



# Full wwPDB X-ray Structure Validation Report i

Nov 24, 2021 – 06:13 pm GMT

PDB ID : 6Z91  
Title : Copper transporter OprC  
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Deposited on : 2020-06-03  
Resolution : 2.60 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](mailto: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 i symbol.

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The following versions of software and data (see [references](#) ①) 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

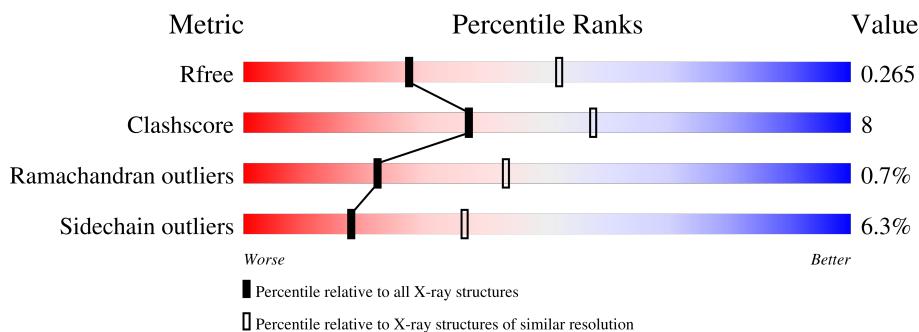
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

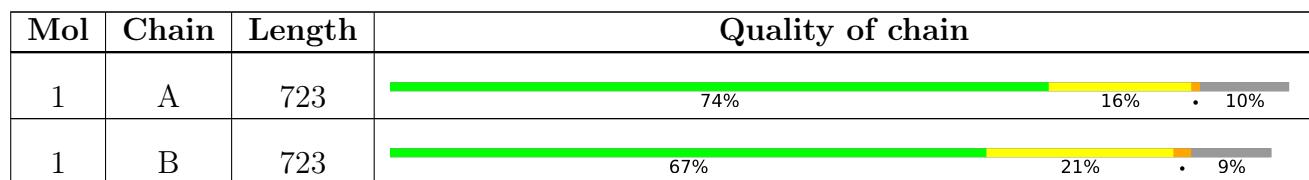
The reported resolution of this entry is 2.60 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10175 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
			Total	C	N	O	S			
1	A	653	5068	3182	895	975	16	4	1	0
1	B	656	5088	3192	900	979	17	4	1	0

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 3 3	0	0
2	B	3	Total Ag 3 3	0	0

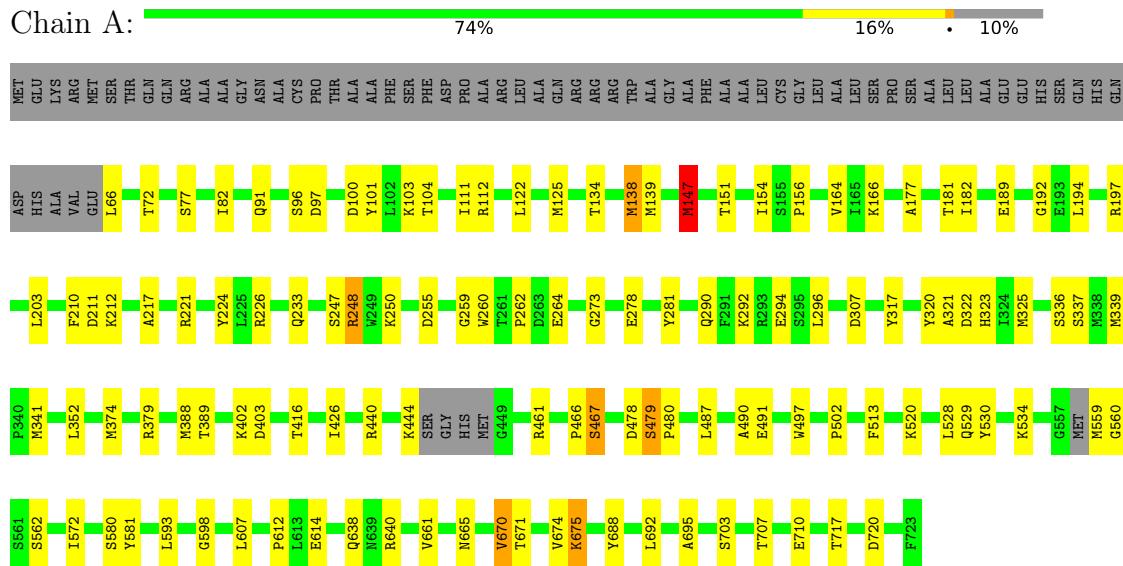
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	5	Total O 5 5	0	0

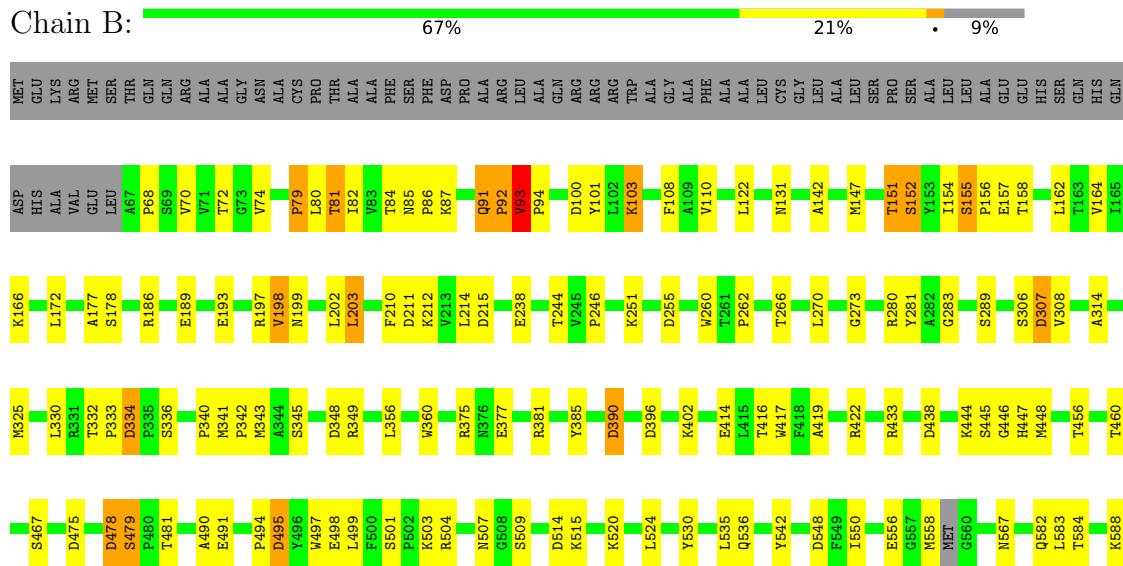
### 3 Residue-property plots [\(i\)](#)

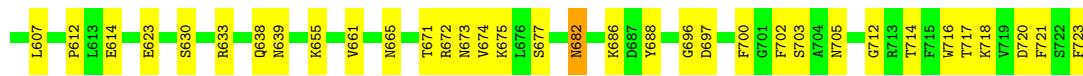
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



- Molecule 1: Putative copper transport outer membrane porin OprC





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.48Å 195.03Å 165.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.74 – 2.60 97.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (82.74-2.60) 99.8 (97.72-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.55 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
$R$ , $R_{free}$	0.222 , 0.262 0.224 , 0.265	Depositor DCC
$R_{free}$ test set	3846 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.9	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/5196	0.67	1/7043 (0.0%)
1	B	0.43	0/5218	0.66	3/7073 (0.0%)
All	All	0.45	0/10414	0.67	4/14116 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	343	MET	CA-CB-CG	-5.79	103.45	113.30
1	A	147	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	343	MET	CG-SD-CE	-5.36	91.62	100.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5068	0	4849	65	0
1	B	5088	0	4863	89	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
All	All	10175	0	9712	154	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 8.

All (154) 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:514:ASP:HB3	1:B:515:LYS:HD2	1.58	0.85
1:A:151:THR:HA	1:A:154:ILE:HD12	1.63	0.79
1:A:147:MET:HG2	1:A:281:TYR:CE2	2.18	0.79
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.69	0.74
1:B:72:THR:HA	1:B:91:GLN:HB3	1.71	0.72
1:B:103:LYS:HE2	1:B:110:VAL:HG21	1.72	0.70
1:B:422:ARG:HG2	1:B:475:ASP:HB2	1.74	0.69
1:B:671:THR:HG23	1:B:673:ASN:H	1.58	0.68
1:B:682:ASN:HD21	1:B:686:LYS:H	1.40	0.68
1:A:210:PHE:HE2	1:A:212:LYS:HE2	1.58	0.68
1:A:670:VAL:HG23	1:A:671:THR:HG23	1.75	0.67
1:B:100:ASP:HA	1:B:103:LYS:HE3	1.77	0.67
1:B:444:LYS:HE2	1:B:448:MET:HA	1.77	0.66
1:A:323:HIS:NE2	1:A:325:MET:HG3	2.10	0.66
1:B:74:VAL:HG11	1:B:84:THR:HB	1.77	0.66
1:B:68:PRO:O	1:B:675:LYS:NZ	2.28	0.66
1:A:255:ASP:OD1	1:A:273:GLY:HA3	1.96	0.66
1:A:189:GLU:OE1	1:A:197:ARG:NH2	2.27	0.64
1:B:612:PRO:HB3	1:B:638:GLN:HB2	1.78	0.64
1:A:670:VAL:HG22	1:A:674:VAL:HB	1.79	0.63
1:B:82:ILE:HB	1:B:164:VAL:HG22	1.78	0.63
1:B:478:ASP:N	1:B:478:ASP:OD1	2.31	0.63
1:A:147:MET:HG2	1:A:281:TYR:HE2	1.62	0.63
1:B:202:LEU:HD12	1:B:721:PHE:HE1	1.64	0.63
1:A:598:GLY:HA3	1:A:607:LEU:HD12	1.80	0.62
1:B:214:LEU:HD12	1:B:215:ASP:H	1.64	0.62
1:B:152:SER:O	1:B:251:LYS:NZ	2.29	0.61
1:B:307:ASP:OD1	1:B:307:ASP:N	2.35	0.60
1:B:238:GLU:HG2	1:B:244:THR:HG22	1.84	0.59
1:A:177:ALA:HB1	1:A:181:THR:HG22	1.84	0.59
1:B:497:TRP:O	1:B:501:SER:HB2	2.03	0.59
1:B:203:LEU:HD12	1:B:718:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ASN:HB3	1:B:655:LYS:HD3	1.84	0.58
1:B:147:MET:HG2	1:B:281:TYR:CE2	2.39	0.58
1:B:495:ASP:HB2	1:B:498:GLU:OE2	2.02	0.58
1:B:101:TYR:OH	1:B:157:GLU:HG2	2.04	0.57
1:B:198:VAL:HG13	1:B:723:PHE:HB2	1.87	0.57
1:A:379:ARG:HG2	1:A:402:LYS:HA	1.87	0.56
1:A:294:GLU:HB2	1:A:320:TYR:HB3	1.87	0.56
1:B:446:GLY:HA2	1:B:503:LYS:HE3	1.88	0.55
1:B:93:VAL:HG22	1:B:716:TRP:CD1	2.42	0.55
1:A:192:GLY:O	1:A:221:ARG:HG3	2.07	0.54
1:B:479:SER:HB2	1:B:481:THR:OG1	2.07	0.54
1:B:494:PRO:HB2	1:B:499:LEU:HG	1.89	0.54
1:A:139:MET:CE	1:A:321:ALA:HB2	2.38	0.54
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.43	0.53
1:B:84:THR:OG1	1:B:85:ASN:N	2.42	0.53
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.89	0.53
1:A:233:GLN:HB3	1:A:250:LYS:HG3	1.89	0.53
1:B:158:THR:HG22	1:B:186:ARG:HE	1.74	0.52
1:B:444:LYS:CE	1:B:448:MET:HA	2.39	0.52
1:B:142:ALA:HB2	1:B:349:ARG:HB2	1.90	0.52
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.45	0.52
1:B:214:LEU:HD12	1:B:215:ASP:N	2.25	0.52
1:B:682:ASN:ND2	1:B:686:LYS:H	2.08	0.52
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.45	0.51
1:B:262:PRO:HD2	1:B:266:THR:HB	1.92	0.51
1:B:438:ASP:OD2	1:B:456:THR:HG23	2.09	0.51
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.46	0.50
1:A:640:ARG:HG2	1:A:640:ARG:HH11	1.76	0.50
1:B:535:LEU:HD12	1:B:536:GLN:N	2.27	0.50
1:A:138:MET:CE	1:A:374:MET:HG3	2.42	0.49
1:B:131:ASN:HB2	1:B:177:ALA:HB2	1.93	0.49
1:B:151:THR:HA	1:B:154:ILE:HG13	1.94	0.49
1:B:671:THR:HG22	1:B:674:VAL:HG13	1.93	0.49
1:B:255:ASP:OD1	1:B:273:GLY:HA3	2.12	0.49
1:B:333:PRO:O	1:B:334:ASP:HB3	2.13	0.48
1:B:91:GLN:HG3	1:B:92:PRO:HG2	1.95	0.48
1:B:155:SER:O	1:B:158:THR:HB	2.13	0.48
1:A:403:ASP:HB2	1:A:440:ARG:HG2	1.95	0.48
1:A:478:ASP:OD2	1:A:478:ASP:N	2.43	0.48
1:B:246:PRO:HG2	1:B:700:PHE:HD2	1.77	0.48
1:A:72:THR:HG22	1:A:91:GLN:CB	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PRO:HD2	1:A:530:TYR:HE1	1.79	0.48
1:B:491:GLU:CD	1:B:520:LYS:HD3	2.34	0.48
1:B:614:GLU:OE1	1:B:633:ARG:NE	2.32	0.48
1:B:280:ARG:HD2	1:B:330:LEU:O	2.13	0.48
1:B:203:LEU:O	1:B:210:PHE:HA	2.13	0.47
1:A:467:SER:HB3	1:A:490:ALA:HA	1.96	0.47
1:A:177:ALA:CB	1:A:181:THR:HG22	2.44	0.47
1:A:203:LEU:HB3	1:A:211:ASP:HB2	1.95	0.47
1:B:82:ILE:HD11	1:B:166:LYS:HE2	1.97	0.46
1:B:467:SER:OG	1:B:490:ALA:HA	2.15	0.46
1:A:125:MET:HE1	1:A:572:ILE:HG21	1.98	0.46
1:B:94:PRO:HB2	1:B:101:TYR:CE1	2.51	0.46
1:A:100:ASP:HA	1:A:103:LYS:HD2	1.96	0.46
1:B:712:GLY:O	1:B:714:THR:HG23	2.16	0.46
1:A:91:GLN:OE1	1:A:665:ASN:HB3	2.16	0.46
1:A:125:MET:CE	1:A:572:ILE:HG21	2.45	0.46
1:A:497:TRP:O	1:A:502:PRO:HD3	2.16	0.46
1:B:84:THR:HG23	1:B:162:LEU:HB3	1.98	0.46
1:B:189:GLU:OE1	1:B:197:ARG:NH1	2.49	0.46
1:B:582:GLN:OE1	1:B:588:LYS:HE2	2.16	0.46
1:B:340:PRO:HD2	1:B:341:MET:CE	2.46	0.46
1:B:548:ASP:HB3	1:B:567:ASN:ND2	2.31	0.45
1:B:283:GLY:HA2	1:B:696:GLY:HA2	1.97	0.45
1:A:111:ILE:HG12	1:A:692:LEU:HB3	1.97	0.45
1:A:534:LYS:HB3	1:A:581:TYR:CE1	2.50	0.45
1:A:675:LYS:HG2	1:A:720:ASP:HB2	1.99	0.45
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.52	0.45
1:B:325:MET:HE3	1:B:345:SER:HB3	1.97	0.45
1:A:125:MET:CE	1:A:572:ILE:HD13	2.47	0.45
1:A:317:TYR:O	1:A:352:LEU:HD12	2.17	0.45
1:B:697:ASP:O	1:B:702:PHE:HB2	2.17	0.44
1:B:308:VAL:O	1:B:360:TRP:HA	2.17	0.44
1:A:290:GLN:CD	1:A:292:LYS:HE3	2.38	0.44
1:B:607:LEU:HD23	1:B:607:LEU:HA	1.88	0.44
1:B:172:LEU:HD21	1:B:414:GLU:HB2	2.00	0.43
1:B:203:LEU:HB3	1:B:211:ASP:HB2	1.99	0.43
1:A:466:PRO:O	1:A:491:GLU:HG3	2.19	0.43
1:A:529:GLN:HE21	1:A:529:GLN:HB3	1.61	0.43
1:A:138:MET:HE1	1:A:374:MET:HG3	2.01	0.43
1:B:444:LYS:NZ	1:B:448:MET:HA	2.34	0.43
1:A:224:TYR:CZ	1:A:259:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:PRO:HD2	1:B:385:TYR:CE1	2.54	0.43
1:B:385:TYR:OH	1:B:390:ASP:OD1	2.21	0.43
1:A:640:ARG:HG2	1:A:640:ARG:NH1	2.34	0.43
1:B:85:ASN:OD1	1:B:87:LYS:HB2	2.18	0.43
1:B:381:ARG:CZ	1:B:396:ASP:HA	2.48	0.43
1:A:307:ASP:OD1	1:A:307:ASP:N	2.50	0.42
1:A:248:ARG:NH2	1:A:278:GLU:OE1	2.52	0.42
1:A:461:ARG:NH1	1:A:513:PHE:O	2.46	0.42
1:A:112:ARG:NH2	1:A:710:GLU:OE1	2.53	0.42
1:B:108:PHE:CE1	1:B:122:LEU:HD13	2.53	0.42
1:B:583:LEU:HB2	1:B:584:THR:HG23	2.01	0.42
1:A:292:LYS:HB2	1:A:322:ASP:HB3	2.00	0.42
1:A:416:THR:HG23	1:A:426:ILE:HG13	2.02	0.42
1:B:498:GLU:HG2	1:B:550:ILE:HG21	2.02	0.42
1:A:260:TRP:CZ2	1:A:262:PRO:HG3	2.55	0.42
1:B:556:GLU:N	1:B:556:GLU:OE2	2.53	0.42
1:A:593:LEU:HA	1:A:614:GLU:O	2.20	0.42
1:A:661:VAL:HG21	1:A:688:TYR:CZ	2.54	0.42
1:A:695:ALA:HA	1:A:707:THR:HA	2.02	0.42
1:B:417:TRP:CE2	1:B:419:ALA:HB2	2.55	0.42
1:B:81:THR:HA	1:B:164:VAL:O	2.20	0.42
1:A:122:LEU:O	1:A:125:MET:HB2	2.20	0.41
1:A:491:GLU:OE1	1:A:520:LYS:HE2	2.21	0.41
1:A:164:VAL:HG22	1:A:182:ILE:HG12	2.03	0.41
1:A:337:SER:C	1:A:339:MET:H	2.23	0.41
1:B:193:GLU:OE1	1:B:193:GLU:N	2.48	0.41
1:A:559:MET:HB2	1:A:560:GLY:H	1.69	0.41
1:B:377:GLU:CD	1:B:402:LYS:HD2	2.41	0.41
1:B:86:PRO:HB2	1:B:156:PRO:O	2.20	0.41
1:B:314:ALA:HB2	1:B:356:LEU:HD13	2.02	0.41
1:A:444:LYS:H	1:A:444:LYS:HG3	1.68	0.41
1:B:199:ASN:HB3	1:B:215:ASP:HB3	2.03	0.41
1:A:82:ILE:HD11	1:A:166:LYS:HE2	2.03	0.40
1:B:332:THR:HA	1:B:333:PRO:HD3	1.97	0.40
1:A:210:PHE:CE2	1:A:212:LYS:HE2	2.47	0.40
1:A:217:ALA:HB2	1:A:226:ARG:HG3	2.02	0.40
1:B:524:LEU:O	1:B:542:TYR:HA	2.22	0.40
1:B:674:VAL:HA	1:B:720:ASP:O	2.21	0.40
1:B:246:PRO:HG2	1:B:700:PHE:CD2	2.55	0.40
1:A:403:ASP:HB2	1:A:440:ARG:CG	2.52	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	648/723 (90%)	607 (94%)	38 (6%)	3 (0%)	29 52
1	B	653/723 (90%)	605 (93%)	42 (6%)	6 (1%)	17 35
All	All	1301/1446 (90%)	1212 (93%)	80 (6%)	9 (1%)	22 43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	PRO
1	A	147	MET
1	B	151	THR
1	A	247	SER
1	B	334	ASP
1	B	445	SER
1	B	93	VAL
1	B	79	PRO
1	A	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	522/572 (91%)	496 (95%)	26 (5%)	24 47
1	B	524/572 (92%)	482 (92%)	42 (8%)	12 24
All	All	1046/1144 (91%)	978 (94%)	68 (6%)	18 34

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	77	SER
1	A	96	SER
1	A	97	ASP
1	A	104	THR
1	A	134	THR
1	A	138	MET
1	A	194	LEU
1	A	248	ARG
1	A	264	GLU
1	A	296	LEU
1	A	336	SER
1	A	341	MET
1	A	388	MET
1	A	389	THR
1	A	467	SER
1	A	479	SER
1	A	487	LEU
1	A	528	LEU
1	A	562	SER
1	A	580	SER
1	A	670	VAL
1	A	675	LYS
1	A	703	SER
1	A	717[A]	THR
1	A	717[B]	THR
1	B	70	VAL
1	B	79	PRO
1	B	80	LEU
1	B	81	THR
1	B	91	GLN
1	B	93	VAL
1	B	103	LYS
1	B	152	SER
1	B	155	SER
1	B	178	SER
1	B	198	VAL
1	B	203	LEU
1	B	212	LYS
1	B	270	LEU
1	B	289	SER
1	B	306	SER

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Mol	Chain	Res	Type
1	B	307	ASP
1	B	336	SER
1	B	375	ARG
1	B	390	ASP
1	B	416	THR
1	B	433	ARG
1	B	447	HIS
1	B	460	THR
1	B	478	ASP
1	B	479	SER
1	B	495	ASP
1	B	504	ARG
1	B	507	ASN
1	B	509	SER
1	B	530	TYR
1	B	558	MET
1	B	623	GLU
1	B	630	SER
1	B	665	ASN
1	B	672	ARG
1	B	677	SER
1	B	682	ASN
1	B	703	SER
1	B	705	ASN
1	B	717[A]	THR
1	B	717[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

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

## 5.6 Ligand geometry [\(i\)](#)

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 [\(i\)](#)

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 [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

### 6.3 Carbohydrates [\(i\)](#)

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

### 6.4 Ligands [\(i\)](#)

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

### 6.5 Other polymers [\(i\)](#)

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