Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:20 PM GMT

PDB ID	:	4OJ6
Title	:	Crystal Structure of a Putative Tailspike Protein (TSP1, orf210) from Escherichia coli O157:H7 Bacteriohage 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

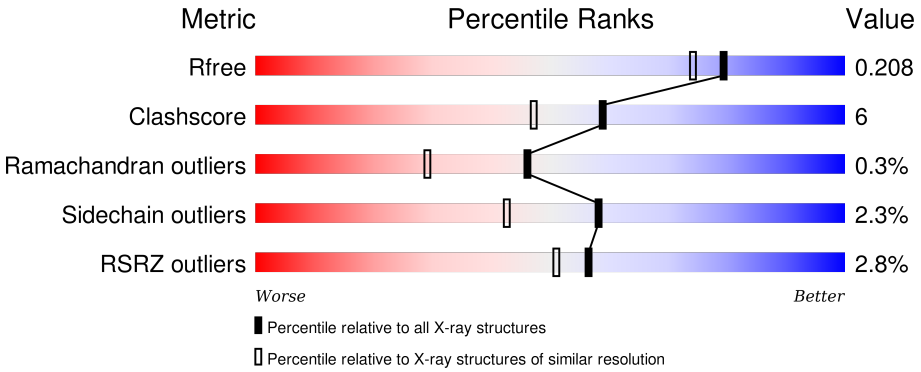
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	3% 87% 10%
1	B	776	3% 87% 10%
1	C	776	2% 89% 7%

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

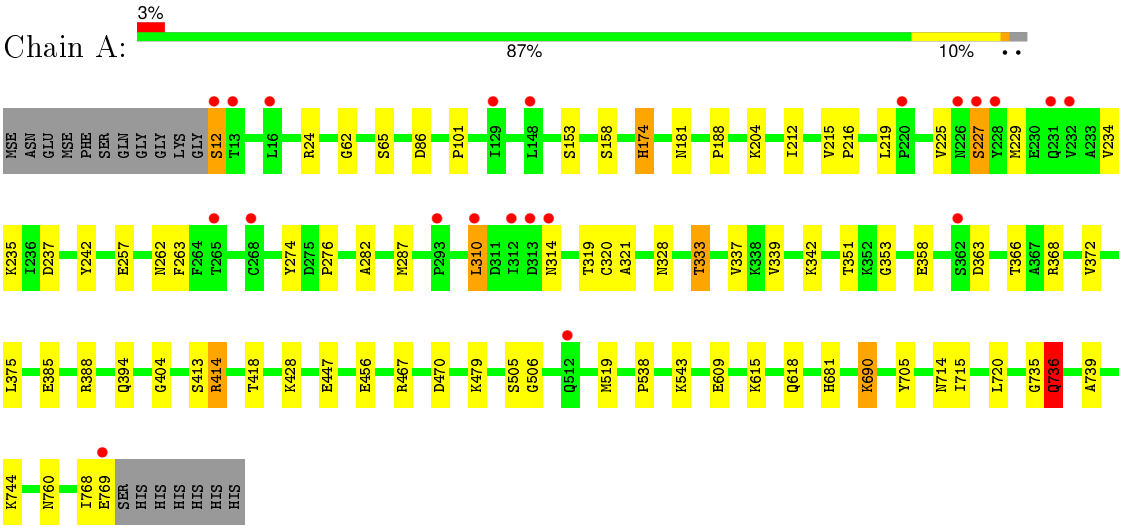
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	707	Total O 707 707	0	0
3	B	828	Total O 828 828	0	1
3	C	827	Total O 827 827	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

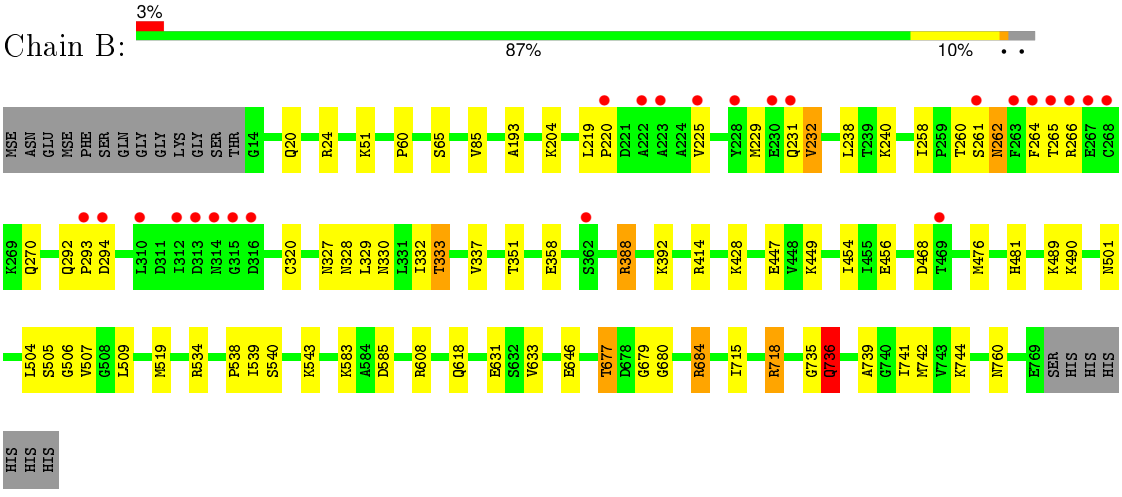
- Molecule 1: Tailspike protein

Chain A:



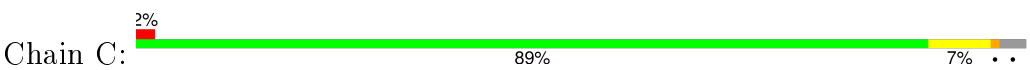
- Molecule 1: Tailspike protein

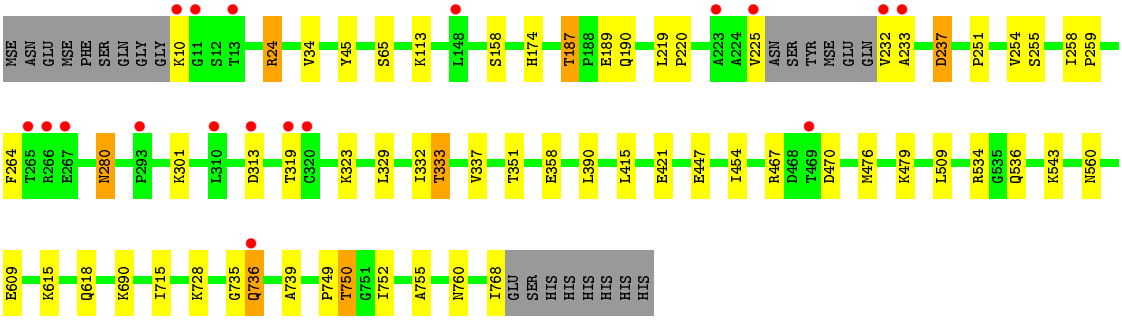
Chain B:



- Molecule 1: Tailspike protein

Chain C:




MSE ASN GLU MSE PHE SER GLN GLY GLY K10 G11 S12 T13 R24 V34 Y45 S65 K113 L148 S158 H174 T187 P188 E189 Q190 L219 P220 A223 A224 V225 ASN SER TYR MSE GLU GLN V232 A233 D237 P251 V254 S255 I258 P259
F264 T265 R266 E267 N280 P293 K301 L310 D313 T319 C320 K323 L329 I332 T333 V337 T351 E358 L390 L415 E421 E447 I454 R467 D468 T469 D470 M476 K479 L509 R534 G535 Q536 K543 N560
E609 K615 Q618 K690 I715 K728 G735 Q736 A739 P749 T750 G751 I752 A755 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	123.30Å 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) 99.7 (19.85-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.187 , 0.209 0.185 , 0.208	Depositor DCC
R_{free} test set	14902 reflections (5.01%)	DCC
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 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 297461 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0/5735	0.55	0/7784
1	B	0.40	0/5718	0.60	3/7761 (0.0%)
1	C	0.40	0/5692	0.57	0/7726
All	All	0.38	0/17145	0.57	3/23271 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	718	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	718	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	684	ARG	NE-CZ-NH2	-6.25	117.17	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	5641	5517	5576	66	0
1	B	5624	5488	5547	77	1
1	C	5600	5482	5536	61	0
2	B	1	0	0	0	0
3	A	707	0	0	30	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	828	0	0	39	1
3	C	827	0	0	34	1
All	All	19228	16487	16659	193	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 (193) 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	1.07
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:OD2	3:C:1521:HOH:O	1.80	0.98
1:C:237:ASP:CG	3:C:1521:HOH:O	2.00	0.94
1:A:319:THR:OG1	3:A:1402:HOH:O	1.84	0.93
1:C:280:ASN:ND2	3:C:1498:HOH:O	1.97	0.93
1:A:543:LYS:HE3	3:A:1504:HOH:O	1.67	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: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:540:SER:HB2	3:B:1681:HOH:O	1.77	0.84
1:B:270:GLN:OE1	1:C:233:ALA:N	2.08	0.84
1:A:227:SER:OG	3:A:1340:HOH:O	1.95	0.84
1:B:501:ASN:CG	3:B:1623:HOH:O	2.16	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:456:GLU:CG	3:B:1687:HOH:O	2.30	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:769:GLU:HB3	3:A:1475:HOH:O	1.90	0.71
1:A:505:SER:N	3:A:1399:HOH:O	1.87	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: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:B:677:THR:HG21	1:B:680:GLY:O	1.93	0.68
1:A:86:ASP:CB	3:A:1428:HOH:O	2.41	0.68
1:C:447:GLU:HG2	1:C:476:MSE:HE2	1.74	0.68
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:C:768:ILE:C	3:C:1504:HOH:O	2.34	0.66
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
1:C:618:GLN:CG	3:C:1540:HOH:O	2.27	0.62
1:B:447:GLU:HG2	1:B:476:MSE:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:506:GLY:O	3:A:907:HOH:O	2.17	0.57
1:A:385:GLU:HG2	3:A:1404:HOH:O	2.03	0.57
1:A:62:GLY:N	3:A:1454:HOH:O	2.14	0.56
1:B:742:MSE:HE3	1:B:744:LYS:HD3	1.88	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: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
1:A:12:SER:OG	3:A:1375:HOH:O	2.18	0.53
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:519:MSE:HE1	1:A:538:PRO:HG2	1.91	0.52
1:A:358:GLU:OE1	1:A:368:ARG:HD3	2.09	0.52
1:C:479:LYS:CE	3:C:1518:HOH:O	2.54	0.52
1:B:231:GLN:NE2	3:B:1688:HOH:O	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:583:LYS:NZ	3:B:1667:HOH:O	2.43	0.50
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:A:744:LYS:NZ	3:A:1507:HOH:O	2.42	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: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:B:260:THR:HG21	1:C:323:LYS:C	2.35	0.47
1:A:229:MSE:HE3	1:A:321:ALA:H	1.80	0.47
1:B:543:LYS:NZ	3:B:1642:HOH:O	2.47	0.46
1:A:506:GLY:N	3:A:1399:HOH:O	2.48	0.46
1:A:342:LYS:HD2	1:A:375:LEU:HD23	1.97	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: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:262:ASN:ND2	3:A:1410:HOH:O	2.50	0.45
1:A:24:ARG:NH2	3:A:842:HOH:O	2.49	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:C:615:LYS:NZ	3:C:967:HOH:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:ALA:HA	1:B:204:LYS:HD3	2.00	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: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:C:536:GLN:HA	1:C:560:ASN:HB3	2.02	0.42
1:A:372:VAL:HA	1:A:394:GLN:O	2.20	0.42
1:C:301:LYS:HG3	3:C:1379:HOH:O	2.18	0.41
1:A:188:PRO:HG2	1:A:242:TYR:CZ	2.55	0.41
1:C:219:LEU:HA	1:C:220:PRO:HD3	1.89	0.41
1:A:174:HIS:HE1	3:C:1266:HOH:O	2.03	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:B:292:GLN:HB3	1:B:293:PRO:HD2	2.04	0.40
1:A:690:LYS:HE2	1:A:714:ASN:OD1	2.21	0.40
1:B:742:MSE:HE2	1:B:744:LYS:HB2	2.03	0.40
1:A:24:ARG:HA	1:A:24:ARG:HD3	1.75	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: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 (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%)	725 (96%)	29 (4%)	2 (0%)	46	29
1	B	754/776 (97%)	726 (96%)	25 (3%)	3 (0%)	39	23
1	C	749/776 (96%)	724 (97%)	23 (3%)	2 (0%)	46	29
All	All	2259/2328 (97%)	2175 (96%)	77 (3%)	7 (0%)	46	29

All (7) Ramachandran outliers are listed below:

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

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	610/625 (98%)	595 (98%)	15 (2%)	55 39
1	B	608/625 (97%)	593 (98%)	15 (2%)	55 39
1	C	606/625 (97%)	594 (98%)	12 (2%)	63 49
All	All	1824/1875 (97%)	1782 (98%)	42 (2%)	58 42

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	65	SER
1	A	174	HIS
1	A	227	SER
1	A	237	ASP
1	A	310	LEU
1	A	333	THR
1	A	351	THR
1	A	414	ARG
1	A	428	LYS
1	A	447	GLU
1	A	615	LYS
1	A	690	LYS
1	A	720	LEU
1	A	736	GLN
1	B	51	LYS
1	B	232	VAL
1	B	240	LYS
1	B	262	ASN
1	B	294	ASP
1	B	327	ASN
1	B	333	THR
1	B	351	THR
1	B	388	ARG
1	B	428	LYS
1	B	608	ARG
1	B	646	GLU
1	B	677	THR
1	B	736	GLN
1	B	741	ILE
1	C	10	LYS
1	C	24	ARG
1	C	65	SER
1	C	158	SER

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Mol	Chain	Res	Type
1	C	187	THR
1	C	237	ASP
1	C	280	ASN
1	C	319	THR
1	C	333	THR
1	C	351	THR
1	C	509	LEU
1	C	750	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	314	ASN
1	A	501	ASN
1	A	681	HIS
1	B	328	ASN
1	C	262	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 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	748/776 (96%)	-0.13	21 (2%)	56	51	18, 31, 50, 70	2 (0%)
1	B	746/776 (96%)	-0.25	24 (3%)	51	45	15, 25, 49, 73	0
1	C	744/776 (95%)	-0.26	18 (2%)	62	57	18, 25, 42, 76	0
All	All	2238/2328 (96%)	-0.21	63 (2%)	56	51	15, 27, 48, 76	2 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	SER	8.1
1	C	232	VAL	6.4
1	A	13	THR	6.2
1	B	264	PHE	6.1
1	B	310	LEU	5.8
1	C	233	ALA	5.8
1	A	310	LEU	5.0
1	B	266	ARG	4.9
1	A	314	ASN	4.8
1	C	10	LYS	4.8
1	B	268	CYS	4.4
1	B	314	ASN	4.3
1	C	293	PRO	4.2
1	C	267	GLU	3.8
1	B	293	PRO	3.6
1	B	265	THR	3.6
1	B	261	SER	3.5
1	C	310	LEU	3.5
1	A	227	SER	3.4
1	C	266	ARG	3.4
1	A	313	ASP	3.4
1	C	320	CYS	3.4
1	C	313	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	769	GLU	3.4
1	A	293	PRO	3.2
1	B	313	ASP	3.1
1	C	223	ALA	3.1
1	B	294	ASP	3.0
1	B	263	PHE	2.9
1	C	13	THR	2.9
1	A	220	PRO	2.9
1	B	267	GLU	2.9
1	A	312	ILE	2.9
1	A	362	SER	2.8
1	C	225	VAL	2.8
1	B	312	ILE	2.7
1	A	268	CYS	2.7
1	A	226	ASN	2.7
1	A	231	GLN	2.7
1	B	231	GLN	2.6
1	A	148	LEU	2.6
1	C	11	GLY	2.6
1	A	265	THR	2.6
1	C	469	THR	2.6
1	B	228	TYR	2.5
1	B	315	GLY	2.5
1	B	223	ALA	2.5
1	A	228	TYR	2.4
1	B	220	PRO	2.4
1	C	319	THR	2.4
1	B	225	VAL	2.3
1	B	469	THR	2.3
1	B	222	ALA	2.3
1	B	362	SER	2.1
1	A	512	GLN	2.1
1	A	129	ILE	2.1
1	B	316	ASP	2.1
1	A	232	VAL	2.1
1	C	736	GLN	2.1
1	B	230	GLU	2.0
1	C	148	LEU	2.0
1	C	265	THR	2.0
1	A	16	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	B	800[A]	1/1	0.99	0.05	-	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.