Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:14 pm GMT

PDB ID	:	6Z99
Title	:	Copper transporter OprC
Authors	:	Bhamidimarri, S.P.; van den Berg, B.
Deposited on	:	2020-06-03
Resolution	:	2.68 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 following versions of software and data (see references ⓘ) were used in the production of this report:

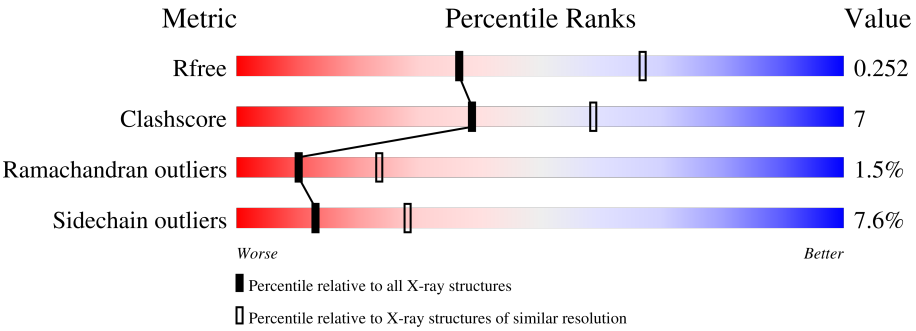
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)

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%

Mol	Chain	Length	Quality of chain
1	A	723	74% 16% • 10%
1	B	723	69% 20% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	802	-	-	X	-
2	AG	B	803	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10196 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 Putative copper transport outer membrane porin OprC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	4	1	0
			5074	3185	896	977	16			
1	B	658	Total	C	N	O	S	4	2	0
			5108	3207	902	981	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	CYS	engineered mutation	UNP G3XD89
B	143	ALA	CYS	engineered mutation	UNP G3XD89

- Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ag	0	0
			3	3		
2	B	3	Total	Ag	0	0
			3	3		

- Molecule 3 is water.

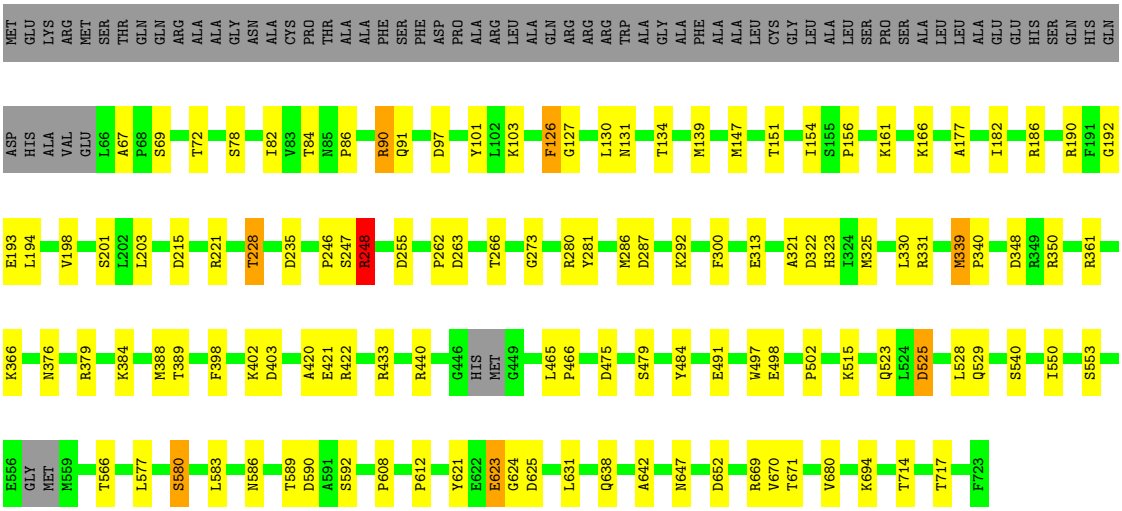
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	2	Total	O	0	0
			2	2		

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. 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. 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.

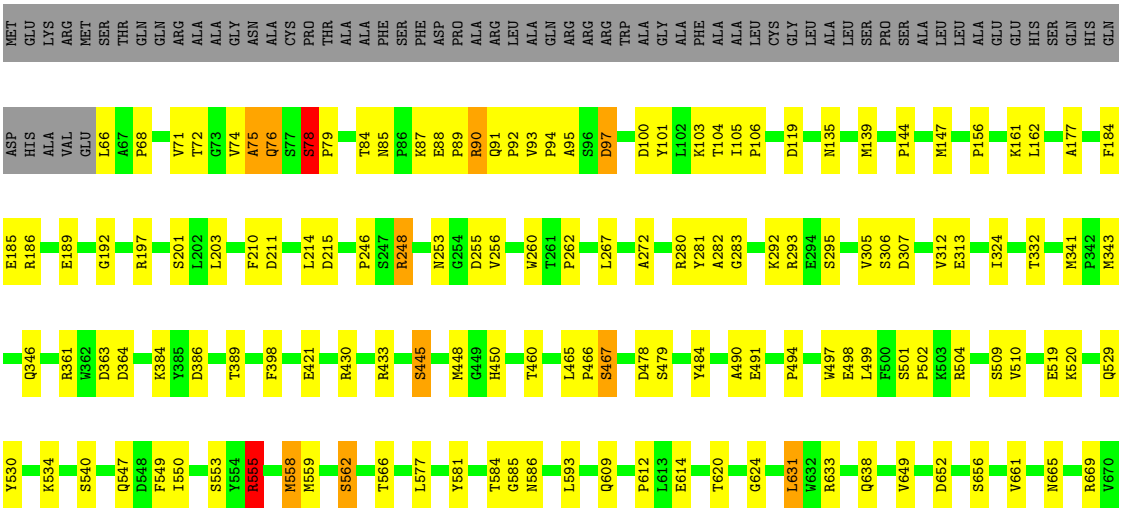
• Molecule 1: Putative copper transport outer membrane porin OprC

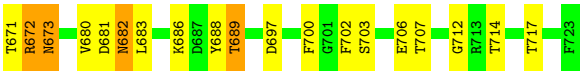
Chain A:



• Molecule 1: Putative copper transport outer membrane porin OprC

Chain B:




T671
R672
N673
V680
D681
N682
L683
K686
D687
Y688
T689
D697
F700
G701
F702
S703
E706
T707
G712
R713
T714
T717
F723

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	154.64Å 195.51Å 165.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.18 – 2.68 84.18 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.18-2.68) 99.8 (84.18-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.215 , 0.252 0.216 , 0.252	Depositor DCC
R_{free} test set	3459 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: AG

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	0.47	1/5202 (0.0%)	0.69	1/7051 (0.0%)
1	B	0.44	0/5242	0.68	1/7107 (0.0%)
All	All	0.46	1/10444 (0.0%)	0.68	2/14158 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	ARG	C-N	-6.14	1.20	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	555	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	348	ASP	CB-CG-OD1	5.87	123.58	118.30

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	5074	0	4854	59	0
1	B	5108	0	4893	92	0
2	A	3	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3	0	0	2	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
All	All	10196	0	9747	149	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 (149) 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:343:MET:HE1	2:B:803:AG:AG	1.39	1.08
1:B:72:THR:HA	1:B:92:PRO:HG3	1.52	0.92
1:A:286:MET:CE	2:A:802:AG:AG	2.12	0.84
1:B:90:ARG:HH11	1:B:101:TYR:HB3	1.41	0.82
1:B:343:MET:CE	2:B:803:AG:AG	2.14	0.82
1:B:467:SER:HB3	1:B:490:ALA:HA	1.64	0.79
1:A:286:MET:HE2	2:A:802:AG:AG	1.71	0.76
1:B:246:PRO:HG2	1:B:282:ALA:HB2	1.68	0.76
1:B:498:GLU:HG2	1:B:550:ILE:HG21	1.66	0.76
1:B:71:VAL:HB	1:B:90:ARG:HA	1.70	0.71
1:B:612:PRO:HB3	1:B:638:GLN:HB2	1.72	0.71
1:A:72:THR:HB	1:A:631:LEU:HD13	1.73	0.70
1:B:614:GLU:OE1	1:B:633:ARG:NE	2.24	0.69
1:B:78:SER:HB3	1:B:79:PRO:CD	2.23	0.68
1:B:90:ARG:HE	1:B:101:TYR:HD2	1.42	0.67
1:B:246:PRO:HG3	1:B:700:PHE:CD1	2.29	0.67
1:B:484:TYR:HH	1:B:540:SER:HG	1.42	0.66
1:A:286:MET:HE3	2:A:802:AG:AG	1.80	0.66
1:B:94:PRO:HD3	1:B:681:ASP:OD2	1.96	0.65
1:B:147:MET:HG2	1:B:281:TYR:CE2	2.32	0.65
1:B:84:THR:HG21	1:B:90:ARG:NH2	2.12	0.65
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.80	0.64
1:B:680:VAL:HG11	1:B:683:LEU:HD13	1.80	0.63
1:A:255:ASP:OD2	1:A:273:GLY:HA3	1.99	0.63
1:B:91:GLN:NE2	1:B:94:PRO:HA	2.14	0.63
1:A:498:GLU:HG2	1:A:550:ILE:HG21	1.81	0.62
1:B:682:ASN:HD21	1:B:686:LYS:H	1.48	0.62
1:A:580:SER:HB2	1:A:590:ASP:HB3	1.83	0.61
1:B:135:ASN:HD21	1:B:186:ARG:HB2	1.65	0.61
1:B:74:VAL:HB	1:B:105:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLN:HE22	1:B:94:PRO:HA	1.66	0.61
1:A:466:PRO:O	1:A:491:GLU:HG3	2.01	0.60
1:A:422:ARG:HB3	1:A:475:ASP:HB2	1.82	0.60
1:B:214:LEU:HD12	1:B:215:ASP:H	1.66	0.60
1:B:84:THR:HG22	1:B:162:LEU:HB3	1.82	0.60
1:B:689:THR:HG21	1:B:707:THR:OG1	2.02	0.60
1:A:151:THR:HA	1:A:154:ILE:HD12	1.84	0.60
1:B:248:ARG:HH21	1:B:280:ARG:NH1	1.98	0.59
1:A:466:PRO:HG2	1:B:466:PRO:HG2	1.85	0.58
1:B:609:GLN:NE2	1:B:652:ASP:OD1	2.37	0.58
1:A:583:LEU:HD11	1:A:589:THR:HG22	1.86	0.57
1:A:484:TYR:OH	1:A:540:SER:HB3	2.04	0.57
1:B:90:ARG:NH1	1:B:101:TYR:O	2.38	0.56
1:B:72:THR:HB	1:B:631:LEU:HD13	1.88	0.56
1:B:497:TRP:O	1:B:502:PRO:HD3	2.06	0.56
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.88	0.56
1:B:253:ASN:HD22	1:B:293:ARG:HH21	1.53	0.56
1:B:491:GLU:CD	1:B:520:LYS:HD3	2.27	0.55
1:A:379:ARG:HG2	1:A:402:LYS:HA	1.88	0.55
1:A:608:PRO:HB3	1:A:642:ALA:HB3	1.88	0.55
1:B:248:ARG:HH21	1:B:280:ARG:HH12	1.55	0.54
1:B:74:VAL:HG21	1:B:90:ARG:NH2	2.22	0.54
1:B:84:THR:HG21	1:B:90:ARG:HH22	1.72	0.54
1:B:534:LYS:HB2	1:B:581:TYR:HE2	1.71	0.54
1:A:193:GLU:HG3	1:A:194:LEU:N	2.24	0.53
1:A:262:PRO:HD2	1:A:266:THR:HB	1.90	0.53
1:A:287:ASP:CG	1:A:331:ARG:HH21	2.12	0.52
1:B:497:TRP:O	1:B:501:SER:HB2	2.09	0.52
1:B:91:GLN:OE1	1:B:94:PRO:HA	2.09	0.52
1:B:384:LYS:HG3	1:B:398:PHE:CZ	2.45	0.52
1:B:386:ASP:HB3	1:B:389:THR:HG22	1.92	0.52
1:B:93:VAL:HA	1:B:681:ASP:OD2	2.10	0.51
1:B:260:TRP:NE1	1:B:262:PRO:HG3	2.26	0.51
1:B:324:ILE:HG13	1:B:346:GLN:HG3	1.90	0.51
1:A:280:ARG:HG3	1:A:330:LEU:HB3	1.93	0.51
1:B:91:GLN:HE22	1:B:94:PRO:CA	2.23	0.50
1:B:363:ASP:OD2	1:B:364:ASP:N	2.44	0.50
1:B:78:SER:HB3	1:B:79:PRO:HD2	1.93	0.50
1:B:92:PRO:HG2	1:B:104:THR:HG22	1.92	0.50
1:B:702:PHE:HD1	1:B:706:GLU:HG2	1.76	0.50
1:A:669:ARG:HG3	1:A:669:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:O	1:B:210:PHE:HA	2.13	0.49
1:A:523:GLN:NE2	1:A:525:ASP:OD2	2.38	0.49
1:B:555:ARG:NE	1:B:555:ARG:HA	2.27	0.49
1:B:577:LEU:HD21	1:B:593:LEU:HD23	1.94	0.49
1:A:465:LEU:HB3	1:A:491:GLU:HB2	1.95	0.48
1:A:287:ASP:OD2	1:A:331:ARG:NE	2.31	0.48
1:A:497:TRP:O	1:A:502:PRO:HD3	2.12	0.48
1:B:91:GLN:CD	1:B:94:PRO:HA	2.34	0.48
1:A:361:ARG:HD2	1:A:366:LYS:HB2	1.96	0.48
1:A:339:MET:H	1:A:340:PRO:HD3	1.79	0.48
1:A:384:LYS:HD2	1:A:398:PHE:CZ	2.49	0.48
1:A:84:THR:HG21	1:A:90:ARG:HH22	1.79	0.48
1:A:130:LEU:HD23	1:A:182:ILE:CD1	2.44	0.48
1:B:75:ALA:HA	1:B:106:PRO:CD	2.44	0.48
1:A:190:ARG:HB3	1:A:190:ARG:NH1	2.29	0.47
1:A:403:ASP:HB2	1:A:440:ARG:CG	2.44	0.47
1:B:555:ARG:HA	1:B:555:ARG:HE	1.79	0.47
1:A:350:ARG:O	1:A:376:ASN:HA	2.14	0.47
1:B:478:ASP:N	1:B:478:ASP:OD1	2.43	0.47
1:B:534:LYS:HB2	1:B:581:TYR:CE2	2.50	0.47
1:A:86:PRO:HA	1:A:90:ARG:NH1	2.30	0.46
1:A:323:HIS:NE2	1:A:325:MET:HG3	2.30	0.46
1:A:139:MET:CE	1:A:321:ALA:HB2	2.44	0.46
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.51	0.46
1:A:235:ASP:HA	1:A:248:ARG:HB2	1.97	0.46
1:B:95:ALA:HA	1:B:100:ASP:HB3	1.98	0.46
1:B:144:PRO:O	1:B:497:TRP:HD1	1.98	0.46
1:B:68:PRO:HG3	1:B:669:ARG:HB2	1.97	0.46
1:A:192:GLY:O	1:A:221:ARG:HG3	2.16	0.46
1:B:577:LEU:CD2	1:B:593:LEU:HB3	2.46	0.46
1:A:433:ARG:NH1	1:B:547:GLN:OE1	2.49	0.46
1:A:529:GLN:HE21	1:A:529:GLN:HB3	1.64	0.45
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.52	0.45
1:A:215:ASP:HB2	1:A:228:THR:HG22	1.97	0.45
1:B:78:SER:HA	1:B:529:GLN:OE1	2.17	0.45
1:B:712:GLY:O	1:B:714:THR:HG23	2.17	0.45
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.52	0.44
1:A:72:THR:HG22	1:A:91:GLN:CB	2.47	0.44
1:B:72:THR:CA	1:B:92:PRO:HG3	2.35	0.44
1:B:519:GLU:HG3	1:B:549:PHE:HA	1.99	0.44
1:A:147:MET:HB3	1:A:281:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:HA	1:A:154:ILE:CD1	2.47	0.44
1:A:624:GLY:O	1:A:625:ASP:HB2	2.16	0.44
1:B:91:GLN:HE22	1:B:94:PRO:HB3	1.81	0.44
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.83	0.43
1:B:702:PHE:CD1	1:B:706:GLU:HG2	2.52	0.43
1:B:162:LEU:HD13	1:B:184:PHE:CD1	2.54	0.43
1:B:88:GLU:O	1:B:90:ARG:N	2.51	0.43
1:B:189:GLU:OE1	1:B:197:ARG:NH2	2.51	0.43
1:B:283:GLY:HA2	1:B:697:ASP:N	2.34	0.43
1:A:623:GLU:HB3	1:A:624:GLY:H	1.53	0.43
1:B:671:THR:HG22	1:B:672:ARG:N	2.34	0.43
1:A:131:ASN:HB2	1:A:177:ALA:HB2	2.01	0.43
1:B:135:ASN:OD1	1:B:186:ARG:N	2.42	0.42
1:B:100:ASP:HA	1:B:103:LYS:HE2	2.00	0.42
1:B:584:THR:HG22	1:B:585:GLY:N	2.34	0.42
1:A:583:LEU:CD1	1:A:589:THR:HG22	2.48	0.42
1:A:586:ASN:O	1:A:621:TYR:HA	2.20	0.42
1:A:670:VAL:HG23	1:A:671:THR:HG23	2.02	0.42
1:B:272:ALA:HA	1:B:295:SER:O	2.20	0.42
1:B:85:ASN:OD1	1:B:87:LYS:HB2	2.19	0.42
1:B:445:SER:O	1:B:445:SER:OG	2.37	0.42
1:A:670:VAL:CG2	1:A:671:THR:HG23	2.50	0.42
1:B:74:VAL:HG11	1:B:84:THR:HB	2.01	0.41
1:B:74:VAL:O	1:B:74:VAL:HG12	2.20	0.41
1:B:161:LYS:HB3	1:B:185:GLU:HG3	2.02	0.41
1:A:82:ILE:HD11	1:A:166:LYS:HE2	2.03	0.41
1:A:669:ARG:HG3	1:A:669:ARG:NH1	2.36	0.41
1:B:494:PRO:HB2	1:B:499:LEU:HG	2.03	0.41
1:B:504:ARG:NH1	1:B:562:SER:OG	2.51	0.41
1:B:671:THR:HG22	1:B:673:ASN:H	1.86	0.41
1:A:126:PHE:CG	1:A:127:GLY:N	2.88	0.41
1:B:465:LEU:HB3	1:B:491:GLU:HB2	2.03	0.41
1:A:642:ALA:O	1:A:652:ASP:HB2	2.21	0.41
1:A:292:LYS:HB2	1:A:322:ASP:HB3	2.02	0.40
1:A:403:ASP:HB2	1:A:440:ARG:HG2	2.03	0.40
1:B:74:VAL:O	1:B:75:ALA:C	2.60	0.40
1:B:203:LEU:HB3	1:B:211:ASP:HB2	2.03	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	649/723 (90%)	610 (94%)	32 (5%)	7 (1%)	14 31
1	B	658/723 (91%)	606 (92%)	40 (6%)	12 (2%)	8 19
All	All	1307/1446 (90%)	1216 (93%)	72 (6%)	19 (2%)	10 23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	MET
1	B	75	ALA
1	B	78	SER
1	B	90	ARG
1	B	558	MET
1	A	421	GLU
1	A	623	GLU
1	B	76	GLN
1	A	67	ALA
1	B	97	ASP
1	B	555	ARG
1	A	246	PRO
1	B	177	ALA
1	B	624	GLY
1	A	248	ARG
1	A	420	ALA
1	B	192	GLY
1	B	89	PRO
1	B	479	SER

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	523/572 (91%)	489 (94%)	34 (6%)	17 35
1	B	527/572 (92%)	479 (91%)	48 (9%)	9 20
All	All	1050/1144 (92%)	968 (92%)	82 (8%)	13 27

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	78	SER
1	A	90	ARG
1	A	97	ASP
1	A	103	LYS
1	A	126	PHE
1	A	134	THR
1	A	161	LYS
1	A	198	VAL
1	A	201	SER
1	A	203	LEU
1	A	228	THR
1	A	247	SER
1	A	248	ARG
1	A	263	ASP
1	A	300	PHE
1	A	313	GLU
1	A	388	MET
1	A	389	THR
1	A	479	SER
1	A	515	LYS
1	A	525	ASP
1	A	528	LEU
1	A	553	SER
1	A	566	THR
1	A	577	LEU
1	A	580	SER
1	A	592	SER
1	A	647	ASN
1	A	680	VAL
1	A	694	LYS
1	A	714	THR
1	A	717[A]	THR

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Mol	Chain	Res	Type
1	A	717[B]	THR
1	B	66	LEU
1	B	76	GLN
1	B	78	SER
1	B	97	ASP
1	B	119	ASP
1	B	139	MET
1	B	201	SER
1	B	248	ARG
1	B	255	ASP
1	B	256	VAL
1	B	267	LEU
1	B	292	LYS
1	B	305	VAL
1	B	306	SER
1	B	307	ASP
1	B	312	VAL
1	B	313	GLU
1	B	332	THR
1	B	341	MET
1	B	361	ARG
1	B	421	GLU
1	B	430	ARG
1	B	445	SER
1	B	448	MET
1	B	450	HIS
1	B	460	THR
1	B	467	SER
1	B	509	SER
1	B	510	VAL
1	B	530	TYR
1	B	553	SER
1	B	558	MET
1	B	559	MET
1	B	562	SER
1	B	566	THR
1	B	586	ASN
1	B	620	THR
1	B	631	LEU
1	B	649	VAL
1	B	656	SER
1	B	665	ASN

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Mol	Chain	Res	Type
1	B	672	ARG
1	B	673	ASN
1	B	682	ASN
1	B	689	THR
1	B	703	SER
1	B	717[A]	THR
1	B	717[B]	THR

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

Mol	Chain	Res	Type
1	A	304	ASN
1	A	531	ASN
1	A	547	GLN
1	B	230	ASN
1	B	253	ASN
1	B	682	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 monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	186:ARG	C	187:GLU	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.