



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:54 AM UTC

PDB ID : 4OJL / pdb_00004ojl
Title : Crystal Structure of Putative Tailspike Protein (TSP1, orf210) from Escherichia coli O157:H7 Bacteriophage CBA120 in Complex with Glucose
Authors : Chen, C.; Herzberg, O.
Deposited on : 2014-01-21
Resolution : 2.00 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

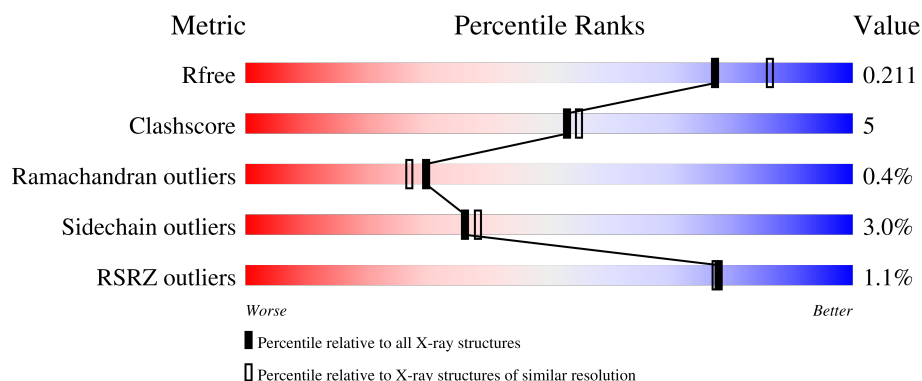
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	% 86% 11% ..
1	B	776	% 85% 10% ..
1	C	776	% 86% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19521 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	758	Total	C	N	O	S	1	0	0
			5673	3577	954	1123	19			
1	B	756	Total	C	N	O	S	0	0	0
			5653	3568	947	1119	19			
1	C	759	Total	C	N	O	S	1	0	0
			5679	3580	958	1122	19			

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 beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	1
			1	1		

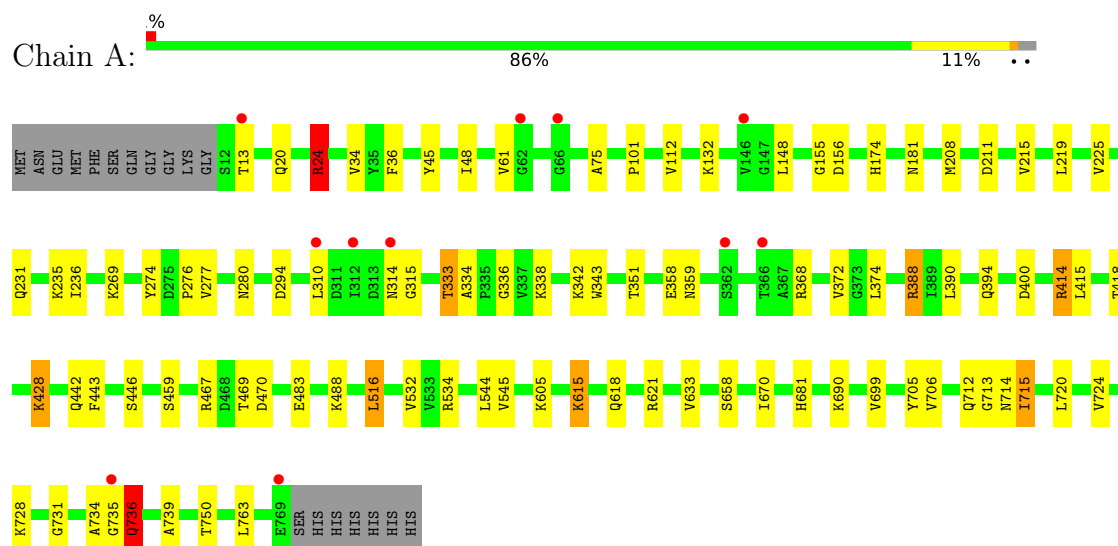
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	756	Total	O	0	0
			756	756		
4	B	841	Total	O	0	0
			841	841		
4	C	870	Total	O	0	0
			870	870		

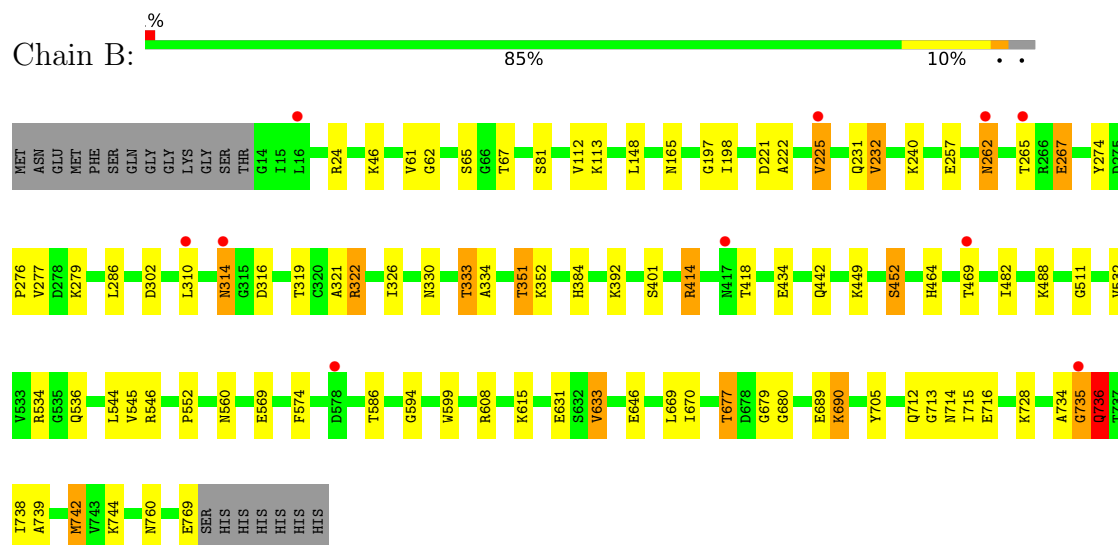
3 Residue-property plots [i](#)

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.

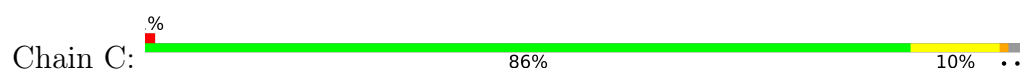
• Molecule 1: Tailspike protein

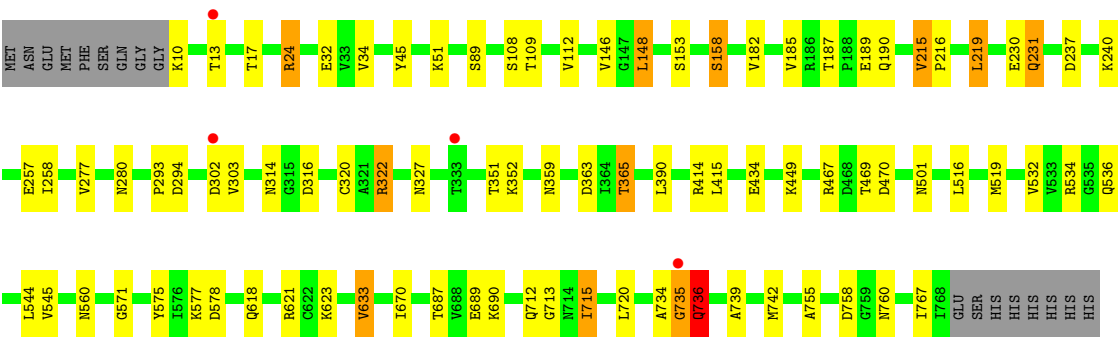


• Molecule 1: Tailspike protein



• 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	123.45Å 152.44Å 171.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.80 – 2.00 43.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (43.80-2.00) 96.2 (43.80-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.178 , 0.211 0.179 , 0.211	Depositor DCC
R_{free} test set	11135 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19521	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: ZN, BGC

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	0.45	0/5777	0.97	22/7854 (0.3%)
1	B	0.49	0/5757	1.00	19/7828 (0.2%)
1	C	0.49	0/5783	0.98	23/7861 (0.3%)
All	All	0.48	0/17317	0.98	64/23543 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	258	ILE	N-CA-C	-9.01	101.80	109.19
1	B	544	LEU	N-CA-C	7.72	119.48	111.14
1	C	544	LEU	N-CA-C	7.27	118.99	111.14
1	A	544	LEU	N-CA-C	6.97	118.76	111.03
1	B	545	VAL	N-CA-C	6.53	117.76	108.42
1	C	734	ALA	N-CA-C	6.53	116.00	108.49
1	A	545	VAL	N-CA-C	6.50	117.71	108.42
1	A	315	GLY	N-CA-C	-6.34	106.97	115.21
1	A	277	VAL	N-CA-C	-6.19	104.71	110.53
1	A	715	ILE	N-CA-C	6.12	117.29	108.48
1	B	65	SER	N-CA-C	-6.10	101.38	110.23
1	A	75	ALA	N-CA-C	-6.09	105.43	112.92
1	C	545	VAL	N-CA-C	6.08	117.11	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	599	TRP	N-CA-C	-6.04	104.27	111.69
1	B	736	GLN	N-CA-C	6.02	123.63	110.80
1	B	198	ILE	CB-CA-C	-6.01	106.60	111.71
1	C	571	GLY	N-CA-C	-6.00	106.15	111.67
1	C	532	VAL	N-CA-C	5.98	117.19	108.58
1	B	469	THR	N-CA-C	5.85	117.34	110.97
1	B	221	ASP	N-CA-C	5.81	115.77	108.45
1	C	736	GLN	N-CA-C	5.75	123.05	110.80
1	B	670	ILE	N-CA-C	5.71	115.81	107.37
1	C	715	ILE	N-CA-C	5.67	116.91	108.46
1	A	736	GLN	N-CA-C	5.67	122.87	110.80
1	A	706	VAL	N-CA-C	-5.59	104.91	111.00
1	C	277	VAL	N-CA-C	-5.58	105.41	110.82
1	B	532	VAL	N-CA-C	5.55	116.22	108.89
1	A	428	LYS	N-CA-C	5.54	113.00	108.07
1	A	155	GLY	N-CA-C	5.53	119.65	112.68
1	C	414	ARG	N-CA-C	-5.53	102.30	110.48
1	C	320	CYS	N-CA-C	-5.49	103.86	110.88
1	C	215	VAL	N-CA-C	5.45	113.87	107.77
1	B	286	LEU	N-CA-C	-5.44	103.51	110.53
1	C	469	THR	N-CA-C	5.43	116.88	111.07
1	C	713	GLY	N-CA-C	5.42	120.90	112.60
1	A	532	VAL	N-CA-C	5.40	116.01	108.89
1	A	469	THR	N-CA-C	5.38	117.22	111.36
1	B	414	ARG	N-CA-C	-5.35	102.56	110.48
1	C	670	ILE	N-CA-C	5.35	115.78	107.28
1	B	734	ALA	N-CA-C	5.34	114.63	108.49
1	A	516	LEU	N-CA-C	5.33	119.89	112.90
1	B	401	SER	N-CA-C	5.32	117.89	109.96
1	A	13	THR	N-CA-C	-5.28	106.34	112.89
1	A	713	GLY	N-CA-C	5.25	121.16	112.66
1	C	755	ALA	CA-C-N	5.23	124.84	119.56
1	C	755	ALA	C-N-CA	5.23	124.84	119.56
1	B	713	GLY	N-CA-C	5.23	120.60	112.60
1	C	219	LEU	CA-C-N	5.21	124.53	118.85
1	C	219	LEU	C-N-CA	5.21	124.53	118.85
1	A	633	VAL	N-CA-C	5.20	117.11	108.99
1	C	182	VAL	N-CA-C	5.19	118.14	113.10
1	A	156	ASP	N-CA-C	5.19	117.34	111.11
1	C	633	VAL	N-CA-C	5.19	116.84	108.85
1	A	443	PHE	N-CA-C	5.15	115.34	108.38
1	A	459	SER	N-CA-C	-5.14	105.59	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	575	TYR	N-CA-C	5.12	119.16	113.01
1	B	586	THR	N-CA-C	5.12	117.79	109.24
1	A	670	ILE	N-CA-C	5.09	115.37	107.28
1	A	338	LYS	N-CA-C	5.08	116.67	111.03
1	C	516	LEU	N-CA-C	5.06	119.72	113.50
1	B	482	ILE	N-CA-C	5.01	115.18	108.17
1	A	414	ARG	N-CA-C	-5.00	103.08	110.48
1	B	452	SER	CA-C-N	-5.00	115.41	120.31
1	B	452	SER	C-N-CA	-5.00	115.41	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	ARG	Sidechain

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	5673	0	5631	51	0
1	B	5653	0	5600	62	0
1	C	5679	0	5641	61	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
2	C	24	0	24	0	0
3	A	1	0	0	0	0
4	A	756	0	0	22	1
4	B	841	0	0	27	3
4	C	870	0	0	38	1
All	All	19521	0	16920	170	3

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 (170) 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:280:ASN:ND2	4:C:1632:HOH:O	1.82	1.09
1:C:690:LYS:NZ	4:C:1739:HOH:O	1.86	1.03
4:A:1615:HOH:O	1:B:690:LYS:HE3	1.58	1.03
1:B:534:ARG:NH1	4:B:1697:HOH:O	1.90	1.02
1:C:314:ASN:ND2	4:C:1701:HOH:O	1.91	1.02
1:C:352:LYS:HE2	4:C:1727:HOH:O	1.58	1.01
1:C:434:GLU:CD	4:C:1760:HOH:O	2.07	0.98
1:B:165:ASN:OD1	4:B:1704:HOH:O	1.81	0.97
1:A:269:LYS:HE2	4:B:1693:HOH:O	1.65	0.96
1:C:294:ASP:OD2	4:C:1697:HOH:O	1.82	0.95
1:C:434:GLU:CG	4:C:1760:HOH:O	2.15	0.95
1:C:434:GLU:HG3	4:C:1760:HOH:O	1.65	0.95
1:A:314:ASN:ND2	4:A:1569:HOH:O	2.01	0.93
1:C:434:GLU:OE1	4:C:1760:HOH:O	1.84	0.92
1:B:677:THR:HG23	1:B:679:GLY:H	1.33	0.92
1:C:280:ASN:CG	4:C:1632:HOH:O	2.11	0.90
1:B:449:LYS:NZ	4:B:1587:HOH:O	2.06	0.89
1:C:148:LEU:HG	4:C:1708:HOH:O	1.71	0.88
1:A:294:ASP:OD1	4:A:1648:HOH:O	1.94	0.85
1:A:294:ASP:CG	4:A:1648:HOH:O	2.18	0.85
1:A:681:HIS:HD2	1:A:705:TYR:H	1.25	0.84
1:C:280:ASN:OD1	4:C:1632:HOH:O	1.97	0.83
1:C:316:ASP:OD1	4:C:1701:HOH:O	1.97	0.81
1:B:546:ARG:NH1	4:B:1724:HOH:O	1.88	0.81
1:B:46:LYS:NZ	4:B:1726:HOH:O	2.13	0.80
1:B:534:ARG:CZ	4:B:1697:HOH:O	2.21	0.80
1:C:578:ASP:OD1	4:C:1710:HOH:O	1.99	0.79
1:C:302:ASP:OD1	4:C:1759:HOH:O	2.00	0.79
1:C:316:ASP:CG	4:C:1701:HOH:O	2.26	0.78
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.52	0.74
1:B:24:ARG:NH2	4:B:1048:HOH:O	2.19	0.74
1:B:279:LYS:HE2	4:B:1590:HOH:O	1.86	0.74
1:A:211:ASP:O	4:A:1624:HOH:O	2.07	0.73
1:C:280:ASN:ND2	4:C:1436:HOH:O	2.21	0.72
1:B:742:MET:HE3	1:B:744:LYS:HB2	1.72	0.71
1:B:488:LYS:NZ	4:B:1605:HOH:O	2.24	0.70
1:B:62:GLY:HA2	4:B:1564:HOH:O	1.92	0.70
1:C:216:PRO:HG2	1:C:219:LEU:HD21	1.76	0.68
1:C:314:ASN:CG	4:C:1701:HOH:O	2.28	0.68
1:A:235:LYS:NZ	4:A:1424:HOH:O	2.27	0.68
1:B:689:GLU:OE1	4:B:1622:HOH:O	2.12	0.67
1:C:24:ARG:NH2	4:C:1056:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:ASP:O	4:C:1758:HOH:O	2.12	0.66
1:B:231:GLN:HB3	4:B:1493:HOH:O	1.94	0.66
1:B:414:ARG:NH2	1:B:418:THR:O	2.29	0.65
1:B:677:THR:HG21	1:B:680:GLY:O	1.96	0.65
1:B:113:LYS:HE3	4:B:1593:HOH:O	1.96	0.64
1:A:534:ARG:CZ	4:B:1697:HOH:O	2.45	0.63
1:B:262:ASN:OD1	1:B:265:THR:OG1	2.07	0.62
1:C:501:ASN:ND2	4:C:1677:HOH:O	2.22	0.61
1:B:769:GLU:O	4:B:1412:HOH:O	2.15	0.60
1:A:181:ASN:O	1:C:187:THR:HG21	2.01	0.60
1:A:618:GLN:HG3	4:A:1507:HOH:O	2.02	0.60
1:C:32:GLU:OE2	4:C:1744:HOH:O	2.16	0.60
1:B:302:ASP:OD2	4:B:1499:HOH:O	2.17	0.58
1:B:314:ASN:ND2	1:B:316:ASP:OD2	2.36	0.58
1:A:280:ASN:OD1	4:A:1586:HOH:O	2.18	0.56
1:C:32:GLU:OE1	4:C:1730:HOH:O	2.17	0.56
1:A:388:ARG:NH2	4:A:1404:HOH:O	2.32	0.56
1:B:712:GLN:HG2	1:B:735:GLY:O	2.06	0.56
1:C:621:ARG:HD3	4:C:1596:HOH:O	2.05	0.56
1:A:467:ARG:HD2	1:A:470:ASP:OD1	2.05	0.56
1:C:736:GLN:HA	1:C:760:ASN:O	2.05	0.56
1:C:467:ARG:HD2	1:C:470:ASP:OD1	2.06	0.55
1:C:293:PRO:HG2	4:C:1536:HOH:O	2.06	0.55
1:C:303:VAL:HG12	4:C:1759:HOH:O	2.06	0.55
1:A:690:LYS:HE3	4:C:1641:HOH:O	2.07	0.55
1:B:677:THR:CG2	1:B:679:GLY:H	2.14	0.54
1:A:488:LYS:NZ	4:A:1565:HOH:O	2.39	0.54
1:B:322:ARG:HH11	1:B:322:ARG:CG	2.20	0.54
1:A:219:LEU:HD12	1:A:225:VAL:HG12	1.88	0.54
1:C:303:VAL:CG1	4:C:1759:HOH:O	2.56	0.54
1:B:267:GLU:HG3	1:C:230:GLU:HB3	1.89	0.54
1:C:153:SER:OG	1:C:158:SER:HB3	2.08	0.53
1:A:333:THR:HG23	1:A:334:ALA:O	2.08	0.53
1:A:414:ARG:NH2	1:A:418:THR:O	2.39	0.53
1:A:681:HIS:CD2	1:A:705:TYR:H	2.16	0.53
1:C:187:THR:HG22	1:C:190:GLN:HG3	1.92	0.52
1:C:13:THR:O	1:C:17:THR:HG23	2.10	0.52
1:A:231:GLN:OE1	4:A:1412:HOH:O	2.19	0.51
1:B:631:GLU:HG2	1:B:633:VAL:HG12	1.92	0.51
1:A:483:GLU:HG2	4:A:1584:HOH:O	2.11	0.50
1:A:605:LYS:NZ	4:A:1403:HOH:O	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:GLN:HA	1:B:760:ASN:O	2.12	0.50
1:C:623:LYS:NZ	4:C:1608:HOH:O	2.45	0.49
4:A:1641:HOH:O	1:B:232:VAL:HG21	2.13	0.49
1:B:351:THR:HG22	1:B:384:HIS:HA	1.95	0.49
1:C:577:LYS:HE2	4:C:1563:HOH:O	2.13	0.49
1:C:302:ASP:HB2	4:C:1729:HOH:O	2.12	0.48
1:B:319:THR:HG22	1:B:321:ALA:H	1.76	0.48
1:A:20:GLN:O	1:A:24:ARG:HG2	2.13	0.48
1:B:714:ASN:HA	1:B:738:ILE:HG13	1.96	0.48
1:C:742:MET:HG3	1:C:767:ILE:HB	1.96	0.48
1:A:336:GLY:HA2	4:A:1516:HOH:O	2.14	0.47
1:B:232:VAL:HG13	4:B:1282:HOH:O	2.14	0.47
1:B:352:LYS:CE	4:C:1592:HOH:O	2.62	0.47
1:A:36:PHE:HB2	1:A:48:ILE:HD11	1.96	0.47
1:B:46:LYS:CE	4:B:1726:HOH:O	2.62	0.47
1:B:552:PRO:HB3	1:B:574:PHE:O	2.15	0.47
1:C:231:GLN:NE2	4:C:1504:HOH:O	2.39	0.47
1:A:488:LYS:HE3	4:A:1565:HOH:O	2.15	0.46
1:B:452:SER:HB3	1:C:449:LYS:HE3	1.97	0.46
1:B:536:GLN:HA	1:B:560:ASN:HB3	1.96	0.46
1:C:32:GLU:CD	4:C:1744:HOH:O	2.58	0.46
1:B:310:LEU:O	1:B:314:ASN:HB2	2.15	0.46
1:A:274:TYR:CE2	1:A:276:PRO:HG3	2.50	0.46
1:A:132:LYS:NZ	4:A:1384:HOH:O	2.49	0.45
1:A:705:TYR:CE2	1:A:731:GLY:HA3	2.51	0.45
1:B:310:LEU:HD23	4:B:1660:HOH:O	2.16	0.45
1:B:67:THR:HG23	1:B:81:SER:HB2	1.97	0.45
1:B:333:THR:HG23	1:B:334:ALA:O	2.16	0.45
1:C:687:THR:OG1	1:C:689:GLU:HG3	2.17	0.45
1:B:314:ASN:HD22	1:B:316:ASP:CG	2.24	0.45
1:B:392:LYS:O	1:B:414:ARG:HD2	2.17	0.45
1:B:434:GLU:OE2	4:B:978:HOH:O	2.21	0.45
1:A:690:LYS:HE2	1:A:714:ASN:OD1	2.17	0.44
1:C:359:ASN:OD1	1:C:415:LEU:HD11	2.18	0.44
1:B:262:ASN:HB3	1:B:330:ASN:OD1	2.18	0.44
1:C:534:ARG:HD3	4:C:1677:HOH:O	2.18	0.44
1:C:712:GLN:HG2	1:C:735:GLY:O	2.18	0.44
1:A:488:LYS:CE	4:A:1565:HOH:O	2.66	0.43
1:A:658:SER:OG	1:A:681:HIS:O	2.29	0.43
4:A:1615:HOH:O	1:B:690:LYS:CE	2.38	0.43
1:C:257:GLU:HA	1:C:327:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ARG:HB3	4:C:1491:HOH:O	2.17	0.43
1:C:108:SER:OG	1:C:109:THR:N	2.51	0.43
1:C:187:THR:OG1	1:C:189:GLU:OE1	2.36	0.43
1:A:615:LYS:HB2	2:A:800:BGC:H6C2	2.01	0.43
1:B:569:GLU:HG3	4:B:1483:HOH:O	2.17	0.43
1:B:442:GLN:O	1:B:464:HIS:HA	2.18	0.43
1:A:358:GLU:OE1	1:A:368:ARG:HD3	2.18	0.43
1:A:715:ILE:O	1:A:739:ALA:HA	2.19	0.43
1:C:363:ASP:OD1	1:C:365:THR:HB	2.19	0.43
1:B:690:LYS:NZ	1:B:716:GLU:OE2	2.52	0.43
1:C:34:VAL:HB	1:C:45:TYR:CD1	2.54	0.43
1:C:618:GLN:HG3	4:C:1747:HOH:O	2.19	0.43
1:B:715:ILE:O	1:B:739:ALA:HA	2.20	0.42
1:A:101:PRO:HB3	4:B:981:HOH:O	2.18	0.42
1:A:621:ARG:NE	4:A:1325:HOH:O	2.51	0.42
1:B:677:THR:HG23	1:B:679:GLY:N	2.16	0.42
1:A:34:VAL:HB	1:A:45:TYR:CD1	2.55	0.42
1:B:274:TYR:CE2	1:B:276:PRO:HG3	2.55	0.42
1:B:594:GLY:C	1:B:608:ARG:HB3	2.45	0.42
1:B:690:LYS:HE2	1:B:714:ASN:OD1	2.20	0.42
1:C:24:ARG:HA	1:C:24:ARG:HD3	1.72	0.42
1:C:215:VAL:HA	1:C:216:PRO:HD2	1.97	0.41
1:A:372:VAL:HA	1:A:394:GLN:O	2.19	0.41
1:B:277:VAL:HG22	4:B:1107:HOH:O	2.19	0.41
1:A:342:LYS:HB3	1:A:342:LYS:HE2	1.89	0.41
1:A:705:TYR:CD1	1:A:728:LYS:HB2	2.54	0.41
1:C:536:GLN:HA	1:C:560:ASN:HB3	2.03	0.41
1:A:359:ASN:OD1	1:A:415:LEU:HD11	2.21	0.41
1:A:534:ARG:HD3	4:A:1109:HOH:O	2.20	0.41
1:A:699:VAL:O	1:A:724:VAL:HA	2.21	0.41
1:B:352:LYS:CE	4:C:1562:HOH:O	2.68	0.41
1:A:174:HIS:HB3	4:A:1620:HOH:O	2.21	0.41
1:B:197:GLY:HA3	4:B:1630:HOH:O	2.20	0.41
1:B:222:ALA:O	1:B:225:VAL:HG23	2.21	0.41
1:B:257:GLU:HG3	4:B:1709:HOH:O	2.20	0.41
1:A:208:MET:HE3	1:A:236:ILE:HD13	2.03	0.41
1:C:519:MET:HE3	1:C:519:MET:HB2	1.91	0.41
1:A:343:TRP:HB2	1:A:374:LEU:HD11	2.03	0.40
1:B:705:TYR:CD1	1:B:728:LYS:HB2	2.56	0.40
1:C:715:ILE:O	1:C:739:ALA:HA	2.20	0.40
1:A:739:ALA:O	1:A:763:LEU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:LEU:HD12	1:C:415:LEU:HA	1.92	0.40
1:A:442:GLN:HG3	1:A:446:SER:HB3	2.03	0.40
1:A:34:VAL:HB	1:A:45:TYR:CG	2.57	0.40
1:A:712:GLN:CD	1:C:720:LEU:HD22	2.47	0.40
4:B:1697:HOH:O	1:C:534:ARG:CZ	2.69	0.40

All (3) 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)
4:B:1303:HOH:O	4:B:1341:HOH:O[2_584]	2.12	0.08
4:A:1626:HOH:O	4:B:1699:HOH:O[4_585]	2.16	0.04
4:B:1350:HOH:O	4:C:1648:HOH:O[2_684]	2.19	0.01

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	756/776 (97%)	727 (96%)	26 (3%)	3 (0%)	30	27
1	B	754/776 (97%)	726 (96%)	25 (3%)	3 (0%)	30	27
1	C	757/776 (98%)	728 (96%)	27 (4%)	2 (0%)	36	35
All	All	2267/2328 (97%)	2181 (96%)	78 (3%)	8 (0%)	30	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	GLN
1	B	736	GLN
1	C	735	GLY
1	C	736	GLN
1	A	735	GLY

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Mol	Chain	Res	Type
1	B	735	GLY
1	A	734	ALA
1	B	511	GLY

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	620/637 (97%)	603 (97%)	17 (3%)	39	42
1	B	615/637 (96%)	594 (97%)	21 (3%)	32	33
1	C	620/637 (97%)	602 (97%)	18 (3%)	37	40
All	All	1855/1911 (97%)	1799 (97%)	56 (3%)	36	38

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	61	VAL
1	A	112	VAL
1	A	148	LEU
1	A	215	VAL
1	A	310	LEU
1	A	333	THR
1	A	351	THR
1	A	388	ARG
1	A	390	LEU
1	A	400	ASP
1	A	428	LYS
1	A	516	LEU
1	A	615	LYS
1	A	720	LEU
1	A	736	GLN
1	A	750	THR
1	B	61	VAL
1	B	112	VAL

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	225	VAL
1	B	232	VAL
1	B	240	LYS
1	B	262	ASN
1	B	267	GLU
1	B	314	ASN
1	B	322	ARG
1	B	326	ILE
1	B	333	THR
1	B	351	THR
1	B	615	LYS
1	B	633	VAL
1	B	646	GLU
1	B	669	LEU
1	B	677	THR
1	B	690	LYS
1	B	736	GLN
1	B	742	MET
1	C	10	LYS
1	C	24	ARG
1	C	51	LYS
1	C	89	SER
1	C	112	VAL
1	C	146	VAL
1	C	148	LEU
1	C	158	SER
1	C	185	VAL
1	C	231	GLN
1	C	237	ASP
1	C	240	LYS
1	C	322	ARG
1	C	351	THR
1	C	365	THR
1	C	390	LEU
1	C	633	VAL
1	C	736	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN

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Mol	Chain	Res	Type
1	A	262	ASN
1	A	419	ASN
1	A	451	ASN
1	A	481	HIS
1	A	681	HIS
1	B	314	ASN
1	B	328	ASN
1	B	409	ASN
1	B	419	ASN
1	B	481	HIS
1	C	20	GLN
1	C	262	ASN
1	C	327	ASN
1	C	451	ASN
1	C	481	HIS
1	C	612	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
2	BGC	C	800	-	12,12,12	0.52	0	17,17,17	0.59	0
2	BGC	B	800	-	12,12,12	0.46	0	17,17,17	0.92	0
2	BGC	A	800	-	12,12,12	0.46	0	17,17,17	0.93	0
2	BGC	C	801	-	12,12,12	0.47	0	17,17,17	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	800	-	-	0/2/22/22	0/1/1/1
2	BGC	B	800	-	-	0/2/22/22	0/1/1/1
2	BGC	A	800	-	-	0/2/22/22	0/1/1/1
2	BGC	C	801	-	-	0/2/22/22	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	BGC	1	0

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	758/776 (97%)	-0.21	11 (1%) 72 71	21, 29, 43, 63	1 (0%)
1	B	756/776 (97%)	-0.36	10 (1%) 75 74	18, 25, 39, 56	0
1	C	759/776 (97%)	-0.45	4 (0%) 87 87	18, 25, 36, 58	0
All	All	2273/2328 (97%)	-0.34	25 (1%) 78 77	18, 26, 39, 63	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	GLY	7.5
1	B	735	GLY	5.6
1	B	262	ASN	4.0
1	C	735	GLY	4.0
1	A	314	ASN	3.4
1	B	417	ASN	3.3
1	B	225	VAL	3.1
1	B	265	THR	3.1
1	A	62	GLY	3.0
1	A	310	LEU	2.8
1	B	16	LEU	2.8
1	A	312	ILE	2.8
1	A	366	THR	2.6
1	B	469	THR	2.6
1	A	769	GLU	2.5
1	C	333	THR	2.4
1	A	13	THR	2.4
1	B	314	ASN	2.4
1	C	13	THR	2.3
1	B	578	ASP	2.2
1	C	302	ASP	2.2
1	B	310	LEU	2.2
1	A	146	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	362	SER	2.1
1	A	66	GLY	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
2	BGC	C	801	12/12	0.92	0.11	40,51,88,98	0
2	BGC	A	800	12/12	0.93	0.08	25,37,42,43	0
2	BGC	C	800	12/12	0.95	0.07	23,30,32,32	0
2	BGC	B	800	12/12	0.95	0.07	24,30,33,38	0
3	ZN	A	802[A]	1/1	0.99	0.04	38,38,38,38	1

6.5 Other polymers [i](#)

There are no such residues in this entry.