



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 6Z8S / pdb_00006z8s
Title : Copper transporter OprC
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Deposited on : 2020-06-02
Resolution : 2.37 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

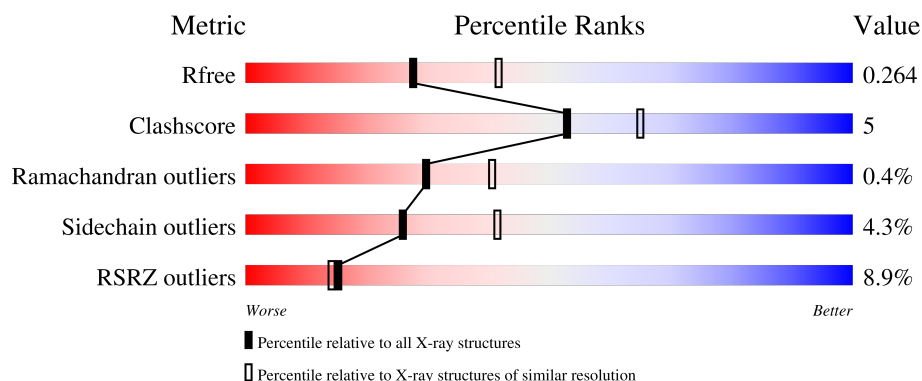
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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% 81% 9% • 9%
1	B	723	10% 76% 14% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10273 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
			5081	3188	899	977	17			
1	B	655	Total	C	N	O	S	0	0	0
			5083	3190	899	976	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	MET	engineered mutation	UNP G3XD89
B	325	HIS	MET	engineered mutation	UNP G3XD89

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (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		

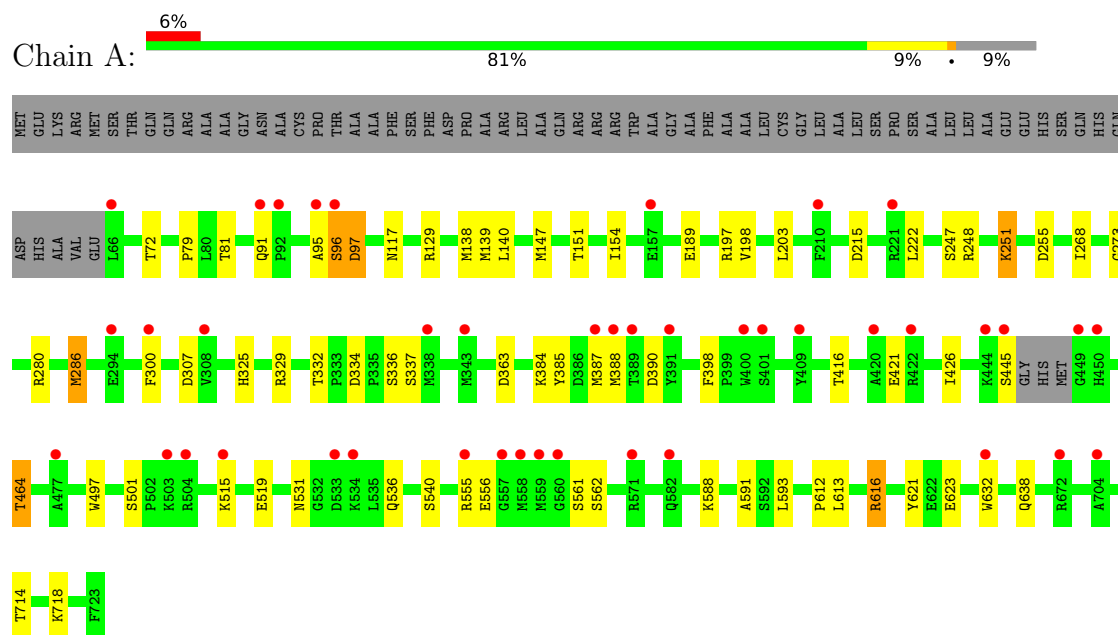
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	35	Total	O	0	0
			35	35		

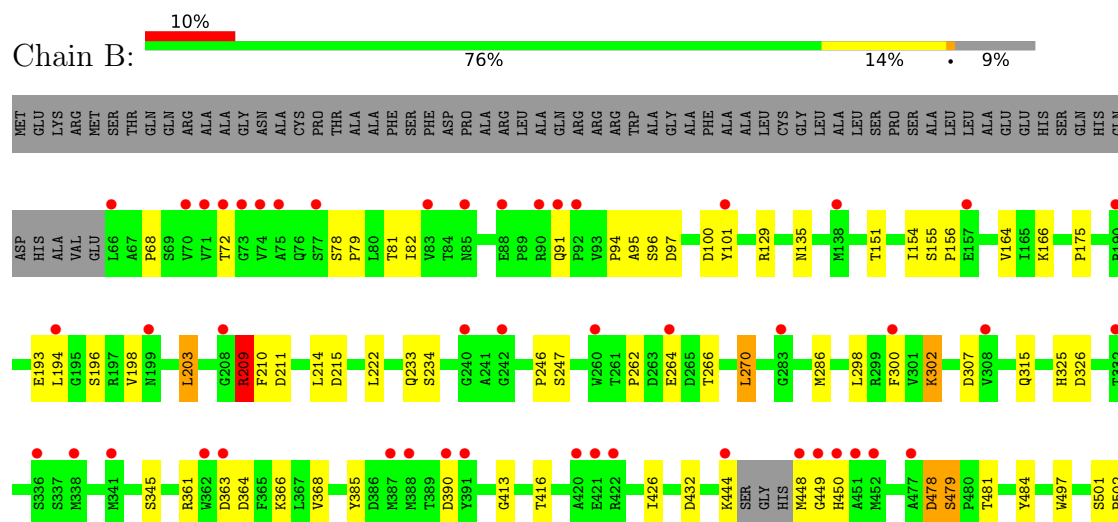
3 Residue-property plots

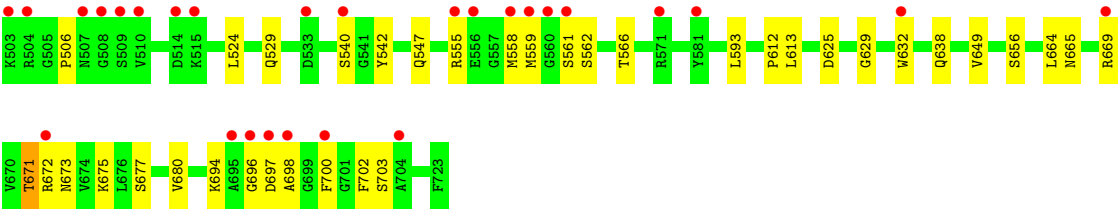
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	156.10Å 195.69Å 166.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.02 – 2.37 61.02 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.7 (61.02-2.37) 99.9 (61.02-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.219 , 0.252 (Not available) , 0.264	Depositor DCC
R_{free} test set	5167 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	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	10273	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: CU1

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	0.40	0/5208	0.60	0/7060
1	B	0.38	1/5210 (0.0%)	0.57	3/7062 (0.0%)
All	All	0.39	1/10418 (0.0%)	0.59	3/14122 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	555	ARG	CD-NE	5.44	1.53	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	555	ARG	CG-CD-NE	8.25	130.15	112.00
1	B	555	ARG	CB-CG-CD	5.42	123.77	111.30
1	B	559	MET	N-CA-C	-5.00	107.03	114.64

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	5081	0	4854	39	0
1	B	5083	0	4858	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	72	0	0	1	0
3	B	35	0	0	0	0
All	All	10273	0	9712	100	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 5.

All (100) 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:671:THR:HG22	1:B:673:ASN:H	1.26	0.96
1:B:151:THR:HA	1:B:154:ILE:HD12	1.59	0.85
1:A:286:MET:HE3	1:A:325:HIS:CD2	2.13	0.83
1:A:117:ASN:OD1	1:A:251:LYS:NZ	2.14	0.80
1:A:555:ARG:HH21	1:A:556:GLU:HB2	1.48	0.78
1:B:94:PRO:O	1:B:209:ARG:NH2	2.19	0.76
1:A:95:ALA:O	1:A:97:ASP:N	2.22	0.72
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.73	0.70
1:A:555:ARG:NH2	1:A:556:GLU:HB2	2.07	0.70
1:B:448:MET:HE2	1:B:450:HIS:HD2	1.57	0.69
1:A:385:TYR:OH	1:A:390:ASP:OD1	2.08	0.67
1:B:286:MET:HE2	1:B:325:HIS:CD2	2.30	0.67
1:A:388:MET:HE3	1:A:388:MET:HA	1.77	0.67
1:A:286:MET:HE3	1:A:325:HIS:HD2	1.58	0.66
1:B:82:ILE:HD11	1:B:166:LYS:HE2	1.78	0.66
1:B:649:VAL:O	1:B:694:LYS:HE2	1.98	0.63
1:A:555:ARG:NE	1:A:556:GLU:H	1.98	0.62
1:B:264:GLU:H	1:B:264:GLU:CD	2.07	0.61
1:B:193:GLU:N	1:B:193:GLU:OE1	2.34	0.60
1:B:72:THR:HG22	1:B:91:GLN:HB2	1.87	0.57
1:B:300:PHE:HE1	1:B:302:LYS:HB2	1.70	0.57
1:B:625:ASP:HB2	1:B:669:ARG:HB2	1.87	0.56
1:A:334:ASP:HB3	1:A:337:SER:HB3	1.87	0.56
1:A:189:GLU:OE2	1:A:197:ARG:NH1	2.39	0.56
1:B:612:PRO:HB3	1:B:638:GLN:HB2	1.87	0.55
1:B:68:PRO:HB3	1:B:675:LYS:HD2	1.89	0.55
1:B:270:LEU:HD12	1:B:298:LEU:HD13	1.89	0.55
1:A:197:ARG:NH2	1:A:215:ASP:OD1	2.40	0.54
1:A:416:THR:HG23	1:A:426:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:MET:HG2	1:B:450:HIS:HB2	1.90	0.54
1:B:95:ALA:HA	1:B:209:ARG:NH2	2.22	0.54
1:A:255:ASP:OD2	1:A:273:GLY:HA3	2.09	0.53
1:A:464:THR:HG23	1:B:547:GLN:OE1	2.09	0.53
1:B:79:PRO:O	1:B:81:THR:HG23	2.09	0.52
1:B:214:LEU:HD12	1:B:215:ASP:H	1.75	0.52
1:B:484:TYR:HH	1:B:540:SER:HG	1.51	0.52
1:A:79:PRO:O	1:A:81:THR:HG23	2.09	0.52
1:A:248:ARG:HD3	1:A:280:ARG:NH2	2.26	0.51
1:B:262:PRO:HD2	1:B:266:THR:HB	1.93	0.51
1:A:621:TYR:OH	1:A:623:GLU:OE2	2.25	0.50
1:B:209:ARG:HA	1:B:233:GLN:O	2.11	0.50
1:B:385:TYR:OH	1:B:390:ASP:OD2	2.22	0.50
1:B:286:MET:CE	1:B:325:HIS:CD2	2.95	0.50
1:B:448:MET:HE2	1:B:450:HIS:CD2	2.44	0.50
1:B:209:ARG:H	1:B:234:SER:HA	1.77	0.49
1:A:96:SER:O	1:A:251:LYS:HE2	2.12	0.49
1:B:72:THR:HG22	1:B:91:GLN:CB	2.42	0.49
1:A:268:ILE:HG12	1:A:300:PHE:HD1	1.77	0.48
1:B:286:MET:HE3	1:B:326:ASP:CA	2.43	0.48
1:A:531:ASN:HD22	1:A:536:GLN:HE21	1.61	0.48
1:B:671:THR:HG22	1:B:673:ASN:N	2.10	0.48
1:B:484:TYR:OH	1:B:540:SER:OG	2.25	0.48
1:B:363:ASP:OD1	1:B:364:ASP:N	2.38	0.48
1:B:286:MET:CE	1:B:325:HIS:HD2	2.27	0.47
1:A:387:MET:O	1:A:387:MET:HE3	2.14	0.47
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.49	0.47
1:A:129:ARG:HD3	1:A:519:GLU:OE2	2.14	0.47
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.96	0.46
1:A:138:MET:CE	1:A:140:LEU:HD21	2.45	0.46
1:B:361:ARG:NH2	1:B:366:LYS:HE3	2.31	0.46
1:B:368:VAL:O	1:B:413:GLY:HA2	2.15	0.46
1:A:388:MET:HA	1:A:388:MET:CE	2.43	0.46
1:B:629:GLY:O	1:B:664:LEU:HD12	2.14	0.46
1:B:81:THR:HA	1:B:164:VAL:O	2.16	0.46
1:B:209:ARG:NH1	1:B:211:ASP:OD1	2.49	0.46
1:B:95:ALA:N	1:B:100:ASP:OD2	2.49	0.45
1:B:697:ASP:O	1:B:698:ALA:HB3	2.16	0.45
1:A:593:LEU:HD11	1:A:613:LEU:HD11	1.98	0.45
1:B:478:ASP:OD1	1:B:478:ASP:N	2.49	0.44
1:B:497:TRP:O	1:B:501:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:LEU:O	1:B:542:TYR:HA	2.18	0.44
1:B:479:SER:HB2	1:B:481:THR:OG1	2.18	0.44
1:B:286:MET:HE3	1:B:326:ASP:HA	1.99	0.44
1:A:307:ASP:OD2	1:A:307:ASP:N	2.42	0.44
1:A:329:ARG:NH2	3:A:913:HOH:O	2.51	0.44
1:B:214:LEU:HD12	1:B:215:ASP:N	2.32	0.44
1:A:151:THR:HA	1:A:154:ILE:HD12	1.99	0.43
1:B:91:GLN:OE1	1:B:665:ASN:ND2	2.30	0.43
1:B:696:GLY:HA3	1:B:702:PHE:CG	2.53	0.43
1:A:189:GLU:CD	1:A:197:ARG:HH12	2.24	0.43
1:B:361:ARG:HE	1:B:361:ARG:HB2	1.68	0.43
1:B:175:PRO:HB3	1:B:432:ASP:CG	2.43	0.43
1:B:203:LEU:HB3	1:B:211:ASP:HB2	2.01	0.43
1:B:325:HIS:NE2	1:B:345:SER:OG	2.52	0.43
1:A:591:ALA:HA	1:A:616:ARG:O	2.18	0.42
1:B:593:LEU:HD11	1:B:613:LEU:HD11	2.01	0.42
1:A:497:TRP:O	1:A:501:SER:HB2	2.19	0.42
1:A:72:THR:HG22	1:A:91:GLN:CB	2.45	0.41
1:A:203:LEU:HD12	1:A:718:LYS:HD2	2.02	0.41
1:A:189:GLU:CD	1:A:197:ARG:NH1	2.78	0.41
1:B:501:SER:N	1:B:502:PRO:HD2	2.35	0.41
1:B:135:ASN:O	1:B:315:GLN:NE2	2.49	0.41
1:B:444:LYS:HE3	1:B:449:GLY:O	2.21	0.41
1:A:147:MET:HE1	1:A:286:MET:HB2	2.02	0.41
1:B:203:LEU:O	1:B:210:PHE:HA	2.21	0.41
1:B:246:PRO:HG2	1:B:700:PHE:CG	2.55	0.41
1:B:416:THR:HG23	1:B:426:ILE:HG13	2.04	0.40
1:B:506:PRO:HA	1:B:566:THR:HG22	2.04	0.40
1:A:384:LYS:HE3	1:A:398:PHE:CZ	2.57	0.40
1:B:129:ARG:HH11	1:B:129:ARG:HD2	1.69	0.40

There are no symmetry-related clashes.

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%)	625 (96%)	24 (4%)	2 (0%)	36	48
1	B	651/723 (90%)	618 (95%)	30 (5%)	3 (0%)	24	34
All	All	1302/1446 (90%)	1243 (96%)	54 (4%)	5 (0%)	30	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	247	SER
1	B	209	ARG
1	B	247	SER
1	B	703	SER

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%)	504 (96%)	20 (4%)	29	46
1	B	524/573 (91%)	499 (95%)	25 (5%)	23	37
All	All	1048/1146 (91%)	1003 (96%)	45 (4%)	26	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASP
1	A	139	MET
1	A	198	VAL
1	A	222	LEU
1	A	251	LYS
1	A	286	MET
1	A	332	THR
1	A	336	SER

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Mol	Chain	Res	Type
1	A	363	ASP
1	A	421	GLU
1	A	445	SER
1	A	464	THR
1	A	515	LYS
1	A	540	SER
1	A	561	SER
1	A	562	SER
1	A	588	LYS
1	A	616	ARG
1	A	632	TRP
1	A	714	THR
1	B	78	SER
1	B	96	SER
1	B	97	ASP
1	B	155	SER
1	B	194	LEU
1	B	196	SER
1	B	198	VAL
1	B	203	LEU
1	B	209	ARG
1	B	222	LEU
1	B	270	LEU
1	B	302	LYS
1	B	307	ASP
1	B	478	ASP
1	B	479	SER
1	B	529	GLN
1	B	558	MET
1	B	561	SER
1	B	562	SER
1	B	632	TRP
1	B	656	SER
1	B	671	THR
1	B	672	ARG
1	B	677	SER
1	B	680	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	407	HIS
1	A	408	ASN
1	A	531	ASN
1	A	536	GLN
1	A	645	GLN
1	A	673	ASN
1	B	76	GLN
1	B	131	ASN
1	B	199	ASN
1	B	304	ASN
1	B	450	HIS

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 [i](#)

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%)	0.65	42 (6%) 25 24	48, 58, 86, 123	0
1	B	655/723 (90%)	0.90	75 (11%) 9 8	52, 67, 94, 117	0
All	All	1310/1446 (90%)	0.77	117 (8%) 15 14	48, 63, 92, 123	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	LEU	8.0
1	A	66	LEU	6.6
1	A	558	MET	6.5
1	B	559	MET	6.1
1	B	510	VAL	5.9
1	A	559	MET	5.5
1	A	445	SER	5.2
1	A	450	HIS	5.2
1	B	448	MET	5.2
1	B	560	GLY	4.8
1	A	338	MET	4.7
1	B	449	GLY	4.5
1	B	338	MET	4.5
1	B	92	PRO	4.5
1	B	452	MET	4.4
1	A	387	MET	4.2
1	A	91	GLN	4.1
1	B	558	MET	4.1
1	B	508	GLY	4.0
1	A	449	GLY	4.0
1	A	95	ALA	3.9
1	B	503	LYS	3.9
1	B	632	TRP	3.9
1	B	695	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	388	MET	3.6
1	B	555	ARG	3.5
1	A	632	TRP	3.5
1	B	391	TYR	3.5
1	B	91	GLN	3.5
1	B	260	TRP	3.4
1	B	71	VAL	3.4
1	B	387	MET	3.4
1	A	96	SER	3.4
1	A	704	ALA	3.4
1	B	698	ALA	3.4
1	B	556	GLU	3.4
1	B	672	ARG	3.4
1	A	92	PRO	3.3
1	B	450	HIS	3.3
1	A	557	GLY	3.3
1	A	477	ALA	3.2
1	A	560	GLY	3.2
1	B	696	GLY	3.1
1	B	208	GLY	3.1
1	B	700	PHE	3.1
1	B	242	GLY	3.1
1	B	444	LYS	3.0
1	B	101	TYR	3.0
1	A	444	LYS	2.9
1	B	515	LYS	2.9
1	B	75	ALA	2.8
1	B	190	ARG	2.8
1	A	571	ARG	2.8
1	B	504	ARG	2.8
1	B	507	ASN	2.7
1	B	533	ASP	2.7
1	B	509	SER	2.7
1	B	88	GLU	2.7
1	A	409	TYR	2.7
1	B	451	ALA	2.7
1	A	533	ASP	2.7
1	B	283	GLY	2.7
1	A	391	TYR	2.6
1	B	571	ARG	2.6
1	A	534	LYS	2.6
1	B	422	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	138	MET	2.5
1	B	390	ASP	2.5
1	B	362	TRP	2.5
1	A	555	ARG	2.5
1	B	388	MET	2.5
1	B	697	ASP	2.5
1	B	73	GLY	2.5
1	A	294	GLU	2.4
1	B	540	SER	2.4
1	A	210	PHE	2.4
1	B	85	ASN	2.4
1	B	477	ALA	2.4
1	B	74	VAL	2.4
1	B	70	VAL	2.4
1	B	341	MET	2.4
1	B	157	GLU	2.4
1	A	400	TRP	2.4
1	B	72	THR	2.3
1	B	332	THR	2.3
1	B	421	GLU	2.3
1	A	308	VAL	2.3
1	A	401	SER	2.3
1	B	300	PHE	2.3
1	B	240	GLY	2.3
1	B	420	ALA	2.3
1	B	90	ARG	2.2
1	A	503	LYS	2.2
1	A	422	ARG	2.2
1	A	157	GLU	2.2
1	B	308	VAL	2.2
1	B	561	SER	2.2
1	A	672	ARG	2.2
1	B	363	ASP	2.2
1	A	515	LYS	2.2
1	B	336	SER	2.1
1	B	704	ALA	2.1
1	B	581	TYR	2.1
1	B	264	GLU	2.1
1	A	300	PHE	2.1
1	A	504	ARG	2.1
1	B	83	VAL	2.1
1	A	389	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	582	GLN	2.1
1	B	194	LEU	2.1
1	B	77	SER	2.0
1	A	343	MET	2.0
1	A	420	ALA	2.0
1	B	514	ASP	2.0
1	A	221	ARG	2.0
1	B	199	ASN	2.0
1	B	669	ARG	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(Å ²)	Q<0.9
2	CU1	B	801	1/1	0.99	0.08	67,67,67,67	0
2	CU1	A	801	1/1	1.00	0.06	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.