



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:01 PM UTC

PDB ID : 6Z8Z / pdb_00006z8z
Title : Copper transporter OprC
Authors : Bhamidimarri, S.P.; van den Berg, B.
Deposited on : 2020-06-02
Resolution : 2.56 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

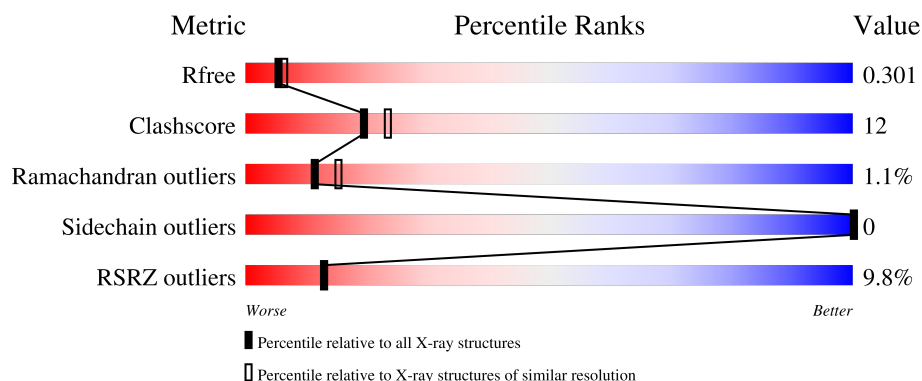
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

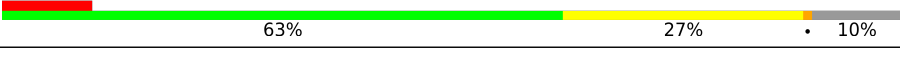
The reported resolution of this entry is 2.56 Å.

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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	
1	B	723	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10187 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	658	Total	C	N	O	S	0	0	0
			5100	3200	902	980	18			
1	B	650	Total	C	N	O	S	0	1	0
			5048	3170	889	972	17			

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

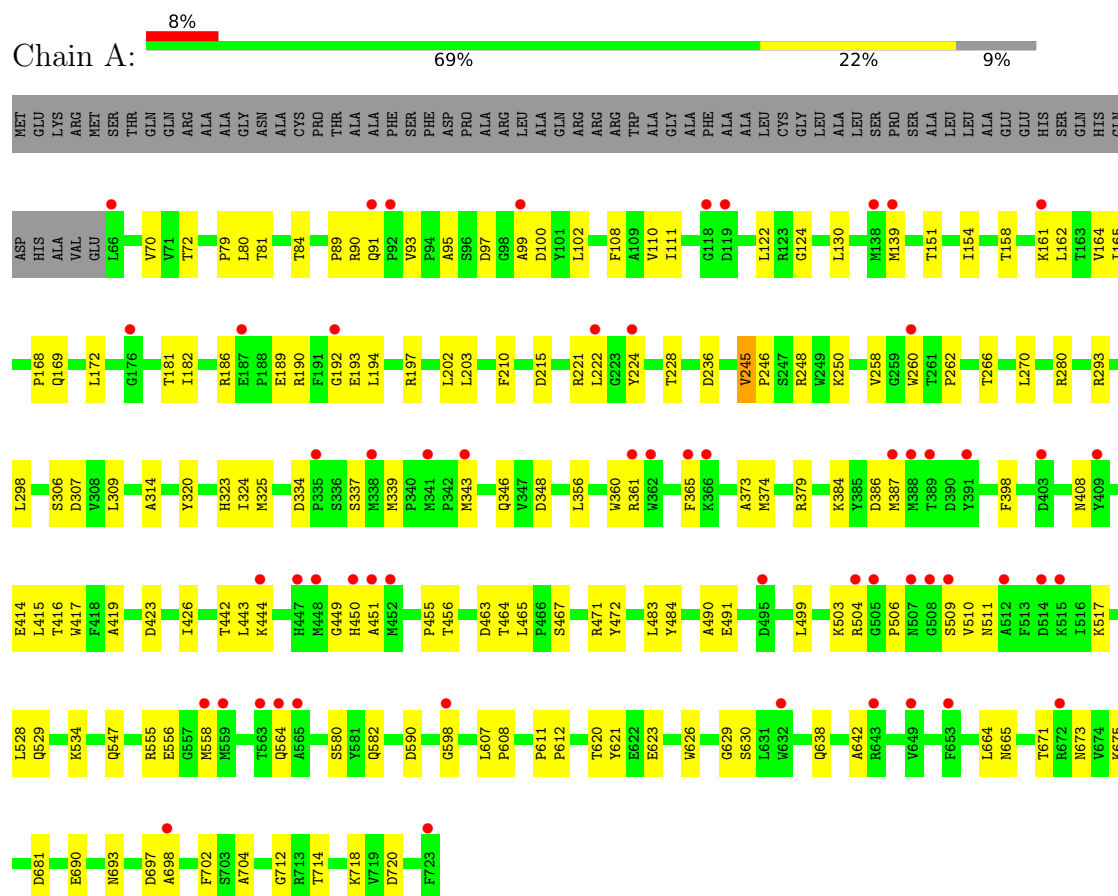
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	19	Total	O	0	0
			19	19		

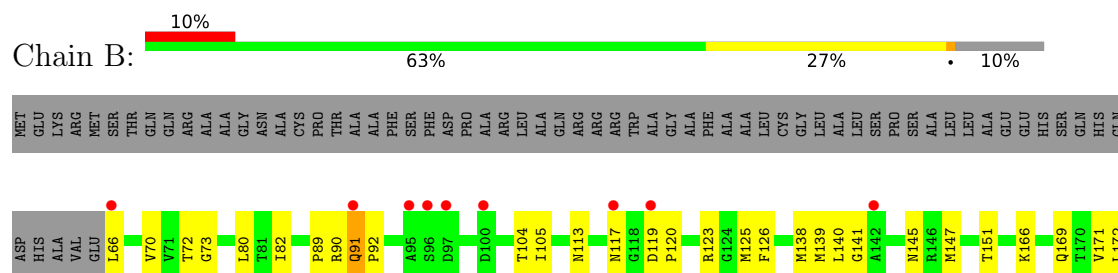
3 Residue-property plots [i](#)

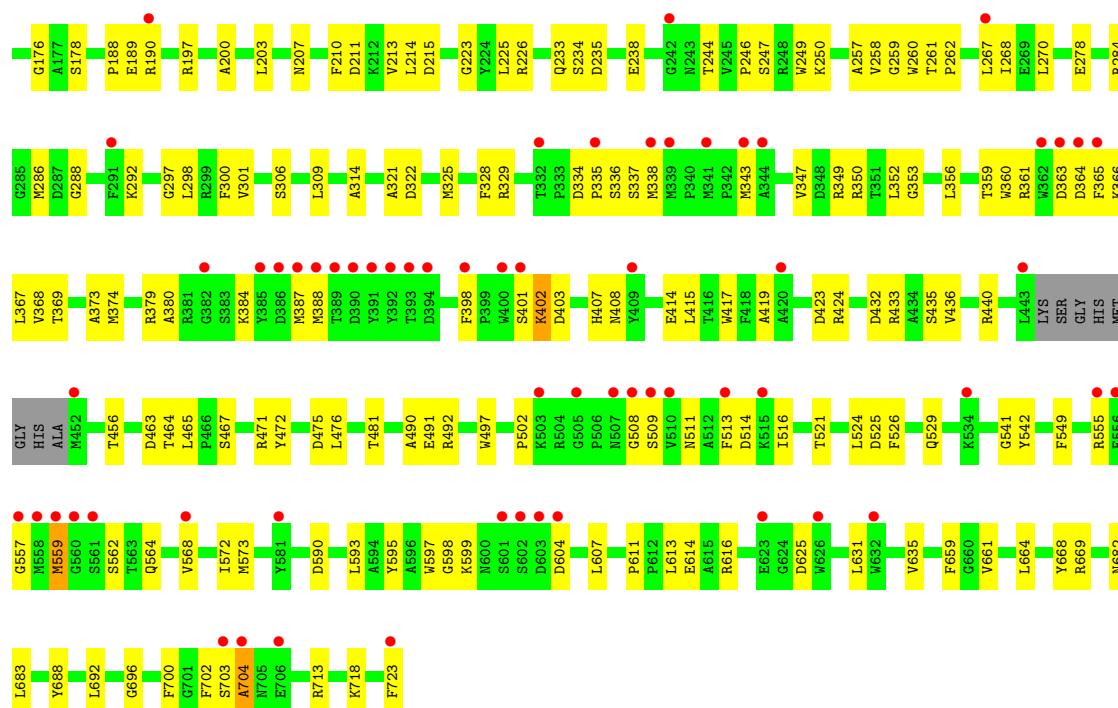
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Putative copper transport outer membrane porin OprC





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	67.02Å 171.22Å 198.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.02 – 2.56 67.02 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.02-2.56) 100.0 (67.02-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.238 , 0.295 0.245 , 0.301	Depositor DCC
R_{free} test set	3729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10187	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 5.57% 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 ⓘ

5.1 Standard geometry ⓘ

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	1/5228 (0.0%)	0.62	1/7087 (0.0%)
1	B	0.40	0/5176	0.65	2/7018 (0.0%)
All	All	0.40	1/10404 (0.0%)	0.64	3/14105 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	VAL	CA-C	-5.67	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	ARG	CA-C-N	6.29	137.16	121.80
1	B	90	ARG	C-N-CA	6.29	137.16	121.80
1	A	245	VAL	O-C-N	-5.20	118.10	121.37

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	5100	0	4877	102	0
1	B	5048	0	4831	131	0
2	A	20	0	0	1	0
2	B	19	0	0	0	0
All	All	10187	0	9708	231	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 12.

All (231) 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:A:139:MET:HE1	1:A:293:ARG:HG3	1.48	0.96
1:B:387:MET:HE2	1:B:388:MET:CG	2.08	0.84
1:A:612:PRO:HG3	1:A:638:GLN:HB2	1.62	0.81
1:B:387:MET:HE2	1:B:388:MET:HG3	1.65	0.78
1:A:151:THR:HA	1:A:154:ILE:HD12	1.66	0.77
1:B:72:THR:HB	1:B:631:LEU:HD13	1.67	0.76
1:B:82:ILE:HD11	1:B:166:LYS:HE2	1.71	0.73
1:B:286:MET:HE2	1:B:325:MET:HE2	1.71	0.72
1:B:91:GLN:HE22	1:B:616:ARG:HH12	1.37	0.71
1:A:306:SER:OG	1:A:307:ASP:N	2.20	0.70
1:A:463:ASP:HB3	1:A:465:LEU:HD11	1.74	0.69
1:B:203:LEU:HD12	1:B:718:LYS:HB2	1.74	0.67
1:B:403:ASP:HB2	1:B:440:ARG:HG3	1.77	0.67
1:B:189:GLU:OE1	1:B:197:ARG:NH2	2.28	0.67
1:B:350:ARG:HH21	1:B:379:ARG:HH12	1.43	0.67
1:B:139:MET:HE3	1:B:321:ALA:HB2	1.77	0.66
1:B:91:GLN:HE22	1:B:616:ARG:NH1	1.93	0.66
1:B:387:MET:CE	1:B:388:MET:HG2	2.26	0.66
1:A:250:LYS:NZ	2:A:801:HOH:O	2.27	0.66
1:B:66:LEU:O	1:B:669:ARG:NH1	2.25	0.65
1:B:387:MET:HE2	1:B:388:MET:HG2	1.79	0.64
1:B:125:MET:HE1	1:B:572:ILE:HG21	1.80	0.64
1:A:193:GLU:HG2	1:A:194:LEU:H	1.62	0.64
1:A:70:VAL:HG21	1:A:665:ASN:HB2	1.79	0.64
1:B:423:ASP:OD2	1:B:472:TYR:OH	2.17	0.63
1:B:314:ALA:HB2	1:B:356:LEU:HD12	1.82	0.62
1:A:456:THR:OG1	1:A:511:ASN:ND2	2.29	0.62
1:B:456:THR:OG1	1:B:511:ASN:ND2	2.33	0.61
1:B:467:SER:HB3	1:B:490:ALA:HA	1.83	0.61
1:A:192:GLY:O	1:A:221:ARG:NH2	2.34	0.61
1:A:547:GLN:OE1	1:B:433:ARG:NH1	2.33	0.60
1:A:384:LYS:HD3	1:A:398:PHE:CZ	2.37	0.60
1:B:597:TRP:CH2	1:B:599:LYS:HB2	2.37	0.59
1:B:123:ARG:HG2	1:B:542:TYR:CE1	2.37	0.59
1:A:97:ASP:OD1	1:A:100:ASP:N	2.35	0.59
1:B:595:TYR:HB2	1:B:613:LEU:HD12	1.85	0.59
1:B:207:ASN:O	1:B:235:ASP:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PRO:O	1:B:190:ARG:NH1	2.36	0.59
1:B:147:MET:HE2	1:B:284:ARG:HD2	1.86	0.58
1:A:215:ASP:OD1	1:A:228:THR:HG22	2.04	0.58
1:A:555:ARG:HG2	1:A:556:GLU:N	2.18	0.58
1:B:465:LEU:HB3	1:B:491:GLU:HB2	1.87	0.57
1:B:292:LYS:HB3	1:B:322:ASP:HB3	1.85	0.57
1:A:203:LEU:HD12	1:A:718:LYS:HB2	1.86	0.57
1:A:348:ASP:OD2	1:A:379:ARG:NH2	2.38	0.57
1:A:442:THR:O	1:A:443:LEU:HD23	2.05	0.57
1:A:248:ARG:HD3	1:A:280:ARG:NH1	2.20	0.56
1:B:387:MET:CE	1:B:388:MET:CG	2.81	0.56
1:A:547:GLN:HE22	1:B:463:ASP:HA	1.71	0.56
1:B:335:PRO:C	1:B:337:SER:H	2.14	0.56
1:A:598:GLY:HA3	1:A:607:LEU:HD12	1.88	0.56
1:A:93:VAL:HG12	1:A:681:ASP:OD2	2.07	0.55
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.89	0.54
1:A:169:GLN:OE1	1:A:471:ARG:NH1	2.38	0.54
1:A:361:ARG:HA	1:A:365:PHE:O	2.08	0.54
1:B:238:GLU:HG2	1:B:244:THR:HG22	1.89	0.54
1:B:614:GLU:HB2	1:B:635:VAL:HG12	1.89	0.54
1:A:221:ARG:HG3	1:A:222:LEU:HD23	1.90	0.53
1:A:236:ASP:HB3	1:A:245:VAL:O	2.08	0.53
1:B:72:THR:HA	1:B:91:GLN:HB2	1.89	0.53
1:A:334:ASP:O	1:A:337:SER:OG	2.18	0.53
1:A:671:THR:HG23	1:A:673:ASN:H	1.74	0.53
1:A:718:LYS:HE3	1:A:720:ASP:OD1	2.09	0.52
1:A:89:PRO:HB3	1:A:718:LYS:HE2	1.92	0.52
1:A:197:ARG:NH1	1:A:215:ASP:OD2	2.42	0.52
1:A:270:LEU:HD13	1:A:298:LEU:CD2	2.39	0.52
1:A:416:THR:HG23	1:A:426:ILE:HG13	1.90	0.52
1:B:338:MET:SD	1:B:338:MET:N	2.78	0.52
1:A:417:TRP:CE2	1:A:419:ALA:HB2	2.44	0.52
1:B:203:LEU:HB3	1:B:211:ASP:HB2	1.90	0.52
1:B:80:LEU:HD13	1:B:169:GLN:HG3	1.92	0.52
1:A:534:LYS:HE2	1:A:582:GLN:O	2.09	0.52
1:A:190:ARG:HB2	1:A:190:ARG:NH1	2.26	0.51
1:B:497:TRP:O	1:B:502:PRO:HD3	2.09	0.51
1:B:379:ARG:HA	1:B:402:LYS:HA	1.93	0.51
1:A:270:LEU:HD13	1:A:298:LEU:HD21	1.93	0.51
1:A:608:PRO:HB3	1:A:642:ALA:HB3	1.92	0.51
1:B:593:LEU:HD21	1:B:613:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:THR:HB	1:A:186:ARG:HH21	1.76	0.51
1:B:169:GLN:HB3	1:B:471:ARG:NH1	2.26	0.51
1:B:598:GLY:HA3	1:B:607:LEU:HD12	1.92	0.51
1:A:324:ILE:HG12	1:A:346:GLN:HG3	1.92	0.51
1:B:509:SER:OG	1:B:511:ASN:O	2.27	0.51
1:A:580:SER:HB2	1:A:590:ASP:HB3	1.93	0.50
1:B:334:ASP:OD2	1:B:337:SER:HB2	2.10	0.50
1:B:120:PRO:HG3	1:B:151:THR:HG21	1.93	0.50
1:B:138:MET:HE1	1:B:374:MET:HE2	1.94	0.50
1:A:260:TRP:CD1	1:A:262:PRO:HG3	2.47	0.50
1:B:407:HIS:HB2	1:B:435:SER:OG	2.12	0.50
1:A:262:PRO:HD2	1:A:266:THR:HB	1.94	0.50
1:B:73:GLY:HA2	1:B:104:THR:O	2.12	0.50
1:B:352:LEU:HD12	1:B:353:GLY:H	1.77	0.50
1:B:350:ARG:NH2	1:B:379:ARG:HH12	2.10	0.49
1:B:171:VAL:HG22	1:B:414:GLU:HG3	1.93	0.49
1:A:450:HIS:CD2	1:A:451:ALA:H	2.30	0.49
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.48	0.49
1:B:268:ILE:HG13	1:B:300:PHE:HD1	1.78	0.49
1:B:476:LEU:HD12	1:B:481:THR:HB	1.94	0.48
1:B:365:PHE:CD2	1:B:415:LEU:HD11	2.48	0.48
1:B:91:GLN:CG	1:B:92:PRO:HD3	2.43	0.48
1:B:270:LEU:HD12	1:B:297:GLY:O	2.13	0.48
1:B:350:ARG:HH21	1:B:379:ARG:NH1	2.10	0.48
1:B:225:LEU:HD13	1:B:258:VAL:HG22	1.95	0.48
1:B:703:SER:O	1:B:704:ALA:C	2.57	0.48
1:A:620:THR:HG22	1:A:629:GLY:HA3	1.95	0.48
1:A:504:ARG:HB2	1:A:564:GLN:HG3	1.95	0.48
1:B:549:PHE:N	1:B:568:VAL:O	2.46	0.48
1:A:483:LEU:HD23	1:A:528:LEU:HB3	1.95	0.48
1:A:84:THR:OG1	1:A:90:ARG:NH1	2.45	0.47
1:B:664:LEU:HD12	1:B:683:LEU:HD22	1.95	0.47
1:B:306:SER:HB2	1:B:309:LEU:H	1.80	0.47
1:B:343:MET:HE3	1:B:343:MET:HB3	1.74	0.47
1:B:401:SER:OG	1:B:402:LYS:N	2.48	0.47
1:A:675:LYS:HG2	1:A:720:ASP:HB2	1.96	0.46
1:B:270:LEU:HD13	1:B:298:LEU:HD12	1.96	0.46
1:B:361:ARG:HD3	1:B:366:LYS:HB2	1.96	0.46
1:B:367:LEU:HD12	1:B:414:GLU:O	2.14	0.46
1:A:386:ASP:OD1	1:A:387:MET:N	2.48	0.46
1:A:108:PHE:HZ	1:A:182:ILE:HD11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLN:HB3	1:B:92:PRO:CD	2.46	0.46
1:B:72:THR:HG22	1:B:91:GLN:HG3	1.97	0.46
1:B:555:ARG:HH21	1:B:562:SER:HB3	1.80	0.46
1:A:81:THR:HG22	1:A:165:ILE:HG12	1.98	0.46
1:A:712:GLY:O	1:A:714:THR:HG23	2.15	0.46
1:A:323:HIS:NE2	1:A:325:MET:HG2	2.31	0.45
1:B:278:GLU:HA	1:B:288:GLY:O	2.15	0.45
1:B:261:THR:HG22	1:B:267:LEU:HD13	1.98	0.45
1:B:365:PHE:CE2	1:B:415:LEU:HD11	2.52	0.45
1:B:555:ARG:NH1	1:B:564:GLN:HG3	2.32	0.45
1:A:423:ASP:OD2	1:A:472:TYR:OH	2.24	0.45
1:A:190:ARG:HB2	1:A:190:ARG:HH11	1.82	0.44
1:A:79:PRO:HB3	1:A:484:TYR:CD2	2.52	0.44
1:A:320:TYR:CE1	1:A:348:ASP:HB2	2.52	0.44
1:A:506:PRO:O	1:A:509:SER:HB3	2.17	0.44
1:A:690:GLU:HB2	1:A:693:ASN:OD1	2.17	0.44
1:A:623:GLU:HB2	1:A:626:TRP:NE1	2.33	0.44
1:B:526:PHE:O	1:B:541:GLY:N	2.43	0.44
1:A:343:MET:HE2	1:A:343:MET:HB3	1.85	0.44
1:B:424:ARG:NH2	1:B:475:ASP:OD1	2.45	0.44
1:B:475:ASP:OD1	1:B:475:ASP:N	2.51	0.44
1:A:84:THR:CG2	1:A:162:LEU:HB3	2.48	0.44
1:A:698:ALA:HA	1:A:702:PHE:H	1.83	0.43
1:B:176:GLY:HA3	1:B:492:ARG:HG3	1.99	0.43
1:B:384:LYS:HG3	1:B:398:PHE:CZ	2.53	0.43
1:A:467:SER:OG	1:A:490:ALA:HA	2.17	0.43
1:B:119:ASP:HB3	1:B:126:PHE:HE1	1.82	0.43
1:B:352:LEU:HD12	1:B:353:GLY:N	2.33	0.43
1:A:84:THR:HG22	1:A:162:LEU:HB3	1.99	0.43
1:A:314:ALA:HB2	1:A:356:LEU:HD23	2.00	0.43
1:B:267:LEU:HB3	1:B:301:VAL:HG22	1.99	0.43
1:B:401:SER:O	1:B:402:LYS:HB3	2.19	0.43
1:A:202:LEU:HD11	1:A:210:PHE:CZ	2.54	0.43
1:B:145:ASN:ND2	1:B:147:MET:HE3	2.33	0.43
1:B:226:ARG:HB3	1:B:257:ALA:HB3	2.00	0.43
1:A:365:PHE:HD1	1:A:415:LEU:HD11	1.83	0.43
1:A:417:TRP:CZ2	1:A:419:ALA:HB2	2.53	0.43
1:A:258:VAL:HG23	1:A:270:LEU:HB3	2.00	0.43
1:A:324:ILE:CG1	1:A:346:GLN:HG3	2.48	0.43
1:A:455:PRO:HG2	1:A:510:VAL:HG12	2.01	0.43
1:B:463:ASP:OD1	1:B:464:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:PRO:HB3	1:B:692:LEU:HD11	2.01	0.43
1:A:450:HIS:CG	1:A:451:ALA:N	2.87	0.43
1:B:661:VAL:HG13	1:B:682:ASN:OD1	2.19	0.43
1:A:467:SER:HG	1:A:490:ALA:HA	1.84	0.43
1:A:630:SER:HB3	1:A:664:LEU:HD23	2.01	0.43
1:B:91:GLN:HG2	1:B:631:LEU:HD22	2.01	0.43
1:A:79:PRO:HB3	1:A:484:TYR:CG	2.54	0.42
1:A:99:ALA:HA	1:A:102:LEU:HD12	2.00	0.42
1:B:91:GLN:HG2	1:B:92:PRO:HD3	2.01	0.42
1:B:328:PHE:HZ	1:B:329:ARG:HH21	1.65	0.42
1:A:172:LEU:HD21	1:A:414:GLU:HB2	2.01	0.42
1:B:359:THR:HG23	1:B:368:VAL:HG22	2.01	0.42
1:B:524:LEU:HD12	1:B:525:ASP:N	2.34	0.42
1:B:138:MET:HE3	1:B:140:LEU:HD21	2.00	0.42
1:B:403:ASP:CB	1:B:440:ARG:HG3	2.47	0.42
1:B:555:ARG:NH2	1:B:562:SER:HB3	2.34	0.42
1:B:557:GLY:O	1:B:559:MET:N	2.48	0.42
1:A:621:TYR:CE2	1:A:623:GLU:HG3	2.54	0.42
1:B:70:VAL:HG22	1:B:89:PRO:HB2	2.01	0.42
1:B:347:VAL:HG12	1:B:380:ALA:HB2	2.00	0.42
1:A:464:THR:C	1:A:465:LEU:HG	2.44	0.42
1:A:580:SER:CB	1:A:590:ASP:HB3	2.49	0.42
1:B:432:ASP:O	1:B:464:THR:HA	2.20	0.42
1:B:529:GLN:HE21	1:B:529:GLN:HB3	1.64	0.42
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.53	0.42
1:A:309:LEU:HB2	1:A:360:TRP:CZ3	2.55	0.42
1:A:503:LYS:C	1:A:504:ARG:HG3	2.45	0.42
1:B:363:ASP:HB3	1:B:364:ASP:H	1.75	0.42
1:A:79:PRO:O	1:A:80:LEU:HB2	2.20	0.42
1:A:517:LYS:HD3	1:A:517:LYS:HA	1.86	0.42
1:B:234:SER:HB3	1:B:249:TRP:NE1	2.35	0.42
1:B:625:ASP:OD2	1:B:668:TYR:HE1	2.02	0.42
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.82	0.42
1:A:124:GLY:HA2	1:A:611:PRO:HD2	2.01	0.41
1:A:444:LYS:HG2	1:A:449:GLY:O	2.19	0.41
1:B:113:ASN:ND2	1:B:117:ASN:O	2.50	0.41
1:B:223:GLY:HA2	1:B:259:GLY:O	2.19	0.41
1:B:246:PRO:HG2	1:B:700:PHE:CG	2.55	0.41
1:B:373:ALA:HA	1:B:408:ASN:O	2.20	0.41
1:A:122:LEU:HB2	1:A:130:LEU:HD21	2.02	0.41
1:A:373:ALA:HA	1:A:408:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:SER:HB2	1:B:521:THR:HG21	2.02	0.41
1:B:214:LEU:HD12	1:B:215:ASP:H	1.83	0.41
1:B:542:TYR:HE2	1:B:572:ILE:HD12	1.85	0.41
1:B:573:MET:O	1:B:597:TRP:N	2.54	0.41
1:B:360:TRP:HE1	1:B:369:THR:HG22	1.85	0.41
1:B:696:GLY:HA3	1:B:702:PHE:CG	2.55	0.41
1:A:374:MET:HE3	1:A:374:MET:HB3	1.82	0.41
1:A:529:GLN:HE21	1:A:529:GLN:HB3	1.54	0.41
1:A:189:GLU:HB2	1:A:224:TYR:CD2	2.55	0.41
1:B:172:LEU:HD21	1:B:414:GLU:HB2	2.02	0.41
1:B:516:ILE:HD12	1:B:516:ILE:HG23	1.88	0.41
1:A:697:ASP:O	1:A:698:ALA:HB3	2.21	0.41
1:B:590:ASP:OD1	1:B:590:ASP:N	2.54	0.41
1:B:683:LEU:O	1:B:713:ARG:HD3	2.20	0.41
1:A:110:VAL:HG12	1:A:111:ILE:O	2.21	0.41
1:A:465:LEU:HB3	1:A:491:GLU:HB2	2.03	0.41
1:B:200:ALA:HA	1:B:213:VAL:O	2.21	0.41
1:B:233:GLN:HB3	1:B:250:LYS:HG3	2.03	0.41
1:B:417:TRP:CE2	1:B:419:ALA:HB2	2.56	0.41
1:A:248:ARG:HD3	1:A:280:ARG:CZ	2.51	0.40
1:A:339:MET:HE3	1:A:343:MET:HB2	2.03	0.40
1:B:105:ILE:HD13	1:B:105:ILE:HG21	1.85	0.40
1:A:161:LYS:HB2	1:A:161:LYS:HE2	1.85	0.40
1:B:366:LYS:HG3	1:B:367:LEU:N	2.35	0.40
1:A:164:VAL:HA	1:A:181:THR:O	2.22	0.40
1:B:436:VAL:HG22	1:B:513:PHE:HE1	1.87	0.40
1:B:635:VAL:HG21	1:B:659:PHE:CZ	2.55	0.40
1:B:723:PHE:CD1	1:B:723:PHE:N	2.89	0.40
1:B:141:GLY:O	1:B:349:ARG:NH1	2.52	0.40
1:B:203:LEU:O	1:B:210:PHE:HA	2.22	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	656/723 (91%)	610 (93%)	41 (6%)	5 (1%)	16	22
1	B	647/723 (90%)	596 (92%)	42 (6%)	9 (1%)	9	11
All	All	1303/1446 (90%)	1206 (93%)	83 (6%)	14 (1%)	11	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ALA
1	B	91	GLN
1	A	168	PRO
1	B	336	SER
1	B	704	ALA
1	A	558	MET
1	B	514	ASP
1	A	704	ALA
1	B	402	LYS
1	B	559	MET
1	B	604	ASP
1	B	247	SER
1	B	508	GLY
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	525/572 (92%)	525 (100%)	0	100	100
1	B	521/572 (91%)	521 (100%)	0	100	100
All	All	1046/1144 (91%)	1046 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	145	ASN
1	A	397	GLN
1	A	450	HIS
1	A	458	ASN
1	A	645	GLN
1	B	91	GLN
1	B	645	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](#)

There are no ligands in this entry.

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	658/723 (91%)	0.84	57 (8%) 16 16	46, 68, 102, 138	0
1	B	650/723 (89%)	0.84	71 (10%) 10 10	35, 67, 103, 143	1 (0%)
All	All	1308/1446 (90%)	0.84	128 (9%) 13 13	35, 67, 103, 143	1 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	LEU	7.0
1	B	66	LEU	6.0
1	B	392	TYR	4.8
1	A	66	LEU	4.7
1	A	723	PHE	4.5
1	B	362	TRP	4.5
1	A	509	SER	4.4
1	A	338	MET	4.3
1	B	452	MET	4.3
1	A	362	TRP	4.2
1	B	385	TYR	4.1
1	B	603	ASP	4.1
1	B	391	TYR	4.1
1	A	559	MET	4.1
1	B	338	MET	4.1
1	B	559	MET	4.1
1	B	393	THR	4.0
1	B	387	MET	4.0
1	A	514	ASP	3.9
1	B	508	GLY	3.9
1	A	387	MET	3.8
1	B	386	ASP	3.8
1	A	391	TYR	3.7
1	A	118	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	96	SER	3.7
1	B	507	ASN	3.6
1	B	509	SER	3.6
1	A	388	MET	3.5
1	A	558	MET	3.5
1	B	390	ASP	3.4
1	B	558	MET	3.3
1	B	119	ASP	3.3
1	A	504	ARG	3.3
1	A	119	ASP	3.3
1	B	335	PRO	3.3
1	A	260	TRP	3.3
1	B	420	ALA	3.2
1	A	632	TRP	3.2
1	A	448	MET	3.2
1	A	138	MET	3.2
1	B	388	MET	3.1
1	B	341	MET	3.1
1	B	632	TRP	3.1
1	B	557	GLY	3.1
1	B	703	SER	3.1
1	A	564	GLN	3.0
1	B	382	GLY	3.0
1	A	653	PHE	3.0
1	B	389	THR	3.0
1	A	565	ALA	3.0
1	B	706	GLU	2.9
1	A	450	HIS	2.9
1	A	505	GLY	2.9
1	A	515	LYS	2.9
1	A	447	HIS	2.9
1	B	398	PHE	2.9
1	A	192	GLY	2.9
1	B	503	LYS	2.9
1	B	534	LYS	2.9
1	B	400	TRP	2.8
1	B	723	PHE	2.8
1	A	409	TYR	2.8
1	A	672	ARG	2.8
1	B	242	GLY	2.8
1	A	99	ALA	2.8
1	B	561	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	510	VAL	2.8
1	A	389	THR	2.8
1	B	513	PHE	2.8
1	B	560	GLY	2.7
1	A	649	VAL	2.7
1	B	95	ALA	2.7
1	A	139	MET	2.6
1	A	366	LYS	2.6
1	B	100	ASP	2.6
1	B	505	GLY	2.6
1	A	452	MET	2.6
1	B	704	ALA	2.6
1	B	365	PHE	2.5
1	B	91	GLN	2.5
1	A	451	ALA	2.5
1	B	190	ARG	2.5
1	B	97	ASP	2.4
1	B	604	ASP	2.4
1	B	363	ASP	2.4
1	A	341	MET	2.4
1	B	626	TRP	2.4
1	A	495	ASP	2.3
1	A	187	GLU	2.3
1	B	623	GLU	2.3
1	A	507	ASN	2.3
1	B	117	ASN	2.3
1	B	401	SER	2.3
1	B	515	LYS	2.3
1	B	339	MET	2.3
1	A	563	THR	2.2
1	A	161	LYS	2.2
1	A	643	ARG	2.2
1	B	581	TYR	2.2
1	A	91	GLN	2.2
1	B	343	MET	2.2
1	B	568	VAL	2.2
1	A	444	LYS	2.2
1	A	598	GLY	2.2
1	A	361	ARG	2.2
1	A	512	ALA	2.2
1	A	176	GLY	2.2
1	A	698	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	2.1
1	B	142	ALA	2.1
1	A	403	ASP	2.1
1	B	291	PHE	2.1
1	A	508	GLY	2.1
1	B	332	THR	2.1
1	B	394	ASP	2.1
1	A	343	MET	2.1
1	B	555	ARG	2.1
1	B	556	GLU	2.1
1	B	409	TYR	2.1
1	B	601	SER	2.1
1	A	92	PRO	2.1
1	A	222	LEU	2.0
1	B	364	ASP	2.0
1	A	365	PHE	2.0
1	B	267	LEU	2.0
1	B	344	ALA	2.0
1	A	335	PRO	2.0
1	B	602	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.