Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:15 pm GMT

PDB ID	:	6Z8R
Title	:	Copper transporter OprC
Authors	:	Bhamidimarri, S.P.; van den Berg, B.
Deposited on	:	2020-06-02
Resolution	:	2.38 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:

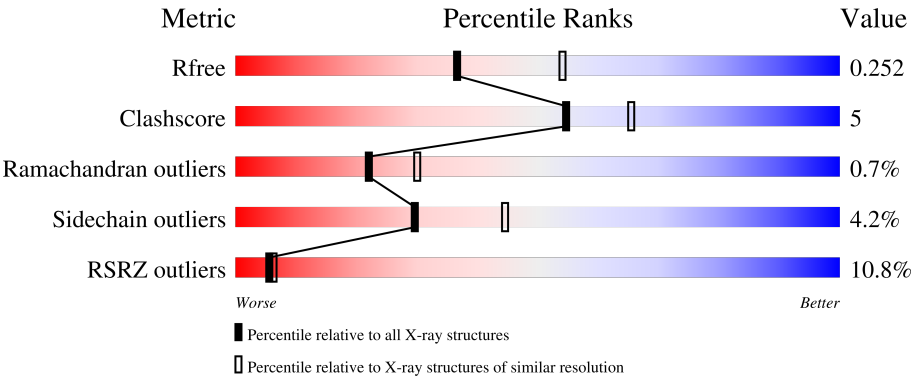
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	723	9% 78% 12% • 9%
1	B	723	10% 76% 14% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10293 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	655	Total	C	N	O	S	0	0	0
			5083	3190	899	976	18			
1	B	654	Total	C	N	O	S	0	0	0
			5075	3185	898	975	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	HIS	MET	engineered mutation	UNP G3XD89
B	147	HIS	MET	engineered mutation	UNP G3XD89

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

- Molecule 3 is water.

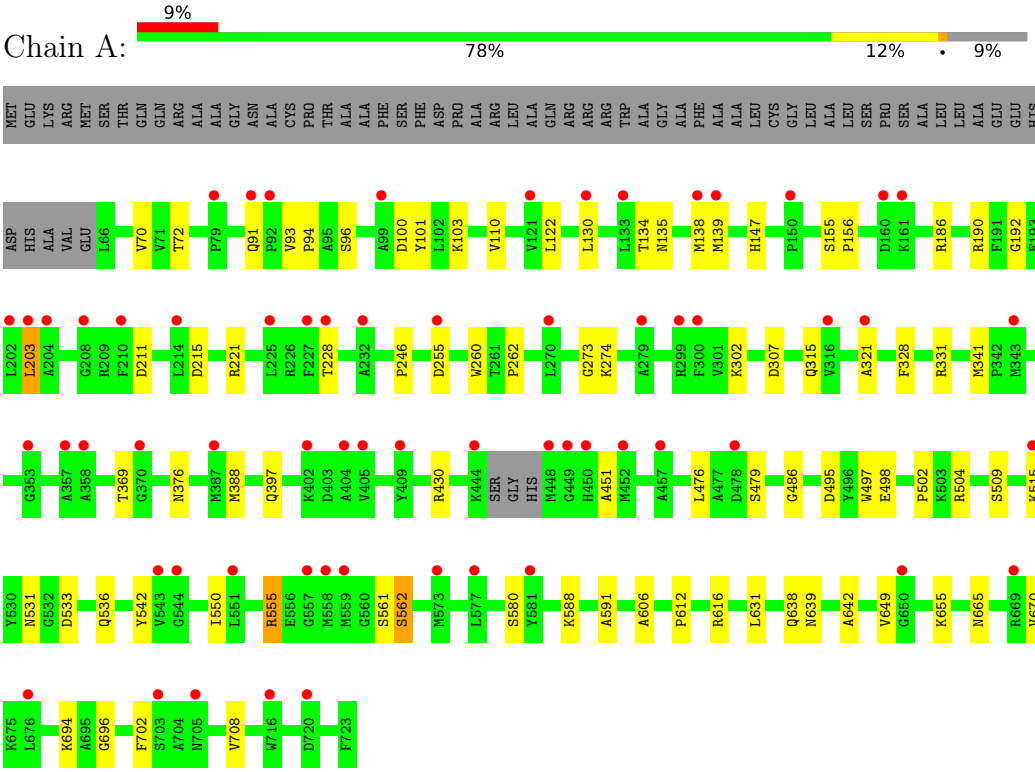
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		
3	B	39	Total	O	0	0
			39	39		

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.

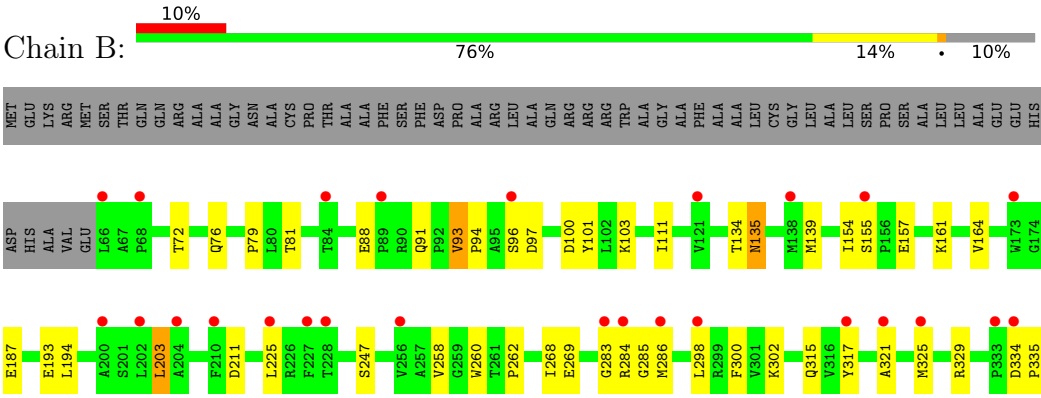
• Molecule 1: Putative copper transport outer membrane porin OprC

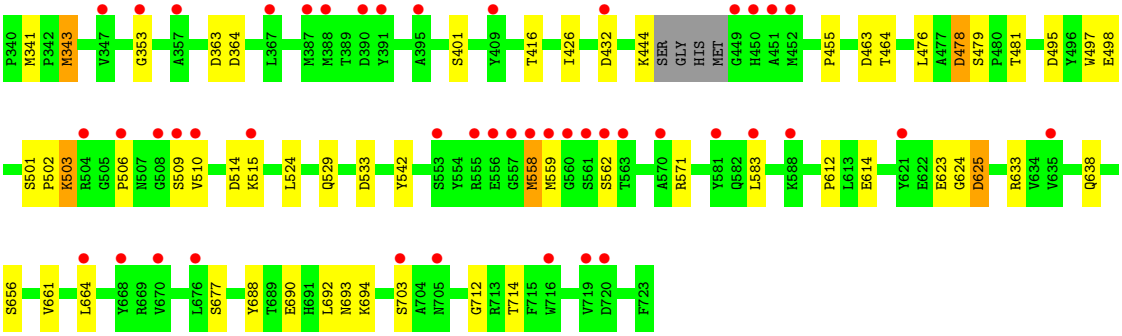
Chain A:



• Molecule 1: Putative copper transport outer membrane porin OprC

Chain B:




P340 M341 P342 M343 V347 G353 A357 D363 D364 L367 M387 M388 T389 D390 Y391 A395 S401 Y409 T416 I426 D432 K444 SER GLY HIS MET G449 H450 A451 M452 P455 D463 T464 L476 A477 D478 S479 P480 T481 D495 Y496 W497 E498
S501 P502 K503 R504 G505 P506 N507 G508 S509 V510 D514 K515 L524 Q529 D533 Y542 S553 Y554 R555 E556 G557 M558 M559 G560 S561 S562 T563 A570 R571 Y581 Q582 L583 K588 P612 L613 E614 Y621 E622 E623 G624 D625 R633 V634 V635 Q638
S656 V661 L664 Y668 R669 V670 L676 S677 Y688 T699 E690 H691 L692 N693 K694 S703 A704 N705 G712 R713 T714 F715 W716 V719 D720 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	155.03Å 196.86Å 165.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.44 – 2.38 98.09 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.44-2.38) 100.0 (98.09-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.217 , 0.252 0.218 , 0.252	Depositor DCC
R_{free} test set	4998 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10293	wwPDB-VP
Average B, all atoms (Å^2)	64.0	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.*

[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: CU

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	0.49	0/5210	0.65	1/7062 (0.0%)
1	B	0.45	0/5202	0.63	0/7052
All	All	0.47	0/10412	0.64	1/14114 (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	A	348	ASP	CB-CG-OD1	5.04	122.84	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	5083	0	4858	45	1
1	B	5075	0	4849	59	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	94	0	0	1	0
3	B	39	0	0	0	0
All	All	10293	0	9707	104	1

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 (104) 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:509:SER:HB3	1:B:515:LYS:HG3	1.69	0.74
1:A:91:GLN:HG3	1:A:665:ASN:HD22	1.54	0.71
1:B:76:GLN:HG2	1:B:529:GLN:HE22	1.57	0.69
1:B:503:LYS:HD3	1:B:562:SER:HB2	1.76	0.68
1:B:203:LEU:HB3	1:B:211:ASP:HB2	1.77	0.67
1:A:504:ARG:HH12	1:A:562:SER:HG	1.42	0.66
1:B:300:PHE:HE2	1:B:302:LYS:HB2	1.62	0.65
1:B:612:PRO:HB3	1:B:638:GLN:HB2	1.79	0.64
1:A:504:ARG:NH1	1:A:562:SER:OG	2.28	0.63
1:B:363:ASP:OD1	1:B:364:ASP:N	2.32	0.63
1:B:478:ASP:N	1:B:478:ASP:OD1	2.31	0.62
1:B:509:SER:CB	1:B:515:LYS:HG3	2.30	0.61
1:B:286:MET:SD	1:B:325:MET:HG3	2.42	0.60
1:A:91:GLN:HG3	1:A:665:ASN:ND2	2.18	0.59
1:B:284:ARG:NH1	1:B:285:GLY:H	2.00	0.59
1:A:671:THR:OG1	1:A:672:ARG:N	2.38	0.56
1:B:339:MET:HG2	1:B:343:MET:CE	2.36	0.56
1:B:72:THR:HG22	1:B:91:GLN:CB	2.36	0.55
1:B:100:ASP:HA	1:B:103:LYS:HD2	1.87	0.55
1:B:614:GLU:OE1	1:B:633:ARG:NE	2.32	0.55
1:A:255:ASP:OD2	1:A:273:GLY:HA3	2.08	0.54
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.89	0.54
1:A:649:VAL:O	1:A:694:LYS:NZ	2.35	0.54
1:B:300:PHE:CE2	1:B:302:LYS:HB2	2.45	0.52
1:A:215:ASP:OD1	1:A:228:THR:HG22	2.10	0.51
1:A:72:THR:HG22	1:A:91:GLN:CB	2.41	0.51
1:B:623:GLU:O	1:B:625:ASP:N	2.44	0.51
1:B:94:PRO:HG2	1:B:101:TYR:CZ	2.45	0.51
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.46	0.51
1:B:455:PRO:HG2	1:B:510:VAL:HB	1.92	0.50
1:B:111:ILE:HG12	1:B:692:LEU:HB3	1.93	0.50
1:B:135:ASN:O	1:B:315:GLN:NE2	2.40	0.50
1:B:164:VAL:HG22	1:B:182:ILE:HG12	1.94	0.49
1:A:72:THR:HB	1:A:631:LEU:HD13	1.94	0.48
1:A:486:GLY:O	1:A:524:LEU:HD12	2.13	0.48
1:A:495:ASP:HB3	1:A:497:TRP:H	1.79	0.48
1:A:94:PRO:HB3	1:A:100:ASP:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:OH	1:B:157:GLU:HG3	2.14	0.48
1:A:203:LEU:HB3	1:A:211:ASP:HB2	1.95	0.47
1:A:671:THR:CG2	1:A:674:VAL:HG13	2.44	0.47
1:B:72:THR:HG22	1:B:91:GLN:HB3	1.95	0.47
1:B:501:SER:N	1:B:502:PRO:HD2	2.29	0.47
1:A:591:ALA:HA	1:A:616:ARG:O	2.13	0.47
1:B:79:PRO:O	1:B:81:THR:HG23	2.14	0.47
1:A:555:ARG:HD2	1:A:555:ARG:HA	1.61	0.47
1:B:317:TYR:CZ	1:B:353:GLY:HA3	2.50	0.47
1:B:268:ILE:HG12	1:B:300:PHE:CD1	2.49	0.47
1:B:638:GLN:H	1:B:656:SER:HB3	1.80	0.47
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.51	0.46
1:B:225:LEU:CD2	1:B:258:VAL:HG22	2.45	0.46
1:B:76:GLN:HE21	1:B:529:GLN:NE2	2.12	0.46
1:A:639:ASN:HA	1:A:655:LYS:HG2	1.97	0.46
1:A:670:VAL:HB	1:A:674:VAL:HG22	1.97	0.46
1:B:495:ASP:HB2	1:B:498:GLU:OE1	2.15	0.46
1:A:199:ASN:HB2	1:A:215:ASP:HB3	1.98	0.45
1:B:571:ARG:HH11	1:B:571:ARG:HB3	1.81	0.45
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.97	0.45
1:B:339:MET:HG2	1:B:343:MET:HE1	1.98	0.45
1:A:103:LYS:HE3	1:A:110:VAL:HG21	1.98	0.45
1:B:476:LEU:HD12	1:B:481:THR:HB	1.99	0.45
1:B:497:TRP:O	1:B:501:SER:HB2	2.17	0.45
1:B:514:ASP:HB3	1:B:515:LYS:HG2	1.99	0.45
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.52	0.45
1:B:81:THR:HA	1:B:164:VAL:O	2.17	0.45
1:B:139:MET:HE1	1:B:321:ALA:HB2	1.99	0.45
1:A:135:ASN:O	1:A:315:GLN:NE2	2.48	0.44
1:A:91:GLN:CG	1:A:665:ASN:HB3	2.47	0.44
1:A:135:ASN:HD21	1:A:186:ARG:H	1.66	0.44
1:A:531:ASN:HA	1:A:536:GLN:OE1	2.18	0.44
1:A:497:TRP:O	1:A:502:PRO:HD3	2.17	0.44
1:B:161:LYS:HE3	1:B:187:GLU:OE2	2.17	0.44
1:B:269:GLU:O	1:B:298:LEU:HD12	2.18	0.44
1:A:606:ALA:O	1:A:642:ALA:HB2	2.18	0.44
1:B:93:VAL:HA	1:B:94:PRO:HD3	1.82	0.43
1:B:134:THR:HG21	1:B:154:ILE:HG12	2.00	0.43
1:B:690:GLU:H	1:B:693:ASN:ND2	2.17	0.43
1:B:506:PRO:O	1:B:509:SER:OG	2.21	0.43
1:B:524:LEU:O	1:B:542:TYR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:THR:HG23	1:B:426:ILE:HG13	2.00	0.43
1:B:515:LYS:HB3	1:B:515:LYS:HE3	1.84	0.43
1:A:192:GLY:O	1:A:221:ARG:HG3	2.18	0.43
1:A:524:LEU:O	1:A:542:TYR:HA	2.18	0.43
1:B:283:GLY:O	1:B:694:LYS:HE3	2.19	0.42
1:A:139:MET:CE	1:A:321:ALA:HB2	2.50	0.42
1:B:571:ARG:HB3	1:B:571:ARG:NH1	2.34	0.42
1:B:614:GLU:CD	1:B:633:ARG:HE	2.22	0.42
1:A:498:GLU:HG2	1:A:550:ILE:HG21	2.01	0.42
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.81	0.42
1:A:350:ARG:O	1:A:376:ASN:HA	2.20	0.41
1:B:463:ASP:OD1	1:B:464:THR:N	2.48	0.41
1:A:509:SER:O	3:A:901:HOH:O	2.22	0.41
1:A:529:GLN:HE21	1:A:529:GLN:HB3	1.60	0.41
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.56	0.41
1:A:70:VAL:HG21	1:A:665:ASN:HB2	2.02	0.41
1:A:122:LEU:HD23	1:A:130:LEU:HD21	2.03	0.41
1:B:334:ASP:HA	1:B:335:PRO:HD3	1.87	0.41
1:B:193:GLU:OE1	1:B:194:LEU:N	2.51	0.41
1:B:503:LYS:HZ2	1:B:503:LYS:HG2	1.79	0.41
1:B:712:GLY:O	1:B:714:THR:HG23	2.21	0.41
1:A:694:LYS:O	1:A:708:VAL:HG23	2.21	0.40
1:A:671:THR:HG23	1:A:674:VAL:H	1.85	0.40
1:A:696:GLY:HA3	1:A:702:PHE:CG	2.56	0.40
1:A:328:PHE:HA	1:A:331:ARG:O	2.21	0.40
1:B:175:PRO:HB3	1:B:432:ASP:CG	2.41	0.40

All (1) 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)
1:A:274:LYS:NZ	1:B:625:ASP:OD1[6_554]	2.13	0.07

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	651/723 (90%)	618 (95%)	30 (5%)	3 (0%)	29	39
1	B	650/723 (90%)	622 (96%)	22 (3%)	6 (1%)	17	23
All	All	1301/1446 (90%)	1240 (95%)	52 (4%)	9 (1%)	22	30

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	A	451	ALA
1	B	93	VAL
1	B	559	MET
1	B	624	GLY
1	B	247	SER
1	B	558	MET
1	B	583	LEU
1	A	246	PRO

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	524/573 (91%)	500 (95%)	24 (5%)	27	40
1	B	523/573 (91%)	503 (96%)	20 (4%)	33	49
All	All	1047/1146 (91%)	1003 (96%)	44 (4%)	30	44

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	134	THR
1	A	138	MET
1	A	147	HIS

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Mol	Chain	Res	Type
1	A	155	SER
1	A	190	ARG
1	A	203	LEU
1	A	302	LYS
1	A	307	ASP
1	A	341	MET
1	A	369	THR
1	A	388	MET
1	A	397	GLN
1	A	430	ARG
1	A	476	LEU
1	A	479	SER
1	A	515	LYS
1	A	533	ASP
1	A	555	ARG
1	A	561	SER
1	A	562	SER
1	A	580	SER
1	A	588	LYS
1	A	672	ARG
1	B	88	GLU
1	B	96	SER
1	B	97	ASP
1	B	135	ASN
1	B	155	SER
1	B	203	LEU
1	B	329	ARG
1	B	341	MET
1	B	343	MET
1	B	401	SER
1	B	444	LYS
1	B	478	ASP
1	B	479	SER
1	B	503	LYS
1	B	533	ASP
1	B	558	MET
1	B	625	ASP
1	B	664	LEU
1	B	677	SER
1	B	703	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	199	ASN
1	A	665	ASN
1	B	529	GLN
1	B	531	ASN
1	B	536	GLN
1	B	673	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 2 ligands modelled in this entry, 2 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

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	655/723 (90%)	1.11	66 (10%) 7 7	47, 57, 85, 130	0
1	B	654/723 (90%)	1.16	75 (11%) 4 5	50, 66, 90, 118	0
All	All	1309/1446 (90%)	1.13	141 (10%) 5 6	47, 62, 89, 130	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	MET	9.8
1	B	557	GLY	9.4
1	B	558	MET	8.0
1	A	559	MET	7.6
1	A	448	MET	7.2
1	B	510	VAL	7.1
1	B	509	SER	7.0
1	A	557	GLY	6.9
1	B	705	ASN	5.7
1	A	558	MET	5.6
1	B	66	LEU	4.8
1	B	338	MET	4.5
1	B	138	MET	4.4
1	B	560	GLY	4.3
1	B	508	GLY	3.8
1	B	84	THR	3.7
1	A	452	MET	3.6
1	B	336	SER	3.6
1	B	391	TYR	3.6
1	B	504	ARG	3.3
1	B	390	ASP	3.3
1	B	555	ARG	3.3
1	B	621	TYR	3.3
1	B	155	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	402	LYS	3.2
1	A	228	THR	3.2
1	B	450	HIS	3.1
1	B	449	GLY	3.1
1	A	92	PRO	3.1
1	A	669	ARG	3.0
1	A	227	PHE	3.0
1	A	91	GLN	3.0
1	A	202	LEU	2.9
1	A	138	MET	2.9
1	A	457	ALA	2.9
1	B	68	PRO	2.9
1	A	478	ASP	2.9
1	A	347	VAL	2.9
1	A	676	LEU	2.9
1	B	670	VAL	2.8
1	A	515	LYS	2.7
1	A	225	LEU	2.7
1	B	452	MET	2.7
1	A	450	HIS	2.7
1	B	334	ASP	2.7
1	B	451	ALA	2.7
1	B	387	MET	2.7
1	A	358	ALA	2.6
1	B	283	GLY	2.6
1	B	210	PHE	2.6
1	A	204	ALA	2.6
1	B	720	ASP	2.6
1	B	298	LEU	2.6
1	A	279	ALA	2.5
1	A	343	MET	2.5
1	B	256	VAL	2.5
1	A	203	LEU	2.5
1	A	79	PRO	2.5
1	B	333	PRO	2.5
1	B	347	VAL	2.5
1	A	214	LEU	2.5
1	A	270	LEU	2.5
1	A	387	MET	2.4
1	A	409	TYR	2.4
1	B	515	LYS	2.4
1	B	719	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	353	GLY	2.4
1	A	577	LEU	2.4
1	B	563	THR	2.4
1	B	409	TYR	2.4
1	A	161	LYS	2.4
1	A	150	PRO	2.4
1	B	506	PRO	2.4
1	B	286	MET	2.4
1	A	581	TYR	2.3
1	B	204	ALA	2.3
1	B	339	MET	2.3
1	B	635	VAL	2.3
1	B	284	ARG	2.3
1	A	543	VAL	2.3
1	B	395	ALA	2.3
1	A	139	MET	2.3
1	B	432	ASP	2.3
1	B	321	ALA	2.3
1	B	553	SER	2.3
1	B	562	SER	2.3
1	A	194	LEU	2.2
1	A	353	GLY	2.2
1	A	449	GLY	2.2
1	A	544	GLY	2.2
1	B	588	LYS	2.2
1	A	300	PHE	2.2
1	A	316	VAL	2.2
1	A	703	SER	2.2
1	A	705	ASN	2.2
1	B	581	TYR	2.2
1	A	208	GLY	2.2
1	A	160	ASP	2.2
1	A	573	MET	2.2
1	B	388	MET	2.2
1	B	668	TYR	2.2
1	A	720	ASP	2.2
1	B	556	GLU	2.2
1	B	173	TRP	2.2
1	B	225	LEU	2.2
1	B	583	LEU	2.2
1	B	703	SER	2.2
1	B	317	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	210	PHE	2.1
1	B	664	LEU	2.1
1	B	89	PRO	2.1
1	B	716	TRP	2.1
1	B	570	ALA	2.1
1	B	96	SER	2.1
1	A	716	TRP	2.1
1	A	357	ALA	2.1
1	A	405	VAL	2.1
1	B	561	SER	2.1
1	B	202	LEU	2.1
1	B	325	MET	2.1
1	A	232	ALA	2.1
1	B	121	VAL	2.1
1	A	370	GLY	2.1
1	B	367	LEU	2.1
1	A	199	ASN	2.1
1	B	200	ALA	2.1
1	A	130	LEU	2.0
1	B	228	THR	2.0
1	A	404	ALA	2.0
1	B	357	ALA	2.0
1	A	133	LEU	2.0
1	B	676	LEU	2.0
1	A	99	ALA	2.0
1	A	299	ARG	2.0
1	A	121	VAL	2.0
1	B	227	PHE	2.0
1	A	551	LEU	2.0
1	A	650	GLY	2.0
1	A	255	ASP	2.0
1	A	321	ALA	2.0
1	A	444	LYS	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

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	CU	B	801	1/1	0.94	0.15	71,71,71,71	0
2	CU	A	801	1/1	0.98	0.13	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.