



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:42 PM UTC

PDB ID : 4OJ6 / pdb_00004oj6
Title : Crystal Structure of a Putative Tailspike Protein (TSP1, orf210) from Escherichia coli O157:H7 Bacteriophage CBA120; Se-Met Protein
Authors : Chen, C.; Herzberg, O.
Deposited on : 2014-01-20
Resolution : 1.80 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

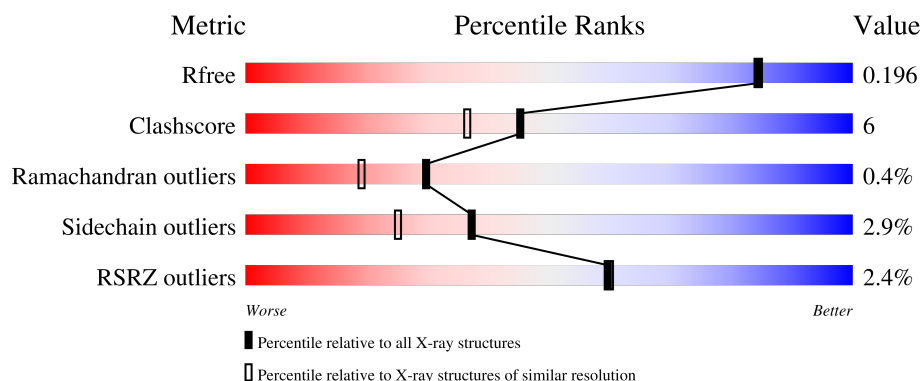
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

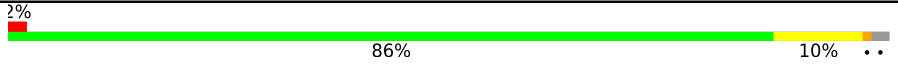
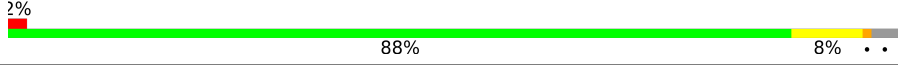
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	776	
1	B	776	
1	C	776	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35715 atoms, of which 16487 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	758	Total	C	H	N	O	S	Se	8	0	0
			11158	3563	5517	944	1115	9	10			
1	B	756	Total	C	H	N	O	S	Se	0	0	0
			11112	3550	5488	941	1115	8	10			
1	C	753	Total	C	H	N	O	S	Se	3	0	0
			11082	3532	5482	940	1110	9	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	771	HIS	-	expression tag	UNP G3M189
A	772	HIS	-	expression tag	UNP G3M189
A	773	HIS	-	expression tag	UNP G3M189
A	774	HIS	-	expression tag	UNP G3M189
A	775	HIS	-	expression tag	UNP G3M189
A	776	HIS	-	expression tag	UNP G3M189
B	771	HIS	-	expression tag	UNP G3M189
B	772	HIS	-	expression tag	UNP G3M189
B	773	HIS	-	expression tag	UNP G3M189
B	774	HIS	-	expression tag	UNP G3M189
B	775	HIS	-	expression tag	UNP G3M189
B	776	HIS	-	expression tag	UNP G3M189
C	771	HIS	-	expression tag	UNP G3M189
C	772	HIS	-	expression tag	UNP G3M189
C	773	HIS	-	expression tag	UNP G3M189
C	774	HIS	-	expression tag	UNP G3M189
C	775	HIS	-	expression tag	UNP G3M189
C	776	HIS	-	expression tag	UNP G3M189

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	1

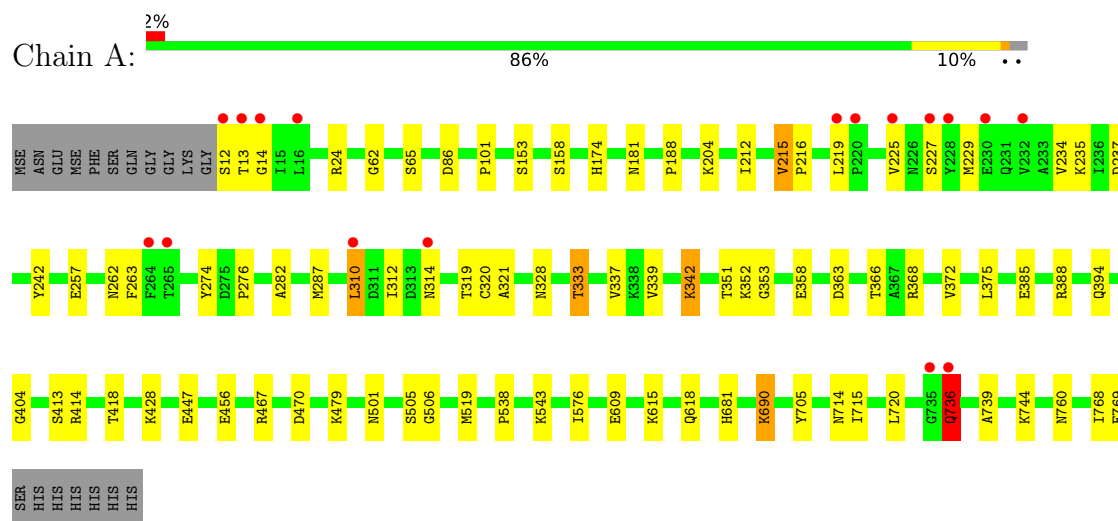
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	707	Total 707	O 707	0	0
3	B	828	Total 828	O 828	0	1
3	C	827	Total 827	O 827	0	0

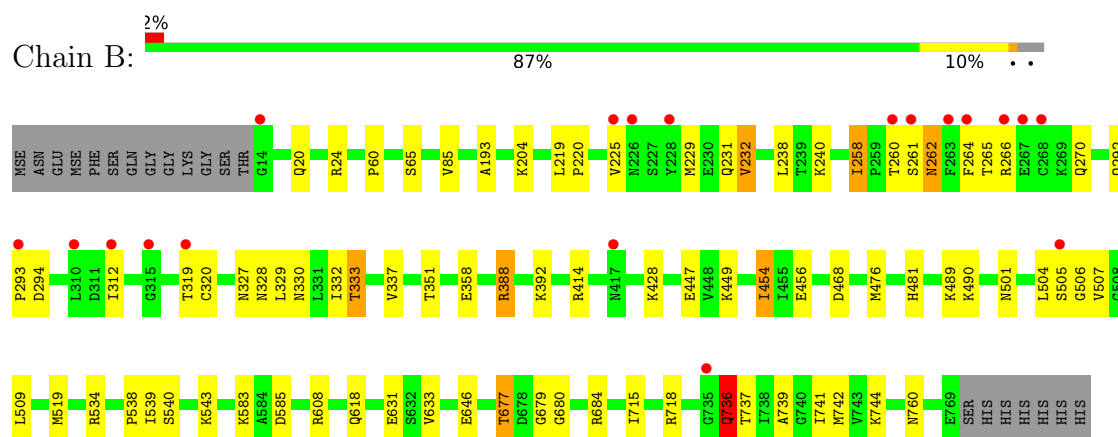
3 Residue-property plots

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.

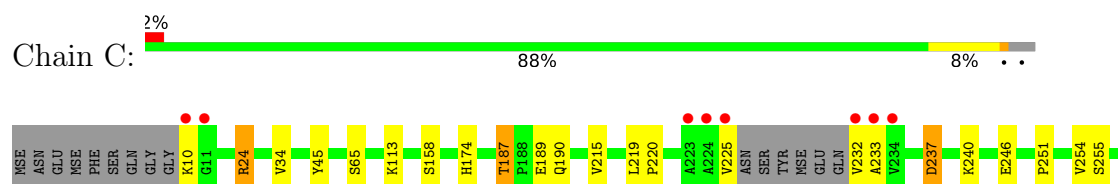
• Molecule 1: Tailspike protein

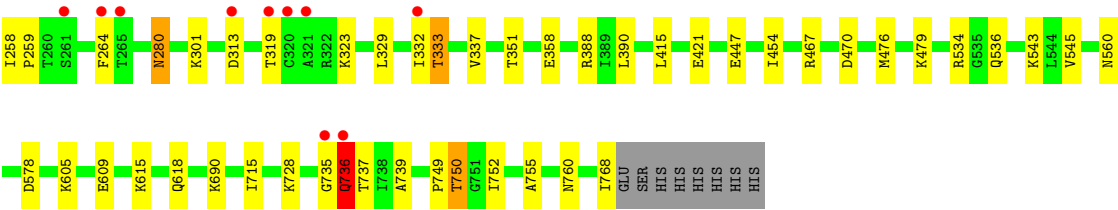


• Molecule 1: Tailspike protein



• 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	123.30Å 153.09Å 171.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 1.80 19.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.85-1.80) 99.6 (19.85-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.187 , 0.209 (Not available) , 0.196	Depositor DCC
R_{free} test set	14894 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35715	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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:
ZN

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	0.42	0/5735	0.81	4/7784 (0.1%)
1	B	0.49	0/5718	0.81	1/7761 (0.0%)
1	C	0.48	0/5692	0.80	2/7726 (0.0%)
All	All	0.47	0/17145	0.80	7/23271 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLY	N-CA-C	-7.75	102.23	113.86
1	A	13	THR	N-CA-C	-6.25	105.30	113.17
1	C	736	GLN	N-CA-C	6.06	123.70	110.80
1	A	736	GLN	N-CA-C	5.79	123.13	110.80
1	B	736	GLN	N-CA-C	5.75	123.05	110.80
1	C	545	VAL	N-CA-C	5.69	115.86	108.35
1	A	576	ILE	CB-CA-C	-5.17	105.03	111.08

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	5641	5517	5576	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5624	5488	5547	77	1
1	C	5600	5482	5536	64	0
2	B	1	0	0	0	0
3	A	707	0	0	32	1
3	B	828	0	0	39	1
3	C	827	0	0	37	1
All	All	19228	16487	16659	199	2

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 6.

All (199) 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:B:264:PHE:CE1	3:B:1572:HOH:O	1.77	1.27
1:C:313:ASP:HA	3:C:1595:HOH:O	1.30	1.25
1:B:330:ASN:HB3	3:B:1637:HOH:O	1.09	1.23
1:B:320:CYS:SG	3:B:1666:HOH:O	2.00	1.19
1:C:237:ASP:HB3	3:C:1521:HOH:O	1.42	1.15
1:C:237:ASP:CB	3:C:1521:HOH:O	1.93	1.15
1:B:490:LYS:NZ	3:B:1656:HOH:O	1.80	1.14
1:B:456:GLU:CD	3:B:1687:HOH:O	1.91	1.10
1:C:618:GLN:HG3	3:C:1540:HOH:O	1.56	1.06
1:B:505:SER:HA	3:B:1625:HOH:O	1.56	1.05
1:B:534:ARG:NE	3:B:1650:HOH:O	1.94	1.00
1:C:237:ASP:CG	3:C:1521:HOH:O	2.00	1.00
1:C:237:ASP:OD2	3:C:1521:HOH:O	1.80	0.98
1:A:319:THR:OG1	3:A:1402:HOH:O	1.84	0.93
1:A:543:LYS:HE3	3:A:1504:HOH:O	1.67	0.93
1:C:280:ASN:ND2	3:C:1498:HOH:O	1.97	0.93
1:B:506:GLY:O	3:B:1629:HOH:O	1.86	0.92
1:C:313:ASP:O	3:C:1595:HOH:O	1.89	0.91
1:A:681:HIS:HD2	1:A:705:TYR:H	1.19	0.90
1:C:728:LYS:NZ	1:C:755:ALA:O	2.06	0.89
1:B:501:ASN:CG	3:B:1623:HOH:O	2.16	0.87
1:A:319:THR:CB	3:A:1402:HOH:O	2.24	0.86
1:B:65:SER:O	3:B:1480:HOH:O	1.94	0.85
1:A:609:GLU:OE1	3:A:1418:HOH:O	1.94	0.85
1:B:270:GLN:OE1	1:C:233:ALA:N	2.08	0.84
1:B:540:SER:HB2	3:B:1681:HOH:O	1.77	0.84
1:A:227:SER:OG	3:A:1340:HOH:O	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LYS:NZ	3:A:1430:HOH:O	2.11	0.82
1:B:332:ILE:HD12	1:B:358:GLU:HB2	1.61	0.82
1:C:332:ILE:HD12	1:C:358:GLU:HB2	1.60	0.82
1:B:264:PHE:HE1	3:B:1572:HOH:O	1.31	0.81
1:B:456:GLU:OE1	3:B:1687:HOH:O	1.90	0.81
1:C:264:PHE:CB	3:C:1580:HOH:O	2.28	0.81
1:C:313:ASP:CA	3:C:1595:HOH:O	2.02	0.81
1:B:677:THR:HG23	1:B:679:GLY:H	1.45	0.79
1:C:113:LYS:NZ	3:C:1569:HOH:O	2.02	0.79
1:C:264:PHE:CA	3:C:1580:HOH:O	2.30	0.79
1:B:583:LYS:HE3	3:B:1727:HOH:O	1.82	0.78
1:B:229:MSE:HG3	3:B:1666:HOH:O	1.85	0.76
1:B:504:LEU:O	3:B:1625:HOH:O	2.02	0.76
1:C:736:GLN:HA	1:C:760:ASN:O	1.86	0.75
1:B:265:THR:O	3:B:1467:HOH:O	2.05	0.74
1:B:481:HIS:CE1	1:B:507:VAL:HG21	2.23	0.73
1:A:229:MSE:HE1	3:A:1402:HOH:O	1.88	0.73
1:C:390:LEU:HD21	1:C:415:LEU:HD13	1.70	0.73
1:C:174:HIS:NE2	3:C:1617:HOH:O	2.21	0.72
1:A:505:SER:N	3:A:1399:HOH:O	1.87	0.71
1:A:769:GLU:HB3	3:A:1475:HOH:O	1.90	0.71
1:B:392:LYS:O	1:B:414:ARG:NH1	2.24	0.71
1:B:468:ASP:OD2	3:B:1474:HOH:O	2.08	0.71
1:C:768:ILE:C	3:C:1504:HOH:O	2.34	0.71
1:B:24:ARG:NH2	3:B:1064:HOH:O	2.23	0.70
1:B:540:SER:CB	3:B:1681:HOH:O	2.38	0.70
1:B:501:ASN:OD1	3:B:1623:HOH:O	2.10	0.69
1:C:543:LYS:HE3	3:C:1501:HOH:O	1.93	0.68
1:A:86:ASP:CB	3:A:1428:HOH:O	2.41	0.68
1:B:677:THR:HG21	1:B:680:GLY:O	1.93	0.68
1:C:447:GLU:HG2	1:C:476:MSE:HE2	1.74	0.68
1:B:456:GLU:CG	3:B:1687:HOH:O	2.30	0.67
1:C:259:PRO:O	3:C:1544:HOH:O	2.13	0.67
1:A:319:THR:HB	3:A:1402:HOH:O	1.90	0.67
1:A:609:GLU:HB3	3:A:1418:HOH:O	1.96	0.66
1:C:255:SER:OG	3:C:1537:HOH:O	2.13	0.66
1:A:618:GLN:HG3	3:A:1394:HOH:O	1.96	0.65
1:C:479:LYS:HE3	3:C:1518:HOH:O	1.95	0.65
1:B:264:PHE:CD1	3:B:1572:HOH:O	2.18	0.64
1:C:333:THR:HG23	1:C:337:VAL:HB	1.79	0.62
1:B:736:GLN:HA	1:B:760:ASN:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:GLU:HG2	1:B:476:MSE:HE2	1.80	0.62
1:C:618:GLN:CG	3:C:1540:HOH:O	2.27	0.62
1:A:181:ASN:O	1:C:187:THR:HG21	2.01	0.61
1:A:229:MSE:CE	3:A:1402:HOH:O	2.47	0.61
1:A:414:ARG:NH2	1:A:418:THR:O	2.34	0.60
1:C:232:VAL:HB	3:C:1541:HOH:O	2.00	0.60
1:B:585:ASP:OD2	3:B:1725:HOH:O	2.16	0.60
1:C:264:PHE:HA	3:C:1580:HOH:O	1.96	0.59
1:B:583:LYS:HE3	3:B:1667:HOH:O	2.01	0.59
1:A:769:GLU:HG2	3:A:1232:HOH:O	2.02	0.59
1:B:238:LEU:HB2	1:B:258:ILE:HD13	1.83	0.59
1:A:768:ILE:HG22	1:A:769:GLU:HG3	1.85	0.59
1:C:421:GLU:OE2	3:C:1610:HOH:O	2.17	0.58
1:C:690:LYS:NZ	3:C:1288:HOH:O	2.22	0.58
1:A:385:GLU:CG	3:A:1404:HOH:O	2.51	0.58
1:A:310:LEU:HD22	1:A:314:ASN:HD21	1.69	0.58
1:A:681:HIS:CD2	1:A:705:TYR:H	2.11	0.57
1:A:736:GLN:HA	1:A:760:ASN:O	2.04	0.57
1:A:385:GLU:HG2	3:A:1404:HOH:O	2.03	0.57
1:A:506:GLY:O	3:A:907:HOH:O	2.17	0.57
1:A:62:GLY:N	3:A:1454:HOH:O	2.14	0.56
1:A:86:ASP:HB3	3:A:1428:HOH:O	2.04	0.56
1:B:261:SER:HB2	1:B:328:ASN:ND2	2.21	0.56
1:B:519:MSE:HE1	1:B:538:PRO:HG2	1.87	0.56
1:B:742:MSE:HE3	1:B:744:LYS:HD3	1.88	0.56
1:B:60:PRO:HG3	1:B:85:VAL:HG21	1.87	0.56
1:C:187:THR:HG23	1:C:189:GLU:H	1.71	0.56
1:A:263:PHE:HD2	1:A:388:ARG:HE	1.55	0.55
1:A:505:SER:CA	3:A:1399:HOH:O	2.45	0.55
1:B:583:LYS:CE	3:B:1667:HOH:O	2.55	0.55
1:B:742:MSE:CE	1:B:744:LYS:HB2	2.37	0.55
1:B:677:THR:CG2	1:B:679:GLY:H	2.17	0.54
1:C:715:ILE:O	1:C:739:ALA:HA	2.07	0.54
3:A:1406:HOH:O	1:B:449:LYS:HB2	2.07	0.53
1:B:258:ILE:HG13	1:B:329:LEU:HA	1.90	0.53
1:C:24:ARG:NH2	3:C:962:HOH:O	2.42	0.53
1:A:744:LYS:HD2	1:B:736:GLN:HG2	1.89	0.53
1:B:715:ILE:O	1:B:739:ALA:HA	2.09	0.53
1:A:358:GLU:OE1	1:A:368:ARG:HD3	2.09	0.52
1:A:519:MSE:HE1	1:A:538:PRO:HG2	1.91	0.52
1:C:479:LYS:CE	3:C:1518:HOH:O	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLN:NE2	3:B:1688:HOH:O	2.42	0.52
1:B:260:THR:HG21	1:C:323:LYS:C	2.35	0.52
1:B:333:THR:HG23	1:B:337:VAL:HB	1.90	0.51
1:B:454:ILE:HG13	3:B:1649:HOH:O	2.10	0.51
1:C:609:GLU:HB3	3:C:1001:HOH:O	2.11	0.51
1:B:20:GLN:NE2	3:B:1693:HOH:O	2.42	0.51
1:B:261:SER:HB2	1:B:328:ASN:HD22	1.76	0.51
1:A:219:LEU:HD12	1:A:225:VAL:HG12	1.94	0.50
1:A:404:GLY:HA3	1:C:454:ILE:HD11	1.94	0.50
1:A:467:ARG:HD2	1:A:470:ASP:OD1	2.11	0.49
1:B:742:MSE:HE1	1:C:736:GLN:HB3	1.93	0.49
1:B:742:MSE:HE1	1:C:736:GLN:CB	2.43	0.49
1:A:153:SER:HB3	1:A:158:SER:OG	2.13	0.49
1:B:583:LYS:CE	3:B:1727:HOH:O	2.49	0.49
1:B:742:MSE:HE3	1:B:744:LYS:HB2	1.92	0.49
1:B:219:LEU:HD12	1:B:225:VAL:HG12	1.95	0.49
1:B:232:VAL:HG13	3:B:1369:HOH:O	2.14	0.48
1:C:219:LEU:HD13	1:C:225:VAL:CA	2.43	0.48
1:A:282:ALA:HA	1:A:339:VAL:O	2.14	0.48
1:A:310:LEU:HD22	1:A:314:ASN:ND2	2.29	0.48
1:B:583:LYS:NZ	3:B:1667:HOH:O	2.43	0.48
1:B:447:GLU:HB3	3:B:1616:HOH:O	2.13	0.47
1:B:618:GLN:HG3	3:B:1135:HOH:O	2.13	0.47
1:A:215:VAL:HG21	1:A:287:MSE:SE	2.64	0.47
1:B:631:GLU:HG2	1:B:633:VAL:HG12	1.97	0.47
1:A:204:LYS:HD3	3:A:890:HOH:O	2.13	0.47
1:A:715:ILE:O	1:A:739:ALA:HA	2.15	0.47
1:C:187:THR:HG22	1:C:190:GLN:H	1.80	0.47
1:A:229:MSE:HE3	1:A:321:ALA:H	1.80	0.47
1:A:86:ASP:CG	3:A:1428:HOH:O	2.58	0.46
1:A:342:LYS:HD2	1:A:375:LEU:HD23	1.97	0.46
1:A:506:GLY:N	3:A:1399:HOH:O	2.48	0.46
1:C:24:ARG:HA	1:C:24:ARG:HD3	1.65	0.46
1:B:501:ASN:CB	3:B:1623:HOH:O	2.59	0.46
1:C:479:LYS:NZ	3:C:1215:HOH:O	2.49	0.46
1:B:543:LYS:NZ	3:B:1642:HOH:O	2.47	0.46
1:C:615:LYS:NZ	3:C:967:HOH:O	2.36	0.46
1:A:235:LYS:HD3	1:A:257:GLU:OE2	2.16	0.45
1:C:174:HIS:CD2	3:C:1617:HOH:O	2.64	0.45
1:B:264:PHE:CZ	1:B:388:ARG:HB3	2.51	0.45
1:A:24:ARG:NH2	3:A:842:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASN:ND2	3:A:1410:HOH:O	2.50	0.45
1:B:539:ILE:HG12	3:B:1629:HOH:O	2.16	0.45
1:C:750:THR:HG23	3:C:1389:HOH:O	2.17	0.45
1:A:229:MSE:HE3	1:A:321:ALA:N	2.32	0.44
1:A:690:LYS:HE2	1:A:714:ASN:CG	2.43	0.44
1:C:467:ARG:HD2	1:C:470:ASP:OD1	2.17	0.44
1:C:333:THR:CG2	1:C:337:VAL:HB	2.48	0.44
1:B:489:LYS:HE3	1:B:509:LEU:HD21	1.99	0.44
1:A:609:GLU:CB	3:A:1418:HOH:O	2.59	0.43
1:B:262:ASN:HA	1:C:323:LYS:HG2	1.99	0.43
1:B:330:ASN:CB	3:B:1637:HOH:O	1.96	0.43
1:A:385:GLU:CD	3:A:1404:HOH:O	2.62	0.43
1:B:193:ALA:HA	1:B:204:LYS:HD3	2.00	0.43
1:C:578:ASP:CG	3:C:1627:HOH:O	2.62	0.43
1:B:742:MSE:HE1	1:C:736:GLN:HG2	2.01	0.43
1:A:229:MSE:HE3	1:A:320:CYS:HA	2.01	0.43
1:B:742:MSE:HE1	1:C:736:GLN:CG	2.49	0.43
1:B:238:LEU:HB2	1:B:258:ILE:CD1	2.49	0.43
1:A:212:ILE:HD12	1:A:234:VAL:HB	2.01	0.42
1:C:246:GLU:CD	3:C:1584:HOH:O	2.62	0.42
1:A:328:ASN:HA	1:A:353:GLY:O	2.20	0.42
1:A:215:VAL:HA	1:A:216:PRO:HD3	1.93	0.42
1:A:363:ASP:O	1:A:366:THR:HG22	2.19	0.42
1:A:681:HIS:HE1	3:A:1139:HOH:O	2.02	0.42
1:C:258:ILE:HD12	1:C:329:LEU:HA	2.01	0.42
1:A:744:LYS:NZ	3:A:1507:HOH:O	2.42	0.42
1:A:372:VAL:HA	1:A:394:GLN:O	2.20	0.42
1:C:536:GLN:HA	1:C:560:ASN:HB3	2.02	0.42
1:A:188:PRO:HG2	1:A:242:TYR:CZ	2.55	0.41
1:C:301:LYS:HG3	3:C:1379:HOH:O	2.18	0.41
1:A:174:HIS:HE1	3:C:1266:HOH:O	2.03	0.41
1:C:219:LEU:HA	1:C:220:PRO:HD3	1.89	0.41
1:B:718:ARG:HD3	3:C:812:HOH:O	2.18	0.41
1:A:333:THR:HG23	1:A:337:VAL:HB	2.01	0.41
1:B:270:GLN:OE1	1:C:232:VAL:HA	2.20	0.41
1:C:534:ARG:NH2	3:C:1172:HOH:O	2.52	0.41
1:C:251:PRO:HD2	1:C:254:VAL:HG21	2.01	0.41
1:A:413:SER:HB2	1:A:456:GLU:HB2	2.03	0.41
1:A:274:TYR:CE2	1:A:276:PRO:HG3	2.55	0.41
1:A:479:LYS:CE	3:A:1441:HOH:O	2.69	0.41
1:A:690:LYS:HE2	1:A:714:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLN:HB3	1:B:293:PRO:HD2	2.04	0.40
1:A:24:ARG:HA	1:A:24:ARG:HD3	1.75	0.40
1:B:742:MSE:HE2	1:B:744:LYS:HB2	2.03	0.40
1:C:749:PRO:HB2	1:C:752:ILE:HG12	2.04	0.40
1:B:219:LEU:HA	1:B:220:PRO:HD3	1.94	0.40
1:C:313:ASP:C	3:C:1595:HOH:O	2.21	0.40
1:A:101:PRO:HB3	3:B:987:HOH:O	2.21	0.40
1:C:34:VAL:HB	1:C:45:TYR:CD1	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1507:HOH:O	3:C:1564:HOH:O[2_585]	2.13	0.07
1:B:684:ARG:HH22	3:B:1090:HOH:O[2_585]	1.57	0.03

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	B	114/776 (15%)	107 (94%)	6 (5%)	1 (1%)	14	5
1	C	563/776 (73%)	540 (96%)	21 (4%)	2 (0%)	30	19
All	All	677/1552 (44%)	647 (96%)	27 (4%)	3 (0%)	30	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	736	GLN
1	C	735	GLY
1	B	266	ARG

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	610/625 (98%)	594 (97%)	16 (3%)	40	28
1	B	608/625 (97%)	589 (97%)	19 (3%)	35	23
1	C	606/625 (97%)	589 (97%)	17 (3%)	38	26
All	All	1824/1875 (97%)	1772 (97%)	52 (3%)	37	25

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	65	SER
1	A	215	VAL
1	A	237	ASP
1	A	310	LEU
1	A	312	ILE
1	A	333	THR
1	A	342	LYS
1	A	351	THR
1	A	428	LYS
1	A	447	GLU
1	A	501	ASN
1	A	615	LYS
1	A	690	LYS
1	A	720	LEU
1	A	736	GLN
1	B	232	VAL
1	B	240	LYS
1	B	258	ILE
1	B	262	ASN
1	B	294	ASP
1	B	312	ILE
1	B	319	THR
1	B	327	ASN
1	B	333	THR
1	B	351	THR

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Mol	Chain	Res	Type
1	B	388	ARG
1	B	428	LYS
1	B	454	ILE
1	B	608	ARG
1	B	646	GLU
1	B	677	THR
1	B	736	GLN
1	B	737	THR
1	B	741	ILE
1	C	10	LYS
1	C	24	ARG
1	C	65	SER
1	C	158	SER
1	C	187	THR
1	C	215	VAL
1	C	237	ASP
1	C	240	LYS
1	C	280	ASN
1	C	319	THR
1	C	333	THR
1	C	351	THR
1	C	388	ARG
1	C	605	LYS
1	C	736	GLN
1	C	737	THR
1	C	750	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	174	HIS
1	A	176	GLN
1	A	314	ASN
1	A	424	GLN
1	A	501	ASN
1	A	681	HIS
1	A	725	ASN
1	B	292	GLN
1	B	314	ASN
1	B	328	ASN
1	B	402	ASN

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Mol	Chain	Res	Type
1	B	692	ASN
1	B	714	ASN
1	C	20	GLN
1	C	165	ASN
1	C	262	ASN
1	C	409	ASN
1	C	501	ASN
1	C	725	ASN

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 1 ligands modelled in this entry, 1 is 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 ⓘ

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	748/776 (96%)	-0.20	17 (2%) 61 61	20, 34, 57, 78	2 (0%)
1	B	746/776 (96%)	-0.39	19 (2%) 58 58	17, 27, 53, 81	0
1	C	744/776 (95%)	-0.37	18 (2%) 59 60	20, 28, 48, 80	0
All	All	2238/2328 (96%)	-0.32	54 (2%) 59 60	17, 30, 52, 81	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	VAL	6.6
1	C	233	ALA	6.6
1	C	320	CYS	5.5
1	C	232	VAL	5.4
1	B	225	VAL	5.0
1	B	264	PHE	4.4
1	A	735	GLY	4.0
1	B	261	SER	3.9
1	A	13	THR	3.8
1	B	735	GLY	3.8
1	B	268	CYS	3.7
1	A	264	PHE	3.4
1	C	735	GLY	3.4
1	B	310	LEU	3.4
1	B	263	PHE	3.3
1	C	234	VAL	3.3
1	C	736	GLN	3.2
1	A	12	SER	3.2
1	C	321	ALA	3.1
1	B	505	SER	3.1
1	B	266	ARG	3.1
1	C	11	GLY	3.0
1	C	319	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	265	THR	2.8
1	A	265	THR	2.7
1	B	260	THR	2.7
1	B	228	TYR	2.6
1	A	14	GLY	2.6
1	A	227	SER	2.6
1	A	225	VAL	2.5
1	A	736	GLN	2.5
1	B	312	ILE	2.5
1	C	261	SER	2.5
1	A	219	LEU	2.4
1	C	224	ALA	2.3
1	A	230	GLU	2.3
1	C	313	ASP	2.3
1	A	314	ASN	2.3
1	C	264	PHE	2.2
1	A	228	TYR	2.2
1	B	267	GLU	2.2
1	A	310	LEU	2.2
1	B	14	GLY	2.2
1	B	315	GLY	2.1
1	A	220	PRO	2.1
1	B	226	ASN	2.1
1	B	319	THR	2.1
1	C	332	ILE	2.1
1	C	10	LYS	2.1
1	A	16	LEU	2.1
1	C	223	ALA	2.0
1	B	417	ASN	2.0
1	B	293	PRO	2.0
1	A	232	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

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
2	ZN	B	800[A]	1/1	0.99	0.02	26,26,26,26	1

6.5 Other polymers

There are no such residues in this entry.