



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:43 AM UTC

PDB ID : 6Z8R / pdb_00006z8r
Title : Copper transporter OprC
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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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

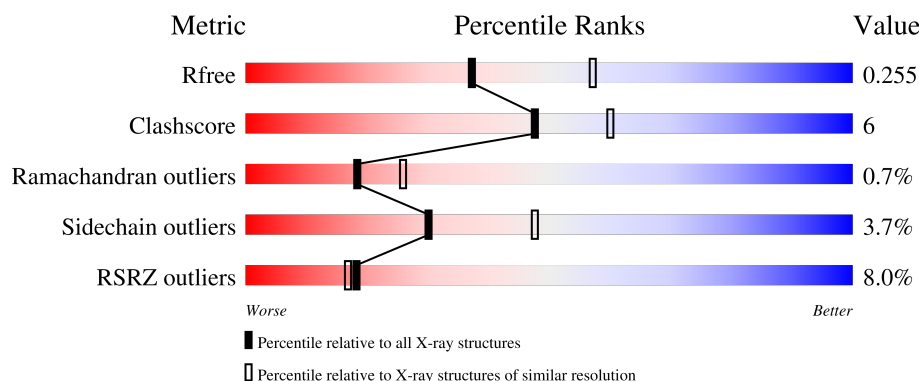
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

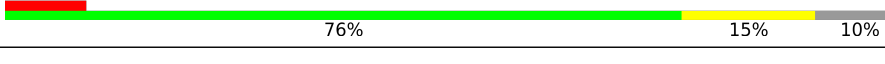
The reported resolution of this entry is 2.38 Å.

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 $\leq 5\%$. 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	 6% 77% 12% 9%
1	B	723	 9% 76% 15% 10%

2 Entry composition

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 (CCD ID: 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		

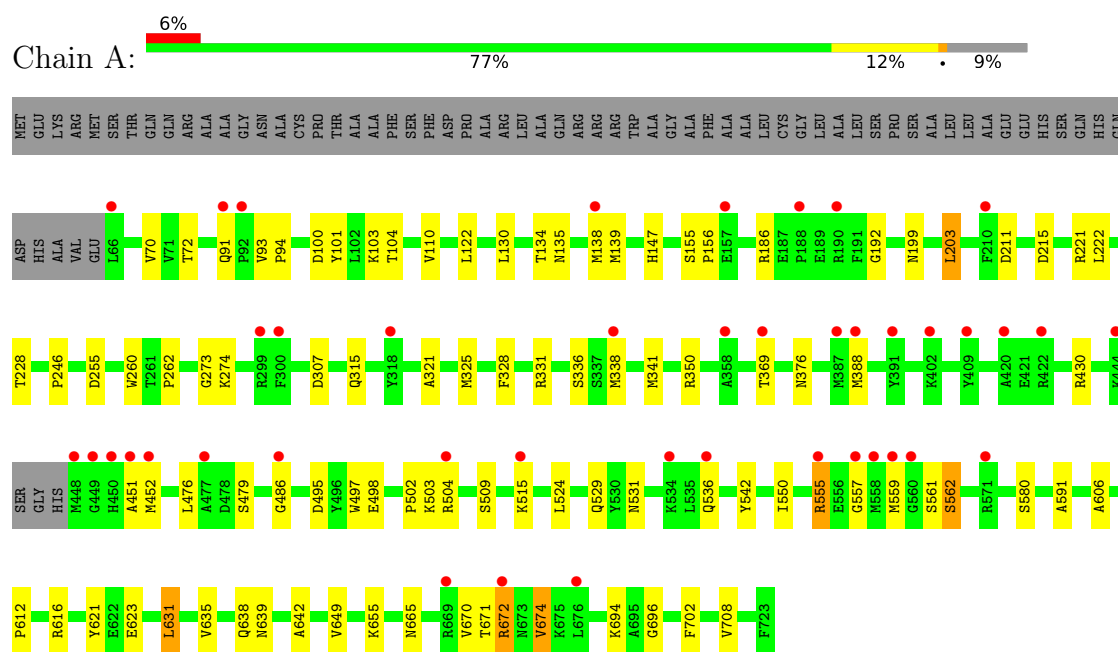
- Molecule 3 is water.

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

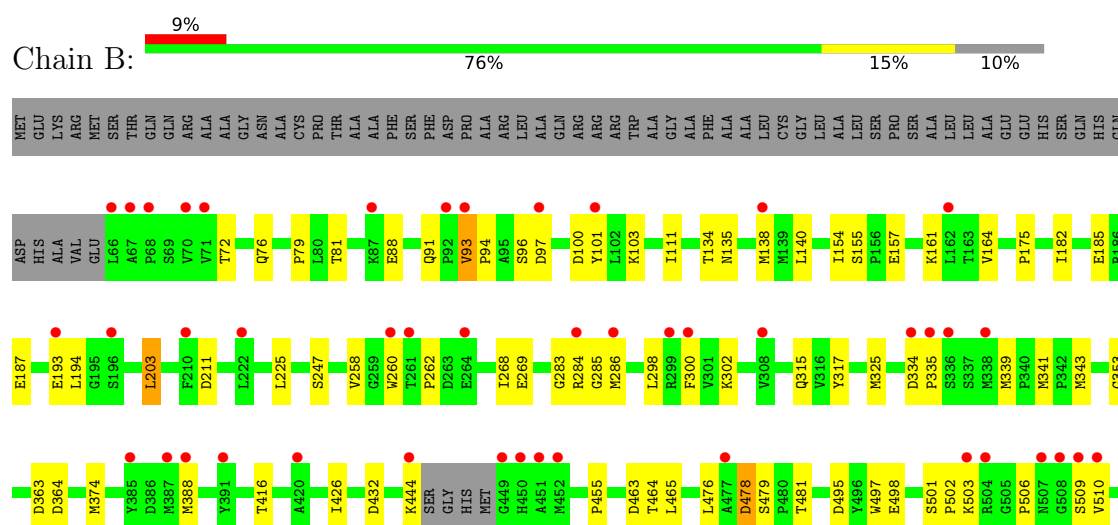
3 Residue-property plots

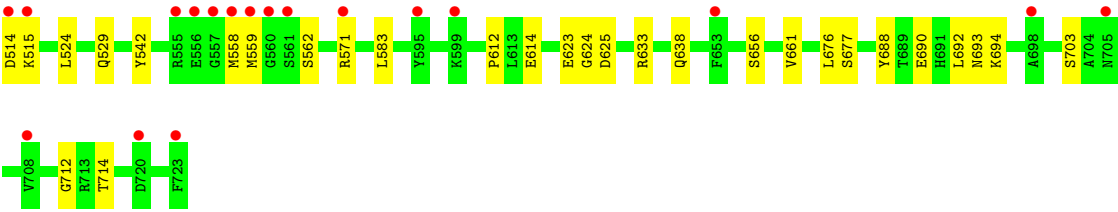
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Putative copper transport outer membrane porin OprC





4 Data and refinement statistics

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 68.44 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.44-2.38) 100.0 (68.44-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.217 , 0.252 0.221 , 0.255	Depositor DCC
R_{free} test set	4999 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)	0.32 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.41	0/5210	0.61	0/7062
1	B	0.37	0/5202	0.58	0/7052
All	All	0.39	0/10412	0.59	0/14114

There are no bond length outliers.

There are no bond angle outliers.

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	5083	0	4858	49	1
1	B	5075	0	4849	62	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	111	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 6.

All (111) 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:A:504:ARG:HH12	1:A:562:SER:HG	1.39	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: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:B:339:MET:HG2	1:B:343:MET:HE1	1.83	0.59
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:138:MET:HE3	1:B:140:LEU:HD11	1.90	0.53
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:614:GLU:CD	1:B:633:ARG:HE	2.22	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:147:HIS:NE2	1:A:325:MET:HE3	2.31	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: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:A:621:TYR:OH	1:A:623:GLU:OE2	2.33	0.45
1:B:175:PRO:HB3	1:B:432:ASP:CG	2.41	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:A:135:ASN:O	1:A:315:GLN:NE2	2.48	0.44
1:B:325:MET:HE2	1:B:325:MET:HB3	1.73	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:A:338:MET:HE1	1:A:559:MET:O	2.18	0.43
1:B:690:GLU:H	1:B:693:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:557:GLY:C	1:A:559:MET:H	2.26	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: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:374:MET:HE3	1:B:374:MET:HB3	1.83	0.41
1:B:676:LEU:HD23	1:B:676:LEU:C	2.45	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

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

5.3.1 Protein backbone

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%)	24	34
1	B	650/723 (90%)	622 (96%)	22 (3%)	6 (1%)	14	20
All	All	1301/1446 (90%)	1240 (95%)	52 (4%)	9 (1%)	18	26

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

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%)	499 (95%)	25 (5%)	23	37
1	B	523/573 (91%)	509 (97%)	14 (3%)	39	59
All	All	1047/1146 (91%)	1008 (96%)	39 (4%)	30	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	134	THR
1	A	138	MET
1	A	155	SER
1	A	203	LEU
1	A	222	LEU
1	A	307	ASP
1	A	336	SER
1	A	341	MET
1	A	369	THR
1	A	388	MET
1	A	430	ARG
1	A	452	MET
1	A	476	LEU
1	A	479	SER
1	A	503	LYS
1	A	515	LYS
1	A	555	ARG
1	A	561	SER
1	A	562	SER
1	A	580	SER
1	A	631	LEU
1	A	635	VAL
1	A	672	ARG
1	A	674	VAL
1	B	88	GLU
1	B	96	SER
1	B	97	ASP
1	B	155	SER
1	B	185	GLU
1	B	203	LEU
1	B	341	MET
1	B	388	MET
1	B	444	LYS
1	B	465	LEU
1	B	478	ASP
1	B	479	SER
1	B	677	SER
1	B	703	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	135	ASN
1	A	199	ASN
1	A	233	GLN
1	A	507	ASN
1	A	529	GLN
1	A	665	ASN
1	B	76	GLN
1	B	408	ASN
1	B	529	GLN
1	B	536	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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, 95th 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%)	0.69	42 (6%)	25 24	47, 57, 85, 130	0
1	B	654/723 (90%)	0.90	63 (9%)	13 12	50, 66, 90, 118	0
All	All	1309/1446 (90%)	0.79	105 (8%)	18 17	47, 62, 89, 130	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	8.9
1	B	557	GLY	7.3
1	A	66	LEU	7.2
1	B	558	MET	6.8
1	A	557	GLY	6.6
1	B	510	VAL	5.8
1	A	559	MET	5.7
1	B	449	GLY	5.5
1	A	448	MET	5.2
1	B	338	MET	5.2
1	A	444	LYS	5.2
1	B	559	MET	4.7
1	A	92	PRO	4.7
1	B	555	ARG	4.7
1	A	450	HIS	4.7
1	A	558	MET	4.6
1	A	91	GLN	4.5
1	B	92	PRO	4.3
1	B	504	ARG	4.2
1	B	560	GLY	4.2
1	B	444	LYS	4.1
1	B	387	MET	3.9
1	B	508	GLY	3.8
1	A	451	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	449	GLY	3.7
1	B	503	LYS	3.6
1	B	284	ARG	3.4
1	B	450	HIS	3.3
1	B	420	ALA	3.3
1	B	509	SER	3.3
1	A	387	MET	3.2
1	B	388	MET	3.2
1	A	388	MET	3.2
1	A	338	MET	3.0
1	B	556	GLU	3.0
1	B	515	LYS	3.0
1	B	391	TYR	2.9
1	A	138	MET	2.9
1	A	560	GLY	2.9
1	B	260	TRP	2.9
1	A	369	THR	2.9
1	B	68	PRO	2.9
1	B	138	MET	2.8
1	B	705	ASN	2.8
1	A	210	PHE	2.8
1	B	210	PHE	2.8
1	B	561	SER	2.7
1	A	534	LYS	2.7
1	B	452	MET	2.7
1	B	70	VAL	2.7
1	A	190	ARG	2.7
1	B	101	TYR	2.7
1	B	514	ASP	2.7
1	A	571	ARG	2.7
1	B	222	LEU	2.7
1	B	334	ASP	2.6
1	B	723	PHE	2.6
1	B	93	VAL	2.6
1	B	477	ALA	2.6
1	B	71	VAL	2.6
1	B	507	ASN	2.5
1	A	486	GLY	2.5
1	B	300	PHE	2.5
1	A	409	TYR	2.5
1	B	595	TYR	2.5
1	A	555	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	391	TYR	2.4
1	B	87	LYS	2.4
1	A	672	ARG	2.4
1	B	336	SER	2.4
1	A	300	PHE	2.4
1	A	318	TYR	2.4
1	A	188	PRO	2.3
1	A	477	ALA	2.3
1	B	308	VAL	2.3
1	A	402	LYS	2.3
1	A	452	MET	2.3
1	B	193	GLU	2.3
1	B	720	ASP	2.3
1	A	536	GLN	2.3
1	B	335	PRO	2.2
1	B	708	VAL	2.2
1	B	97	ASP	2.2
1	B	571	ARG	2.2
1	A	358	ALA	2.2
1	B	286	MET	2.2
1	B	261	THR	2.2
1	B	385	TYR	2.2
1	A	422	ARG	2.2
1	A	669	ARG	2.2
1	B	653	PHE	2.2
1	B	698	ALA	2.1
1	A	515	LYS	2.1
1	B	599	LYS	2.1
1	A	157	GLU	2.1
1	B	299	ARG	2.1
1	A	420	ALA	2.1
1	B	67	ALA	2.1
1	A	299	ARG	2.1
1	B	196	SER	2.0
1	B	451	ALA	2.0
1	A	676	LEU	2.0
1	A	504	ARG	2.0
1	B	264	GLU	2.0
1	B	162	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	CU	B	801	1/1	0.97	0.05	71,71,71,71	0
2	CU	A	801	1/1	0.99	0.04	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.