Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 01:18 PM EST

PDB ID	:	4OJ5
Title	:	Crystal Structure of a Putative Tailspike Protein (TSP1, orf210) from Escherichia coli O157:H7 Bacteriohage CBA120
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:

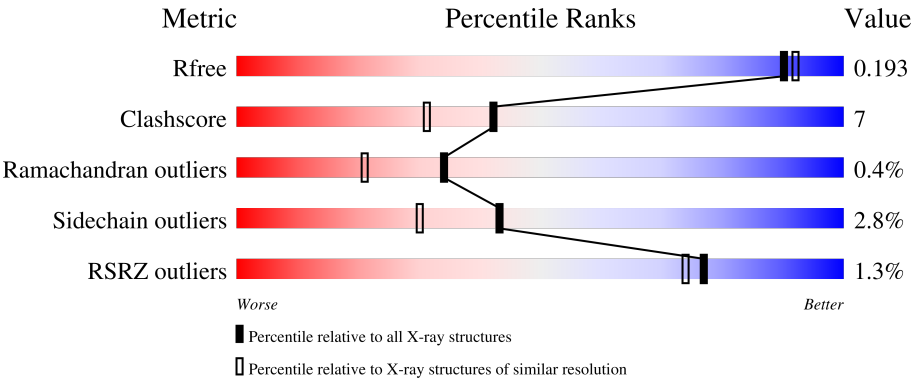
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	2% 87% 10%
1	B	776	3% 86% 11%
1	C	776	3% 88% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 36271 atoms, of which 16849 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	1	0	0
			11300	3575	5633	952	1121	19			
1	B	756	Total	C	H	N	O	S	0	0	0
			11250	3566	5603	946	1116	19			
1	C	757	Total	C	H	N	O	S	3	0	0
			11271	3569	5613	950	1120	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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

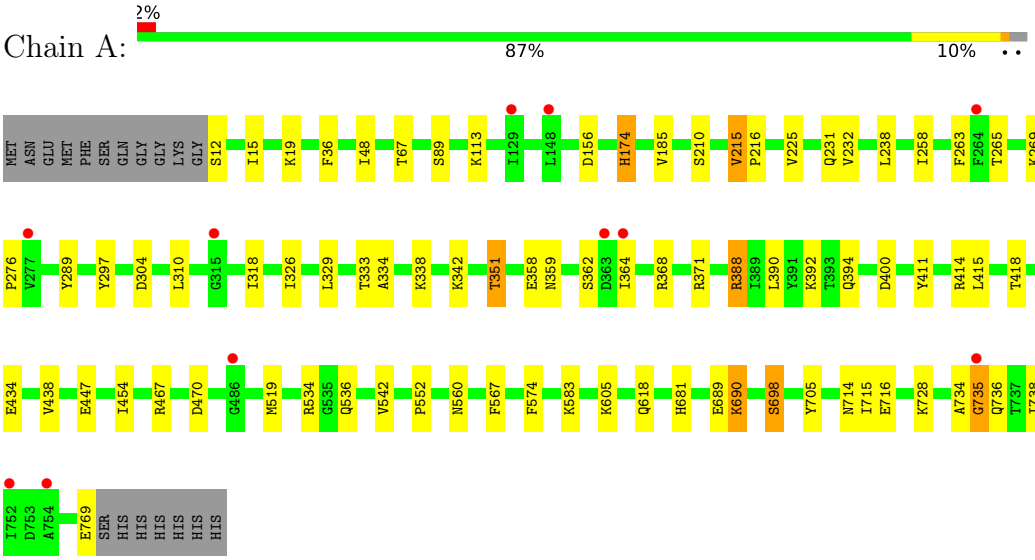
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	734	Total O 734 734	0	0
3	B	815	Total O 815 815	0	0
3	C	900	Total O 900 900	0	0

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.

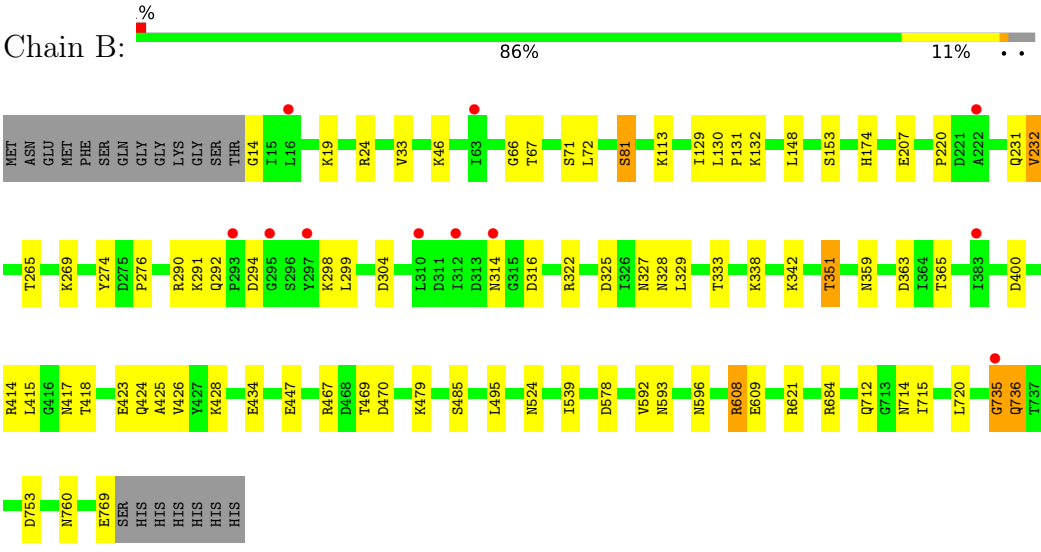
• Molecule 1: Tailspike protein

Chain A:



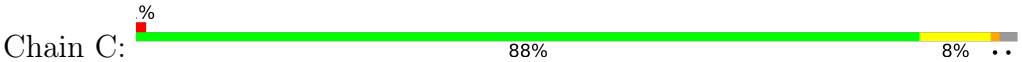
• Molecule 1: Tailspike protein

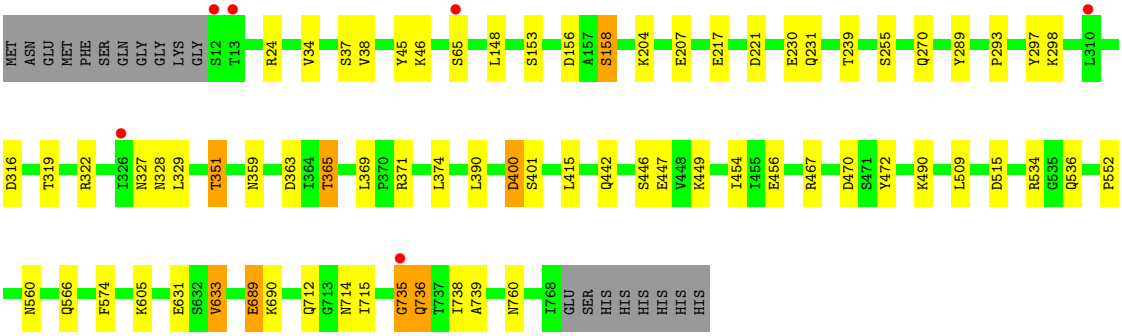
Chain B:



• Molecule 1: Tailspike protein

Chain C:




MET ASN GLU MET PHE SER GLN GLY GLY GLY LYS GLY S12 T13 R24 V34 S37 V38 Y45 K46 S65 L148 S153 D156 A157 S158 K204 E207 E217 D221 E230 Q231 T239 S255 Q270 Y289 P293 Y297 K298 L310
D316 T319 R322 I326 N327 N328 L329 T351 N359 D363 I364 T365 L369 P370 R371 L374 L390 D400 S401 L415 Q442 S446 E447 V448 K449 I454 I455 E456 R467 D470 S471 Y472 K490 L509 D515 R534 G535 Q536 P552
N560 Q566 F574 K605 E631 S632 V633 E689 K690 Q712 G713 N714 I715 G735 Q736 T737 I738 A739 N760 I768 GLU SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	123.62Å 147.82Å 170.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.44 – 1.80 63.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.44-1.80) 99.8 (63.44-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.187 , 0.203 0.194 , 0.193	Depositor DCC
R_{free} test set	14399 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36271	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.35	0/5771	0.65	0/7846
1	B	0.37	0/5751	0.67	1/7820 (0.0%)
1	C	0.39	0/5762	0.67	0/7836
All	All	0.37	0/17284	0.66	1/23502 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	684	ARG	NE-CZ-NH2	-5.53	117.53	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5667	5633	5624	73	0
1	B	5647	5603	5594	94	0
1	C	5658	5613	5604	71	0
2	A	1	0	0	0	0
3	A	734	0	0	43	0
3	B	815	0	0	73	0
3	C	900	0	0	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19422	16849	16822	234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (234) 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:400:ASP:HB3	3:C:1590:HOH:O	1.29	1.28
1:A:364:ILE:HD12	3:A:1553:HOH:O	1.11	1.28
1:B:434:GLU:HG2	3:B:1388:HOH:O	1.33	1.26
1:B:539:ILE:HG12	3:B:1598:HOH:O	1.28	1.25
1:C:369:LEU:HD12	3:C:1591:HOH:O	1.41	1.19
1:C:298:LYS:CA	3:C:1625:HOH:O	1.95	1.14
1:B:426:VAL:CG2	3:B:1509:HOH:O	1.92	1.13
1:C:38:VAL:N	3:C:1595:HOH:O	1.81	1.10
1:C:298:LYS:HA	3:C:1625:HOH:O	1.47	1.10
1:B:426:VAL:N	3:B:1509:HOH:O	1.83	1.09
1:C:328:ASN:C	3:C:1446:HOH:O	1.92	1.08
1:C:369:LEU:CG	3:C:1591:HOH:O	2.00	1.08
1:C:37:SER:CA	3:C:1595:HOH:O	1.98	1.07
1:C:369:LEU:CD1	3:C:1591:HOH:O	1.97	1.07
1:C:329:LEU:N	3:C:1446:HOH:O	1.86	1.06
1:B:322:ARG:NH1	3:B:1330:HOH:O	1.90	1.05
1:B:131:PRO:C	3:B:1352:HOH:O	1.95	1.03
1:A:605:LYS:HE2	3:A:1497:HOH:O	1.58	1.02
1:B:426:VAL:HG23	3:B:1509:HOH:O	1.51	1.02
1:B:71:SER:CA	3:B:1484:HOH:O	2.07	1.00
1:B:609:GLU:OE2	3:B:1459:HOH:O	1.81	0.99
1:A:67:THR:N	3:A:1475:HOH:O	1.95	0.97
1:C:297:TYR:O	3:C:1625:HOH:O	1.81	0.97
1:A:415:LEU:O	3:A:1553:HOH:O	1.81	0.97
1:C:369:LEU:O	3:C:1591:HOH:O	1.83	0.96
1:C:156:ASP:HB2	3:C:1451:HOH:O	1.65	0.96
1:B:71:SER:CB	3:B:1484:HOH:O	2.09	0.96
1:B:769:GLU:O	3:B:1496:HOH:O	1.81	0.96
1:A:67:THR:O	3:A:1475:HOH:O	1.83	0.95
1:B:71:SER:HA	3:B:1484:HOH:O	1.67	0.95
1:A:583:LYS:CD	3:B:1430:HOH:O	2.14	0.94
1:B:71:SER:HB2	3:B:1484:HOH:O	1.63	0.93
1:C:689:GLU:OE1	3:C:1450:HOH:O	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:N	3:B:1334:HOH:O	1.99	0.93
1:B:130:LEU:HA	3:B:1352:HOH:O	1.68	0.92
1:B:524:ASN:OD1	3:B:1434:HOH:O	1.86	0.91
1:B:327:ASN:O	3:B:1334:HOH:O	1.88	0.91
1:B:328:ASN:C	3:B:1334:HOH:O	2.08	0.91
1:B:129:ILE:O	3:B:1352:HOH:O	1.88	0.91
1:A:351:THR:CG2	3:A:1385:HOH:O	2.17	0.91
1:A:371:ARG:O	3:A:1392:HOH:O	1.89	0.91
1:C:293:PRO:O	3:C:1513:HOH:O	1.88	0.90
1:B:237:ASP:OD1	3:B:1563:HOH:O	1.89	0.90
1:C:297:TYR:C	3:C:1625:HOH:O	2.09	0.88
1:B:66:GLY:C	3:B:1567:HOH:O	2.10	0.88
1:A:269:LYS:NZ	3:A:1461:HOH:O	2.06	0.88
1:A:534:ARG:NH2	3:A:1520:HOH:O	2.07	0.87
1:C:401:SER:N	3:C:1590:HOH:O	2.05	0.87
1:B:292:GLN:NE2	3:B:1378:HOH:O	2.06	0.87
1:C:369:LEU:CA	3:C:1591:HOH:O	2.23	0.86
1:C:369:LEU:C	3:C:1591:HOH:O	2.10	0.84
1:C:255:SER:OG	3:C:1502:HOH:O	1.88	0.84
1:C:37:SER:HA	3:C:1595:HOH:O	1.70	0.84
1:A:681:HIS:HD2	1:A:705:TYR:H	1.25	0.83
1:C:298:LYS:CG	3:C:1625:HOH:O	2.25	0.83
1:B:291:LYS:NZ	3:B:1492:HOH:O	2.00	0.83
1:B:524:ASN:CG	3:B:1434:HOH:O	2.16	0.82
1:C:207:GLU:OE2	3:C:1588:HOH:O	1.96	0.82
1:B:495:LEU:O	3:B:1549:HOH:O	1.97	0.82
1:A:388:ARG:NH2	3:A:1361:HOH:O	2.14	0.80
1:A:605:LYS:CE	3:A:1497:HOH:O	2.22	0.80
1:B:426:VAL:CA	3:B:1509:HOH:O	2.27	0.80
1:B:316:ASP:OD2	3:B:1432:HOH:O	2.00	0.79
1:B:524:ASN:ND2	3:B:1434:HOH:O	2.13	0.79
1:B:237:ASP:CG	3:B:1563:HOH:O	2.20	0.79
1:B:298:LYS:NZ	3:B:1335:HOH:O	2.16	0.79
1:A:89:SER:OG	3:A:1400:HOH:O	2.01	0.78
1:B:207:GLU:OE1	3:B:1502:HOH:O	2.02	0.78
1:B:299:LEU:O	3:B:1316:HOH:O	2.03	0.76
1:C:328:ASN:CA	3:C:1446:HOH:O	2.32	0.75
1:A:415:LEU:HB3	3:A:1553:HOH:O	1.86	0.75
1:C:351:THR:HG23	3:C:1441:HOH:O	1.85	0.75
1:C:37:SER:HB2	3:C:1595:HOH:O	1.86	0.75
1:A:231:GLN:HE21	1:A:232:VAL:H	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:NZ	3:A:1477:HOH:O	2.16	0.74
1:C:351:THR:CG2	3:C:1441:HOH:O	2.34	0.74
1:A:689:GLU:OE1	3:A:1422:HOH:O	2.05	0.74
1:B:237:ASP:CB	3:B:1563:HOH:O	2.35	0.74
1:B:327:ASN:ND2	3:B:1331:HOH:O	1.92	0.74
1:C:690:LYS:NZ	3:C:978:HOH:O	2.20	0.73
1:B:131:PRO:O	3:B:1352:HOH:O	1.98	0.73
1:C:217:GLU:OE1	3:C:1579:HOH:O	2.07	0.73
1:B:81:SER:CB	3:B:1420:HOH:O	2.35	0.73
1:C:37:SER:CB	3:C:1595:HOH:O	2.30	0.73
1:A:769:GLU:N	3:A:1476:HOH:O	1.88	0.72
1:B:237:ASP:HB2	3:B:1563:HOH:O	1.89	0.71
3:A:1610:HOH:O	1:B:174:HIS:HE1	1.72	0.71
1:B:479:LYS:NZ	3:B:945:HOH:O	2.23	0.70
1:A:605:LYS:HG3	3:A:1497:HOH:O	1.91	0.70
1:B:265:THR:HA	3:C:1457:HOH:O	1.90	0.70
1:B:578:ASP:OD2	3:B:1364:HOH:O	2.10	0.68
1:B:539:ILE:HG13	1:C:472:TYR:HD1	1.59	0.68
1:C:515:ASP:OD1	3:C:1578:HOH:O	2.12	0.67
1:C:369:LEU:HG	3:C:1591:HOH:O	1.75	0.67
1:C:298:LYS:HG2	3:C:1625:HOH:O	1.89	0.67
1:A:567:PHE:O	3:A:1585:HOH:O	2.11	0.66
1:A:67:THR:CA	3:A:1475:HOH:O	2.39	0.65
1:A:414:ARG:NH2	1:A:418:THR:O	2.29	0.65
1:A:735:GLY:O	3:A:917:HOH:O	2.13	0.65
1:A:351:THR:HG23	3:A:1385:HOH:O	1.87	0.65
1:B:269:LYS:NZ	1:C:230:GLU:O	2.28	0.64
1:B:425:ALA:C	3:B:1509:HOH:O	2.22	0.64
1:B:24:ARG:NH2	3:B:937:HOH:O	2.30	0.64
1:B:753:ASP:HB3	3:B:1550:HOH:O	1.96	0.64
1:A:415:LEU:C	3:A:1553:HOH:O	2.31	0.64
1:C:631:GLU:HG2	1:C:633:VAL:HG12	1.79	0.63
1:A:269:LYS:CE	3:A:1461:HOH:O	2.44	0.63
1:A:690:LYS:NZ	1:A:716:GLU:OE1	2.32	0.62
1:B:414:ARG:NH2	1:B:418:THR:O	2.31	0.62
1:C:298:LYS:N	3:C:1625:HOH:O	2.12	0.62
1:B:66:GLY:CA	3:B:1567:HOH:O	2.48	0.61
1:C:371:ARG:NH1	3:C:1071:HOH:O	2.33	0.61
1:B:14:GLY:N	3:B:1134:HOH:O	2.34	0.60
1:C:369:LEU:N	3:C:1591:HOH:O	2.30	0.60
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ASN:ND2	1:B:485:SER:O	2.34	0.60
1:A:368:ARG:NH2	3:A:1329:HOH:O	2.35	0.59
1:B:424:GLN:O	3:B:1509:HOH:O	2.16	0.59
1:A:358:GLU:OE1	1:A:368:ARG:HD3	2.02	0.59
1:A:605:LYS:CG	3:A:1497:HOH:O	2.49	0.59
1:A:434:GLU:OE1	3:A:1495:HOH:O	2.17	0.59
1:B:265:THR:HG22	3:C:1457:HOH:O	2.03	0.58
1:C:327:ASN:C	3:C:1446:HOH:O	2.41	0.58
1:B:72:LEU:N	3:B:1484:HOH:O	2.34	0.58
1:A:269:LYS:HE3	3:A:1461:HOH:O	2.04	0.58
1:A:681:HIS:CD2	1:A:705:TYR:H	2.15	0.58
1:B:231:GLN:CG	3:B:1391:HOH:O	2.52	0.57
1:B:621:ARG:CD	3:B:1608:HOH:O	2.51	0.57
1:A:263:PHE:H	1:A:265:THR:HG23	1.69	0.57
1:C:363:ASP:OD1	1:C:365:THR:HB	2.05	0.56
1:C:328:ASN:N	3:C:1446:HOH:O	2.39	0.56
1:A:618:GLN:HG3	3:A:1573:HOH:O	2.04	0.56
1:A:534:ARG:HD3	3:A:1376:HOH:O	2.06	0.56
1:B:351:THR:CG2	3:B:1326:HOH:O	2.54	0.56
1:A:552:PRO:HB3	1:A:574:PHE:O	2.06	0.55
3:A:1610:HOH:O	1:B:174:HIS:CE1	2.52	0.55
1:B:304:ASP:OD1	1:B:338:LYS:NZ	2.32	0.54
1:C:217:GLU:CB	3:C:1579:HOH:O	2.54	0.54
1:A:304:ASP:OD1	1:A:338:LYS:NZ	2.39	0.54
1:B:81:SER:CA	3:B:1420:HOH:O	2.55	0.54
1:C:369:LEU:CB	3:C:1591:HOH:O	2.36	0.54
1:B:753:ASP:CG	3:B:1550:HOH:O	2.45	0.53
1:A:415:LEU:CA	3:A:1553:HOH:O	2.56	0.53
1:B:753:ASP:CB	3:B:1550:HOH:O	2.53	0.53
1:C:736:GLN:HA	1:C:760:ASN:O	2.08	0.53
1:B:325:ASP:OD1	3:B:1469:HOH:O	2.19	0.53
1:A:113:LYS:HD3	3:A:1533:HOH:O	2.09	0.52
1:A:583:LYS:CG	3:B:1430:HOH:O	2.51	0.52
1:B:423:GLU:HA	3:B:1569:HOH:O	2.10	0.51
1:B:327:ASN:C	3:B:1334:HOH:O	2.39	0.51
1:B:290:ARG:NH1	3:B:1389:HOH:O	1.93	0.51
1:C:204:LYS:NZ	3:C:1633:HOH:O	2.43	0.51
1:C:449:LYS:NZ	3:C:801:HOH:O	2.39	0.51
1:C:536:GLN:HA	1:C:560:ASN:HB3	1.93	0.51
1:C:552:PRO:HB3	1:C:574:PHE:O	2.11	0.51
1:B:593:ASN:ND2	3:B:1014:HOH:O	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TYR:CE2	1:A:276:PRO:HG3	2.46	0.50
1:B:712:GLN:HG2	1:B:735:GLY:O	2.12	0.50
1:B:467:ARG:HD2	1:B:470:ASP:OD1	2.13	0.49
1:B:274:TYR:CE2	1:B:276:PRO:HG3	2.48	0.49
1:B:715:ILE:O	1:B:739:ALA:HA	2.13	0.49
1:A:690:LYS:HE3	3:C:1007:HOH:O	2.12	0.49
1:B:434:GLU:CG	3:B:1388:HOH:O	2.18	0.49
1:A:67:THR:C	3:A:1475:HOH:O	2.35	0.48
1:A:519:MET:HE3	1:A:542:VAL:HG21	1.96	0.48
1:C:712:GLN:HG2	1:C:735:GLY:O	2.14	0.48
1:A:238:LEU:HB2	1:A:258:ILE:HG12	1.96	0.48
3:B:1249:HOH:O	1:C:534:ARG:HD2	2.13	0.48
1:A:715:ILE:O	1:A:739:ALA:HA	2.14	0.47
1:C:442:GLN:HG3	1:C:446:SER:HB3	1.95	0.47
1:A:698:SER:HB2	3:A:1473:HOH:O	2.15	0.47
1:B:736:GLN:HA	1:B:760:ASN:O	2.14	0.47
1:C:153:SER:OG	1:C:158:SER:HB3	2.15	0.47
1:C:239:THR:O	1:C:270:GLN:HG2	2.15	0.47
1:B:19:LYS:HE3	1:B:33:VAL:O	2.15	0.46
1:B:426:VAL:HG22	3:B:1509:HOH:O	1.83	0.46
1:B:424:GLN:NE2	1:B:428:LYS:HE2	2.31	0.46
1:A:113:LYS:HD3	3:A:1400:HOH:O	2.14	0.46
1:A:705:TYR:CD1	1:A:728:LYS:HB2	2.50	0.46
1:A:215:VAL:HA	1:A:216:PRO:HD3	1.83	0.46
1:A:434:GLU:CD	3:A:1495:HOH:O	2.54	0.46
1:A:364:ILE:CG1	3:A:1553:HOH:O	2.51	0.45
1:C:714:ASN:HA	1:C:738:ILE:HG13	1.97	0.45
1:A:174:HIS:HB3	3:A:1615:HOH:O	2.15	0.45
1:A:351:THR:HG22	3:A:1385:HOH:O	2.01	0.45
1:A:467:ARG:HD2	1:A:470:ASP:OD1	2.16	0.45
1:B:359:ASN:OD1	1:B:415:LEU:HD11	2.16	0.45
1:C:217:GLU:HB2	3:C:1579:HOH:O	2.16	0.45
1:C:359:ASN:OD1	1:C:415:LEU:HD11	2.15	0.45
1:B:113:LYS:HE3	3:B:1336:HOH:O	2.15	0.45
1:B:342:LYS:HB3	1:B:342:LYS:HE2	1.76	0.45
1:A:15:ILE:O	1:A:19:LYS:HG3	2.17	0.45
1:B:363:ASP:OD1	1:B:365:THR:OG1	2.31	0.45
1:B:578:ASP:CG	3:B:1364:HOH:O	2.51	0.45
1:C:289:TYR:HB3	1:C:297:TYR:HB3	1.99	0.44
1:C:217:GLU:HB3	3:C:1579:HOH:O	2.16	0.44
1:A:270:GLN:NE2	1:B:232:VAL:HG23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:THR:HG22	3:B:1326:HOH:O	2.16	0.44
1:A:156:ASP:HB2	3:C:1451:HOH:O	2.17	0.44
1:C:467:ARG:HD2	1:C:470:ASP:OD1	2.18	0.44
1:A:289:TYR:HB3	1:A:297:TYR:HB3	2.00	0.43
1:B:132:LYS:N	3:B:1352:HOH:O	2.32	0.43
1:B:714:ASN:HA	1:B:738:ILE:HG13	2.01	0.43
1:C:415:LEU:HD12	1:C:415:LEU:HA	1.80	0.43
1:A:371:ARG:NH1	3:A:1199:HOH:O	2.25	0.43
1:B:434:GLU:HG3	3:B:1458:HOH:O	2.18	0.42
1:C:24:ARG:HD3	1:C:24:ARG:HA	1.75	0.42
1:A:536:GLN:HA	1:A:560:ASN:HB3	2.01	0.42
1:C:34:VAL:HB	1:C:45:TYR:CG	2.54	0.42
1:B:290:ARG:NH2	3:B:1389:HOH:O	2.52	0.42
1:C:37:SER:C	3:C:1595:HOH:O	2.13	0.42
1:C:454:ILE:HD12	3:C:1566:HOH:O	2.20	0.42
1:C:715:ILE:O	1:C:739:ALA:HA	2.19	0.42
1:B:81:SER:OG	3:B:1420:HOH:O	1.86	0.42
3:B:917:HOH:O	1:C:690:LYS:HE2	2.19	0.41
1:A:342:LYS:HB3	1:A:342:LYS:HE2	1.75	0.41
1:C:204:LYS:NZ	3:C:1640:HOH:O	2.52	0.41
1:B:46:LYS:NZ	3:B:1487:HOH:O	2.53	0.41
1:B:592:VAL:O	1:B:608:ARG:NH2	2.53	0.41
1:B:46:LYS:HE3	3:B:1487:HOH:O	2.19	0.41
1:A:333:THR:HG23	1:A:334:ALA:O	2.20	0.41
1:A:714:ASN:HA	1:A:738:ILE:HG13	2.01	0.41
1:B:67:THR:N	3:B:1567:HOH:O	2.45	0.41
1:A:454:ILE:HD11	1:B:404:GLY:HA3	2.03	0.41
1:C:319:THR:HG22	3:C:1142:HOH:O	2.20	0.41
1:C:566:GLN:O	1:C:605:LYS:HD2	2.21	0.41
1:A:36:PHE:HB2	1:A:48:ILE:HD11	2.02	0.41
1:A:392:LYS:N	3:A:1392:HOH:O	1.97	0.41
1:A:359:ASN:OD1	1:A:415:LEU:HD11	2.21	0.40
1:B:596:ASN:OD1	1:B:609:GLU:HG2	2.22	0.40
1:A:258:ILE:HD12	1:A:329:LEU:HA	2.03	0.40
1:C:46:LYS:HA	1:C:46:LYS:HD3	1.81	0.40
1:A:185:VAL:HG23	3:A:1404:HOH:O	2.21	0.40
1:A:394:GLN:HA	1:A:438:VAL:O	2.21	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	756/776 (97%)	729 (96%)	24 (3%)	3 (0%)	34	21
1	B	754/776 (97%)	717 (95%)	34 (4%)	3 (0%)	34	21
1	C	755/776 (97%)	728 (96%)	25 (3%)	2 (0%)	41	27
All	All	2265/2328 (97%)	2174 (96%)	83 (4%)	8 (0%)	34	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	GLN
1	B	735	GLY
1	B	736	GLN
1	C	735	GLY
1	C	736	GLN
1	A	735	GLY
1	B	220	PRO
1	A	734	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	618/637 (97%)	600 (97%)	18 (3%)	42	29
1	B	613/637 (96%)	597 (97%)	16 (3%)	46	32
1	C	616/637 (97%)	598 (97%)	18 (3%)	42	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1847/1911 (97%)	1795 (97%)	52 (3%)	43 30

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

Mol	Chain	Res	Type
1	A	12	SER
1	A	174	HIS
1	A	210	SER
1	A	215	VAL
1	A	225	VAL
1	A	310	LEU
1	A	318	ILE
1	A	326	ILE
1	A	351	THR
1	A	362	SER
1	A	388	ARG
1	A	390	LEU
1	A	400	ASP
1	A	411	TYR
1	A	428	LYS
1	A	447	GLU
1	A	690	LYS
1	A	698	SER
1	B	81	SER
1	B	148	LEU
1	B	153	SER
1	B	232	VAL
1	B	240	LYS
1	B	294	ASP
1	B	314	ASN
1	B	333	THR
1	B	351	THR
1	B	400	ASP
1	B	411	TYR
1	B	447	GLU
1	B	469	THR
1	B	608	ARG
1	B	720	LEU
1	B	748	ARG
1	C	65	SER
1	C	148	LEU
1	C	158	SER

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Mol	Chain	Res	Type
1	C	221	ASP
1	C	231	GLN
1	C	316	ASP
1	C	322	ARG
1	C	351	THR
1	C	365	THR
1	C	374	LEU
1	C	390	LEU
1	C	400	ASP
1	C	447	GLU
1	C	456	GLU
1	C	490	LYS
1	C	509	LEU
1	C	633	VAL
1	C	689	GLU

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	174	HIS
1	A	231	GLN
1	A	262	ASN
1	A	327	ASN
1	A	419	ASN
1	A	424	GLN
1	A	681	HIS
1	B	174	HIS
1	B	262	ASN
1	B	292	GLN
1	B	328	ASN
1	B	409	ASN
1	B	424	GLN
1	C	20	GLN
1	C	192	ASN
1	C	262	ASN
1	C	550	ASN

5.3.3 RNA

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 monosaccharides 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 (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	758/776 (97%)	0.03	12 (1%)	72	68	14, 27, 46, 79	1 (0%)
1	B	756/776 (97%)	0.04	11 (1%)	73	70	10, 24, 47, 74	0
1	C	757/776 (97%)	-0.13	6 (0%)	86	84	9, 20, 39, 88	0
All	All	2271/2328 (97%)	-0.02	29 (1%)	77	74	9, 23, 44, 88	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	12	SER	4.6
1	B	735	GLY	4.3
1	A	129	ILE	4.1
1	A	735	GLY	4.0
1	B	310	LEU	3.8
1	C	310	LEU	3.6
1	B	295	GLY	3.2
1	C	735	GLY	3.1
1	B	312	ILE	3.0
1	A	486	GLY	3.0
1	B	314	ASN	2.9
1	B	222	ALA	2.9
1	C	13	THR	2.7
1	B	16	LEU	2.7
1	B	293	PRO	2.5
1	A	364	ILE	2.4
1	B	383	ILE	2.4
1	A	148	LEU	2.4
1	A	277	VAL	2.3
1	A	754	ALA	2.3
1	A	264	PHE	2.3
1	B	63	ILE	2.2
1	B	297	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	363	ASP	2.1
1	A	315	GLY	2.1
1	A	422	LEU	2.1
1	C	65	SER	2.1
1	A	752	ILE	2.0
1	C	326	ILE	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	ZN	A	801[A]	1/1	0.99	0.07	27,27,27,27	1

6.5 Other polymers (i)

There are no such residues in this entry.