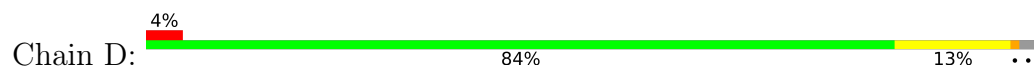
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	211	Total 211	O 211	0	0
4	B	183	Total 183	O 183	0	0
4	C	204	Total 204	O 204	0	0
4	D	119	Total 119	O 119	0	0
4	E	73	Total 73	O 73	0	0
4	F	87	Total 87	O 87	0	0

- Molecule 1: Tailspike protein

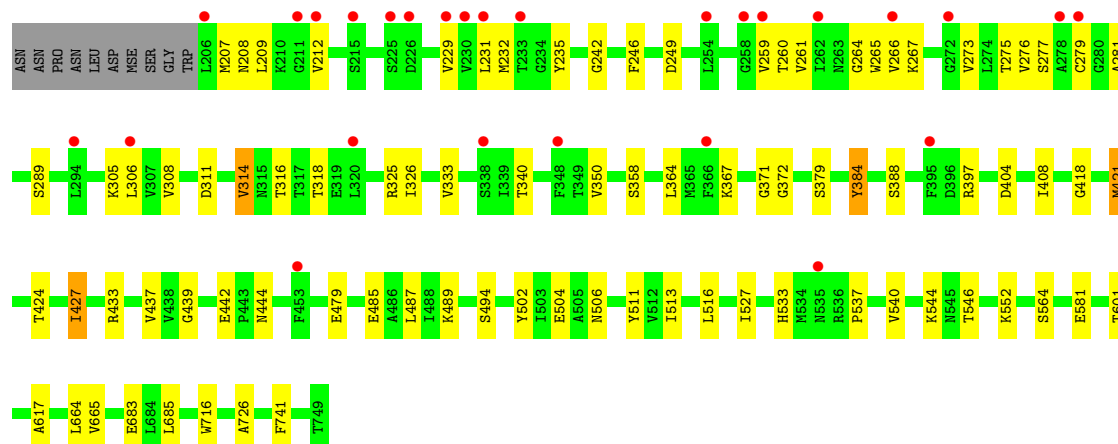
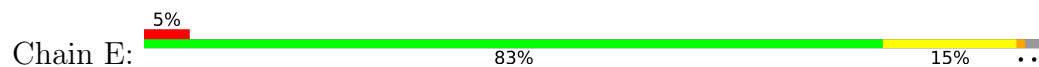




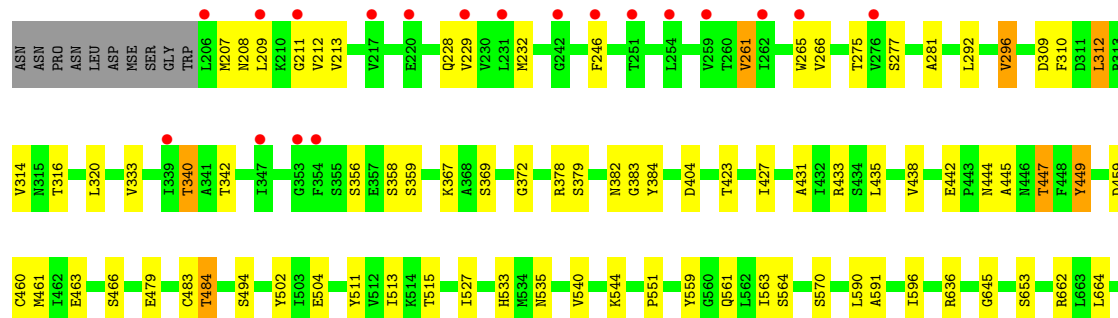
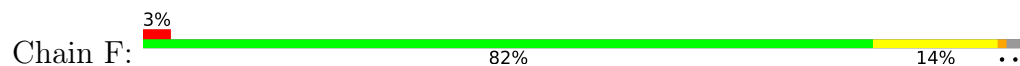
• Molecule 1: Tailspike protein



• Molecule 1: Tailspike protein



• Molecule 1: Tailspike protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.12Å 90.02Å 508.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.69 49.12 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.12-2.69) 99.5 (49.12-2.69)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.200 , 0.237 0.200 , 0.239	Depositor DCC
R_{free} test set	3641 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	1.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25193	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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](#)

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

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	0.09	0/4119	0.31	0/5571
1	B	0.09	0/4112	0.31	0/5563
1	C	0.09	0/4119	0.31	0/5571
1	D	0.10	0/4119	0.32	0/5571
1	E	0.10	0/4119	0.33	0/5571
1	F	0.11	0/4119	0.32	0/5571
All	All	0.10	0/24707	0.32	0/33418

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4053	0	3966	44	0
1	B	4045	0	3955	41	0
1	C	4053	0	3966	40	0
1	D	4053	0	3966	50	0
1	E	4053	0	3966	52	0
1	F	4053	0	3966	57	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	1	0
2	F	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	211	0	0	0	0
4	B	183	0	0	0	0
4	C	204	0	0	3	0
4	D	119	0	0	0	0
4	E	73	0	0	3	0
4	F	87	0	0	6	0
All	All	25193	0	23785	250	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 (250) 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:397:ARG:HD2	1:C:421:MSE:HE3	1.64	0.79
1:C:340:THR:HG23	1:C:367:LYS:HB2	1.66	0.78
1:A:397:ARG:HD2	1:A:421:MSE:HE3	1.67	0.77
1:D:397:ARG:HB3	1:D:421:MSE:HE3	1.68	0.74
1:E:397:ARG:HE	1:E:421:MSE:HE3	1.53	0.73
1:B:397:ARG:NH1	1:B:418:GLY:O	2.22	0.73
1:D:232:MSE:HE2	1:D:235:TYR:HA	1.72	0.72
1:F:423:THR:O	4:F:901:HOH:O	2.09	0.70
1:A:229:VAL:HG21	1:C:233:THR:HG21	1.72	0.70
2:C:802:CL:CL	4:C:949:HOH:O	2.45	0.70
1:F:207:MSE:HE1	1:F:229:VAL:H	1.57	0.69
1:D:494:SER:HG	1:F:533:HIS:HD1	1.42	0.68
1:D:210:LYS:NZ	1:D:223:SER:O	2.28	0.67
1:E:340:THR:HG22	1:E:367:LYS:HB2	1.78	0.65
1:F:459:ASP:O	4:F:902:HOH:O	2.13	0.65
1:E:533:HIS:HD1	1:F:494:SER:HG	1.41	0.65
1:D:220:GLU:HB2	1:D:263:ASN:HD22	1.61	0.65
1:D:320:LEU:HD12	1:D:356:SER:HB3	1.78	0.65
1:D:340:THR:HG23	1:D:367:LYS:HB2	1.79	0.65
1:D:208:ASN:HA	1:F:211:GLY:HA2	1.79	0.65
1:E:439:GLY:N	1:E:442:GLU:OE2	2.30	0.64
1:E:397:ARG:NH1	1:E:418:GLY:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:VAL:HG12	1:E:266:VAL:HG12	1.79	0.64
1:F:340:THR:HG23	1:F:367:LYS:HB2	1.79	0.63
1:C:421:MSE:HE2	1:C:425:ASN:HB3	1.80	0.63
1:C:353:GLY:HA2	1:C:441:ARG:HH21	1.64	0.63
1:E:232:MSE:HE2	1:E:235:TYR:HA	1.80	0.63
1:A:320:LEU:HD22	1:A:356:SER:HB3	1.79	0.62
1:C:404:ASP:OD2	1:C:433:ARG:NH2	2.33	0.61
1:D:453:PHE:HB2	1:D:478:LEU:HD13	1.82	0.61
1:A:739:GLU:OE1	1:B:745:ASN:ND2	2.34	0.60
1:B:397:ARG:HE	1:B:421:MSE:HE3	1.68	0.59
1:A:378:ARG:NH1	1:A:404:ASP:OD2	2.36	0.59
1:E:267:LYS:NZ	4:E:801:HOH:O	2.36	0.58
1:D:494:SER:OG	1:F:533:HIS:ND1	2.27	0.58
1:A:212:VAL:HG12	1:A:231:LEU:HB3	1.85	0.58
1:C:210:LYS:NZ	1:C:223:SER:O	2.37	0.58
1:B:662:ARG:HG2	1:B:743:THR:HB	1.85	0.57
1:F:442:GLU:N	1:F:442:GLU:OE1	2.37	0.57
1:C:384:TYR:OH	1:C:442:GLU:N	2.37	0.57
1:F:378:ARG:NH1	1:F:404:ASP:OD2	2.38	0.57
1:B:207:MSE:HE1	1:B:228:GLN:HA	1.87	0.57
1:E:246:PHE:HB3	1:E:265:TRP:HB3	1.86	0.57
1:D:414:LYS:NZ	1:E:388:SER:O	2.36	0.56
1:F:404:ASP:OD2	1:F:433:ARG:NH2	2.37	0.56
1:A:254:LEU:HB2	1:D:521:THR:HG23	1.88	0.56
1:D:277:SER:HA	1:D:281:ALA:HB3	1.88	0.56
1:F:484:THR:N	4:F:902:HOH:O	2.38	0.55
1:E:533:HIS:ND1	1:F:494:SER:OG	2.29	0.55
1:C:536:ARG:NH1	1:C:561:GLN:OE1	2.39	0.55
1:F:379:SER:HB3	1:F:383:GLY:N	2.22	0.55
1:B:378:ARG:NH1	1:B:404:ASP:OD2	2.40	0.55
1:A:662:ARG:HH21	1:C:664:LEU:HB2	1.72	0.55
1:A:536:ARG:NH1	1:A:561:GLN:OE1	2.40	0.54
1:D:404:ASP:OD2	1:D:433:ARG:NH2	2.40	0.54
1:C:277:SER:HA	1:C:281:ALA:HB3	1.90	0.54
1:F:460:CYS:SG	1:F:463:GLU:HB2	2.48	0.54
1:C:540:VAL:C	1:C:564:SER:HB2	2.33	0.54
1:F:653:SER:OG	4:F:903:HOH:O	2.18	0.54
1:E:277:SER:HA	1:E:281:ALA:HB3	1.90	0.54
1:D:662:ARG:HG2	1:D:743:THR:HB	1.89	0.53
1:F:372:GLY:O	1:F:427:ILE:HD11	2.09	0.53
1:C:510:PRO:HA	1:C:540:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:GLU:OE1	1:E:489:LYS:NZ	2.25	0.53
1:B:216:LYS:HG3	1:B:262:ILE:HD13	1.91	0.53
1:C:213:VAL:HG13	1:C:218:GLU:HB3	1.91	0.53
1:E:404:ASP:OD2	1:E:433:ARG:NH2	2.42	0.53
1:A:414:LYS:NZ	1:B:388:SER:O	2.42	0.53
1:D:745:ASN:ND2	1:F:739:GLU:OE1	2.42	0.52
1:F:277:SER:HA	1:F:281:ALA:HB3	1.91	0.52
1:C:397:ARG:HB3	1:C:421:MSE:HG3	1.92	0.52
1:E:259:VAL:HG22	1:E:279:CYS:HA	1.91	0.51
1:A:247:LYS:O	1:A:266:VAL:HG23	2.11	0.51
1:B:277:SER:HA	1:B:281:ALA:HB3	1.93	0.51
1:B:421:MSE:HE2	1:B:425:ASN:HB3	1.93	0.51
1:D:208:ASN:OD1	1:D:209:LEU:N	2.42	0.51
1:B:739:GLU:OE2	1:C:745:ASN:ND2	2.44	0.51
1:E:540:VAL:C	1:E:564:SER:HB2	2.35	0.51
1:B:510:PRO:HA	1:B:540:VAL:HG23	1.94	0.50
1:A:421:MSE:HE2	1:A:425:ASN:HB3	1.92	0.50
1:A:397:ARG:HB3	1:A:421:MSE:HG3	1.93	0.50
1:D:212:VAL:N	1:E:207:MSE:O	2.39	0.50
1:F:208:ASN:OD1	1:F:209:LEU:N	2.45	0.50
1:C:662:ARG:HG2	1:C:743:THR:HB	1.92	0.50
1:E:249:ASP:N	1:E:264:GLY:O	2.45	0.50
1:B:540:VAL:C	1:B:564:SER:HB2	2.37	0.50
1:E:716:TRP:CZ3	1:E:726:ALA:HB2	2.47	0.49
1:B:384:TYR:OH	1:B:442:GLU:N	2.45	0.49
1:A:513:ILE:HD13	1:A:527:ILE:HD13	1.94	0.49
1:D:662:ARG:HH22	1:F:664:LEU:HB2	1.77	0.49
1:E:260:THR:O	1:E:267:LYS:N	2.40	0.49
1:E:511:TYR:CD1	1:E:544:LYS:HB2	2.48	0.49
1:A:384:TYR:OH	1:A:442:GLU:N	2.46	0.49
1:B:716:TRP:CZ3	1:B:726:ALA:HB2	2.48	0.49
1:A:596:ILE:HD11	1:A:604:MSE:HG3	1.95	0.48
1:B:247:LYS:O	1:B:266:VAL:HG23	2.14	0.48
1:F:320:LEU:HD22	1:F:356:SER:HB3	1.94	0.48
1:A:309:ASP:OD1	1:A:309:ASP:N	2.42	0.48
1:A:292:LEU:O	1:A:296:VAL:HG23	2.13	0.48
1:A:665:VAL:HG11	1:A:716:TRP:CH2	2.48	0.48
1:D:665:VAL:HG11	1:D:716:TRP:CH2	2.49	0.48
1:D:662:ARG:NH2	1:F:683:GLU:OE1	2.46	0.47
1:D:636:ARG:NH1	1:D:645:GLY:O	2.43	0.47
1:E:208:ASN:OD1	1:E:209:LEU:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:665:VAL:HG11	1:E:716:TRP:CH2	2.49	0.47
1:F:540:VAL:C	1:F:564:SER:HB2	2.39	0.47
1:E:276:VAL:HG22	1:E:306:LEU:HD11	1.96	0.47
1:C:378:ARG:NH1	1:C:404:ASP:OD2	2.47	0.47
1:A:401:TYR:OH	1:A:433:ARG:NH2	2.48	0.47
1:D:350:VAL:HB	1:D:379:SER:HA	1.97	0.47
1:F:636:ARG:NH1	1:F:645:GLY:O	2.43	0.47
1:D:212:VAL:HG11	1:E:229:VAL:HG21	1.97	0.46
1:A:503:ILE:HD12	1:A:534:MSE:HE3	1.98	0.46
1:B:259:VAL:HG22	1:B:279:CYS:HA	1.97	0.46
1:B:596:ILE:HD11	1:B:604:MSE:HG3	1.97	0.46
1:C:665:VAL:HG11	1:C:716:TRP:CH2	2.51	0.46
1:F:309:ASP:N	4:F:906:HOH:O	2.49	0.46
1:A:460:CYS:HA	1:A:486:ALA:O	2.16	0.46
1:C:292:LEU:O	1:C:296:VAL:HG23	2.15	0.46
1:E:326:ILE:HG12	1:E:364:LEU:HD11	1.97	0.46
1:F:431:ALA:HB2	1:F:461:MSE:HE3	1.98	0.46
1:A:213:VAL:HG23	1:A:232:MSE:HG3	1.97	0.46
1:D:310:PHE:O	1:D:312:LEU:HD13	2.16	0.46
1:F:246:PHE:HB3	1:F:265:TRP:HB3	1.97	0.46
1:F:309:ASP:N	1:F:309:ASP:OD1	2.42	0.45
1:E:552:LYS:HB3	1:E:581:GLU:HB2	1.98	0.45
1:B:397:ARG:NE	1:B:421:MSE:HE3	2.32	0.45
1:D:408:ILE:HA	1:D:444:ASN:O	2.16	0.45
1:F:379:SER:HB3	1:F:383:GLY:H	1.80	0.45
1:D:326:ILE:HG12	1:D:364:LEU:HD11	1.97	0.45
1:F:213:VAL:HG23	1:F:232:MSE:HG3	1.98	0.45
1:F:292:LEU:O	1:F:296:VAL:HG23	2.17	0.45
1:A:485:GLU:OE1	1:A:489:LYS:NZ	2.44	0.45
1:A:408:ILE:HA	1:A:444:ASN:O	2.17	0.45
1:A:487:LEU:HD11	1:A:506:ASN:ND2	2.32	0.45
1:D:246:PHE:HB3	1:D:265:TRP:HB3	1.99	0.45
1:E:276:VAL:HG21	1:E:308:VAL:HG22	1.97	0.45
1:A:545:ASN:CG	1:A:551:PRO:HD2	2.42	0.45
1:D:515:THR:O	1:D:546:THR:OG1	2.30	0.45
1:A:511:TYR:CD1	1:A:544:LYS:HB2	2.52	0.44
1:F:662:ARG:HD3	1:F:683:GLU:OE2	2.17	0.44
1:E:212:VAL:HG22	1:E:231:LEU:HB3	1.98	0.44
1:B:513:ILE:HD13	1:B:527:ILE:HD13	1.98	0.44
1:B:379:SER:HB3	1:B:383:GLY:N	2.33	0.44
1:B:502:TYR:CE1	1:C:445:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:THR:HG21	1:D:551:PRO:HD3	2.00	0.44
1:D:577:VAL:HG21	1:D:598:ASP:HB2	1.99	0.44
1:D:540:VAL:C	1:D:564:SER:HB2	2.42	0.44
1:E:513:ILE:HD13	1:E:527:ILE:HD13	1.99	0.44
1:F:483:CYS:HB3	4:F:902:HOH:O	2.17	0.44
1:C:246:PHE:HB3	1:C:265:TRP:HB3	2.00	0.44
1:C:437:VAL:N	1:C:441:ARG:O	2.43	0.43
1:D:513:ILE:HD13	1:D:527:ILE:HD13	1.99	0.43
1:F:207:MSE:HE1	1:F:228:GLN:HA	2.00	0.43
1:F:535:ASN:HA	1:F:561:GLN:H	1.83	0.43
1:F:342:THR:HA	1:F:369:SER:HB3	1.99	0.43
1:A:612:SER:HA	1:B:617:ALA:O	2.18	0.43
1:B:408:ILE:HA	1:B:444:ASN:O	2.18	0.43
1:C:511:TYR:CD1	1:C:544:LYS:HB2	2.53	0.43
1:C:697:GLN:NE2	4:C:913:HOH:O	2.51	0.43
1:D:716:TRP:CZ3	1:D:726:ALA:HB2	2.53	0.43
1:E:664:LEU:HB3	1:E:741:PHE:HB2	1.99	0.43
1:F:515:THR:HG21	1:F:551:PRO:HG3	2.00	0.43
1:C:379:SER:HB3	1:C:383:GLY:N	2.33	0.43
1:D:384:TYR:OH	1:D:442:GLU:N	2.51	0.43
1:D:510:PRO:HA	1:D:540:VAL:HG23	1.99	0.43
1:E:371:GLY:HA3	1:E:424:THR:O	2.18	0.43
1:E:384:TYR:OH	1:E:442:GLU:N	2.52	0.43
1:E:397:ARG:HB2	1:E:421:MSE:HG3	2.00	0.43
1:A:246:PHE:HB3	1:A:265:TRP:HB3	2.00	0.43
1:C:716:TRP:CZ3	1:C:726:ALA:HB2	2.54	0.43
1:E:408:ILE:HA	1:E:444:ASN:O	2.18	0.43
1:E:506:ASN:HB2	1:E:537:PRO:O	2.18	0.43
1:F:716:TRP:CZ3	1:F:726:ALA:HB2	2.54	0.43
1:B:506:ASN:HB2	1:B:537:PRO:O	2.19	0.43
1:E:289:SER:HA	1:E:314:VAL:HG22	2.00	0.43
1:F:382:ASN:ND2	1:F:435:LEU:O	2.52	0.43
1:B:397:ARG:NH1	1:B:455:LYS:HD2	2.33	0.43
1:D:460:CYS:HA	1:D:486:ALA:O	2.19	0.43
1:F:590:LEU:HD21	1:F:596:ILE:HG23	2.00	0.43
1:A:257:ASN:HD21	1:A:261:VAL:HG23	1.83	0.42
1:B:210:LYS:HB3	1:B:230:VAL:HG12	2.00	0.42
1:B:460:CYS:HA	1:B:486:ALA:O	2.19	0.42
1:C:357:GLU:HG3	1:C:386:SER:HB3	2.00	0.42
1:A:479:GLU:HA	1:A:504:GLU:O	2.18	0.42
1:B:447:THR:HB	1:B:449:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:TYR:CE1	1:B:445:ALA:HB2	2.54	0.42
1:B:665:VAL:HG11	1:B:716:TRP:CH2	2.54	0.42
1:F:310:PHE:O	1:F:312:LEU:HD13	2.20	0.42
1:B:246:PHE:HB3	1:B:265:TRP:HB3	2.00	0.42
1:D:207:MSE:HB2	1:F:212:VAL:H	1.85	0.42
1:D:245:HIS:HB2	1:D:268:GLN:HB2	2.01	0.42
1:F:563:ILE:HG22	1:F:591:ALA:HB3	2.01	0.42
1:A:459:ASP:HA	1:A:484:THR:OG1	2.20	0.42
1:F:447:THR:HB	1:F:449:TYR:HE2	1.83	0.42
1:A:371:GLY:HA3	1:A:424:THR:O	2.19	0.42
1:B:635:ASN:OD1	1:B:735:ARG:NH1	2.53	0.42
1:C:408:ILE:HA	1:C:444:ASN:O	2.19	0.42
1:D:445:ALA:HB2	1:F:502:TYR:CE1	2.55	0.42
1:B:479:GLU:HA	1:B:504:GLU:O	2.20	0.42
1:E:305:LYS:HG2	1:E:306:LEU:N	2.33	0.42
1:A:296:VAL:HG13	1:A:324:LEU:HD13	2.02	0.42
1:A:540:VAL:C	1:A:564:SER:HB2	2.44	0.42
1:D:612:SER:HA	1:E:617:ALA:O	2.20	0.42
1:E:502:TYR:CE2	1:F:445:ALA:HB2	2.55	0.42
1:F:438:VAL:HG22	1:F:466:SER:HA	2.01	0.42
1:D:261:VAL:HG22	1:D:266:VAL:HG13	2.01	0.41
1:F:513:ILE:HD13	1:F:527:ILE:HD13	2.00	0.41
1:B:487:LEU:HD11	1:B:506:ASN:ND2	2.35	0.41
1:E:311:ASP:HB3	4:E:826:HOH:O	2.20	0.41
1:E:479:GLU:HA	1:E:504:GLU:O	2.20	0.41
1:C:487:LEU:HD11	1:C:506:ASN:ND2	2.35	0.41
1:E:502:TYR:OH	1:F:444:ASN:HB3	2.20	0.41
1:A:511:TYR:HA	1:A:541:ALA:O	2.20	0.41
1:B:216:LYS:HE3	1:B:258:GLY:HA2	2.03	0.41
1:B:220:GLU:HB2	1:B:263:ASN:HD22	1.86	0.41
1:E:487:LEU:HD11	1:E:506:ASN:ND2	2.36	0.41
1:E:516:LEU:HD23	1:E:546:THR:HG21	2.03	0.41
1:E:683:GLU:OE2	1:F:662:ARG:NE	2.53	0.41
1:E:350:VAL:HB	1:E:379:SER:HA	2.03	0.41
1:C:603:THR:C	1:C:605:PRO:HD3	2.46	0.41
1:C:515:THR:HG23	4:C:906:HOH:O	2.20	0.41
1:D:308:VAL:HG12	1:D:337:ARG:HD2	2.03	0.41
1:A:212:VAL:HG21	1:B:207:MSE:HE2	2.03	0.41
1:A:528:LYS:NZ	1:C:556:GLU:OE2	2.45	0.41
1:B:511:TYR:CD1	1:B:544:LYS:HB2	2.56	0.41
1:E:305:LYS:HE2	1:E:325:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ALA:HB2	1:C:502:TYR:CE1	2.55	0.40
1:A:716:TRP:CZ3	1:A:726:ALA:HB2	2.56	0.40
1:D:525:PRO:HG3	1:F:559:TYR:HB2	2.02	0.40
1:E:372:GLY:O	1:E:427:ILE:HD12	2.21	0.40
1:C:452:ILE:HG21	1:C:454:ARG:NH1	2.35	0.40
1:D:444:ASN:HB3	1:F:502:TYR:OH	2.21	0.40
1:D:455:LYS:HE3	1:D:480:GLN:HB3	2.02	0.40
1:D:478:LEU:O	1:D:503:ILE:HA	2.21	0.40
1:A:452:ILE:HG21	1:A:454:ARG:NH1	2.36	0.40
1:A:497:MSE:SE	1:C:530:GLN:HG2	2.71	0.40
1:C:460:CYS:HA	1:C:486:ALA:O	2.20	0.40
1:D:487:LEU:HD11	1:D:506:ASN:ND2	2.37	0.40
1:E:685:LEU:HD23	1:E:685:LEU:HA	1.95	0.40
1:F:511:TYR:CD1	1:F:544:LYS:HB2	2.56	0.40
1:B:534:MSE:HE3	1:B:558:CYS:SG	2.61	0.40
1:D:329:ASP:O	1:E:305:LYS:N	2.52	0.40
1:D:662:ARG:NH1	1:F:662:ARG:HH21	2.19	0.40
1:E:242:GLY:O	4:E:801:HOH:O	2.22	0.40
1:B:530:GLN:HG2	1:C:497:MSE:SE	2.71	0.40
1:C:513:ILE:HD13	1:C:527:ILE:HD13	2.03	0.40
1:C:515:THR:HG21	1:C:551:PRO:HG3	2.04	0.40
1:F:261:VAL:HG13	1:F:266:VAL:HG22	2.03	0.40
1:F:479:GLU:HA	1:F:504:GLU:O	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	542/554 (98%)	521 (96%)	20 (4%)	1 (0%)	43 68
1	B	541/554 (98%)	521 (96%)	19 (4%)	1 (0%)	43 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	542/554 (98%)	522 (96%)	19 (4%)	1 (0%)	43	68
1	D	542/554 (98%)	521 (96%)	20 (4%)	1 (0%)	43	68
1	E	542/554 (98%)	519 (96%)	21 (4%)	2 (0%)	30	54
1	F	542/554 (98%)	520 (96%)	20 (4%)	2 (0%)	30	54
All	All	3251/3324 (98%)	3124 (96%)	119 (4%)	8 (0%)	43	68

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	B	333	VAL
1	C	333	VAL
1	D	333	VAL
1	E	333	VAL
1	F	333	VAL
1	E	358	SER
1	F	358	SER

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	438/435 (101%)	427 (98%)	11 (2%)	42	71
1	B	437/435 (100%)	425 (97%)	12 (3%)	39	69
1	C	438/435 (101%)	428 (98%)	10 (2%)	44	73
1	D	438/435 (101%)	426 (97%)	12 (3%)	39	69
1	E	438/435 (101%)	427 (98%)	11 (2%)	42	71
1	F	438/435 (101%)	425 (97%)	13 (3%)	36	66
All	All	2627/2610 (101%)	2558 (97%)	69 (3%)	40	70

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	VAL
1	A	261	VAL
1	A	266	VAL
1	A	273	VAL
1	A	276	VAL
1	A	318	THR
1	A	384	TYR
1	A	424	THR
1	A	447	THR
1	A	507	THR
1	A	589	THR
1	B	261	VAL
1	B	266	VAL
1	B	276	VAL
1	B	316	THR
1	B	318	THR
1	B	384	TYR
1	B	447	THR
1	B	449	TYR
1	B	494	SER
1	B	507	THR
1	B	540	VAL
1	B	589	THR
1	C	212	VAL
1	C	273	VAL
1	C	340	THR
1	C	384	TYR
1	C	427	ILE
1	C	447	THR
1	C	494	SER
1	C	507	THR
1	C	540	VAL
1	C	601	THR
1	D	259	VAL
1	D	266	VAL
1	D	312	LEU
1	D	340	THR
1	D	380	THR
1	D	384	TYR
1	D	437	VAL
1	D	484	THR
1	D	540	VAL
1	D	546	THR

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Mol	Chain	Res	Type
1	D	547	MSE
1	D	589	THR
1	E	273	VAL
1	E	275	THR
1	E	314	VAL
1	E	316	THR
1	E	318	THR
1	E	384	TYR
1	E	421	MSE
1	E	427	ILE
1	E	437	VAL
1	E	494	SER
1	E	601	THR
1	F	261	VAL
1	F	275	THR
1	F	296	VAL
1	F	312	LEU
1	F	314	VAL
1	F	316	THR
1	F	340	THR
1	F	359	SER
1	F	384	TYR
1	F	447	THR
1	F	449	TYR
1	F	484	THR
1	F	570	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	745	ASN
1	B	666	ASN
1	B	697	GLN
1	C	214	ASN
1	C	387	GLN
1	C	587	HIS
1	C	666	ASN
1	C	745	ASN
1	D	450	ASN
1	D	587	HIS
1	D	622	ASN

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Mol	Chain	Res	Type
1	D	635	ASN
1	E	587	HIS
1	F	535	ASN
1	F	587	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	533/554 (96%)	-0.16	2 (0%) 88 87	29, 42, 68, 180	0
1	B	532/554 (96%)	-0.11	0 100 100	29, 44, 77, 112	0
1	C	533/554 (96%)	-0.18	0 100 100	29, 41, 75, 96	0
1	D	533/554 (96%)	0.30	21 (3%) 43 39	33, 71, 135, 207	0
1	E	533/554 (96%)	0.48	27 (5%) 33 29	29, 81, 135, 190	0
1	F	533/554 (96%)	0.44	19 (3%) 46 42	32, 81, 135, 186	0
All	All	3197/3324 (96%)	0.13	69 (2%) 62 59	29, 50, 124, 207	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	5.3
1	F	206	LEU	4.5
1	E	206	LEU	4.3
1	D	206	LEU	4.2
1	D	242	GLY	4.1
1	E	259	VAL	4.1
1	D	212	VAL	4.0
1	F	242	GLY	3.6
1	D	272	GLY	3.2
1	D	273	VAL	3.1
1	F	209	LEU	3.1
1	E	229	VAL	3.1
1	E	366	PHE	3.1
1	E	212	VAL	3.1
1	E	211	GLY	3.0
1	E	231	LEU	3.0
1	F	259	VAL	3.0
1	E	230	VAL	2.9
1	F	254	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	209	LEU	2.8
1	F	353	GLY	2.7
1	F	251	THR	2.7
1	E	453	PHE	2.7
1	F	262	ILE	2.7
1	F	231	LEU	2.7
1	E	338	SER	2.6
1	F	354	PHE	2.6
1	D	364	LEU	2.5
1	D	259	VAL	2.5
1	D	310	PHE	2.5
1	D	267	LYS	2.5
1	E	278	ALA	2.5
1	E	306	LEU	2.4
1	E	320	LEU	2.4
1	E	254	LEU	2.4
1	F	265	TRP	2.4
1	F	220	GLU	2.4
1	F	229	VAL	2.4
1	E	294	LEU	2.3
1	D	255	ILE	2.3
1	D	261	VAL	2.3
1	D	231	LEU	2.3
1	E	395	PHE	2.3
1	F	276	VAL	2.2
1	F	246	PHE	2.2
1	E	225	SER	2.2
1	E	258	GLY	2.2
1	D	438	VAL	2.2
1	F	339	ILE	2.2
1	D	251	THR	2.2
1	E	226	ASP	2.2
1	D	213	VAL	2.2
1	D	250	SER	2.2
1	F	217	VAL	2.2
1	A	222	LEU	2.1
1	F	211	GLY	2.1
1	E	233	THR	2.1
1	D	219	LEU	2.1
1	D	229	VAL	2.1
1	E	348	PHE	2.1
1	D	274	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	535	ASN	2.0
1	D	248	TYR	2.0
1	E	279	CYS	2.0
1	E	215	SER	2.0
1	E	262	ILE	2.0
1	E	272	GLY	2.0
1	F	347	ILE	2.0
1	E	266	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](#)

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
3	NA	B	801	1/1	0.77	0.17	55,55,55,55	0
3	NA	D	801	1/1	0.78	0.09	50,50,50,50	0
2	CL	C	802	1/1	0.81	0.15	94,94,94,94	0
2	CL	F	801	1/1	0.86	0.16	71,71,71,71	0
2	CL	A	801	1/1	0.89	0.12	58,58,58,58	0
3	NA	C	801	1/1	0.96	0.18	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.