



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:13 pm GMT

PDB ID : 6Z8Y
Title : Copper transporter OprC
Authors : Bhamidimarri, S.P.; van den Berg, B.
Deposited on : 2020-06-02
Resolution : 2.78 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

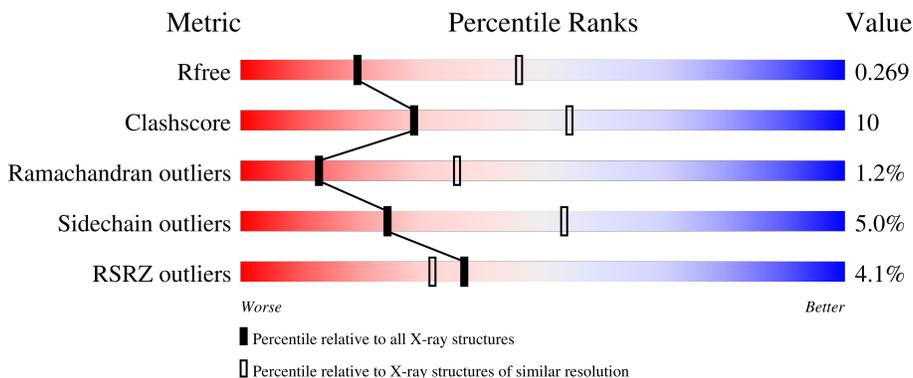
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	 4% 67% 23% 9%
1	B	723	 3% 66% 21% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10142 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	658	5104	3203	902	981	18	0	1	0
1	B	645	5015	3151	884	965	15	0	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

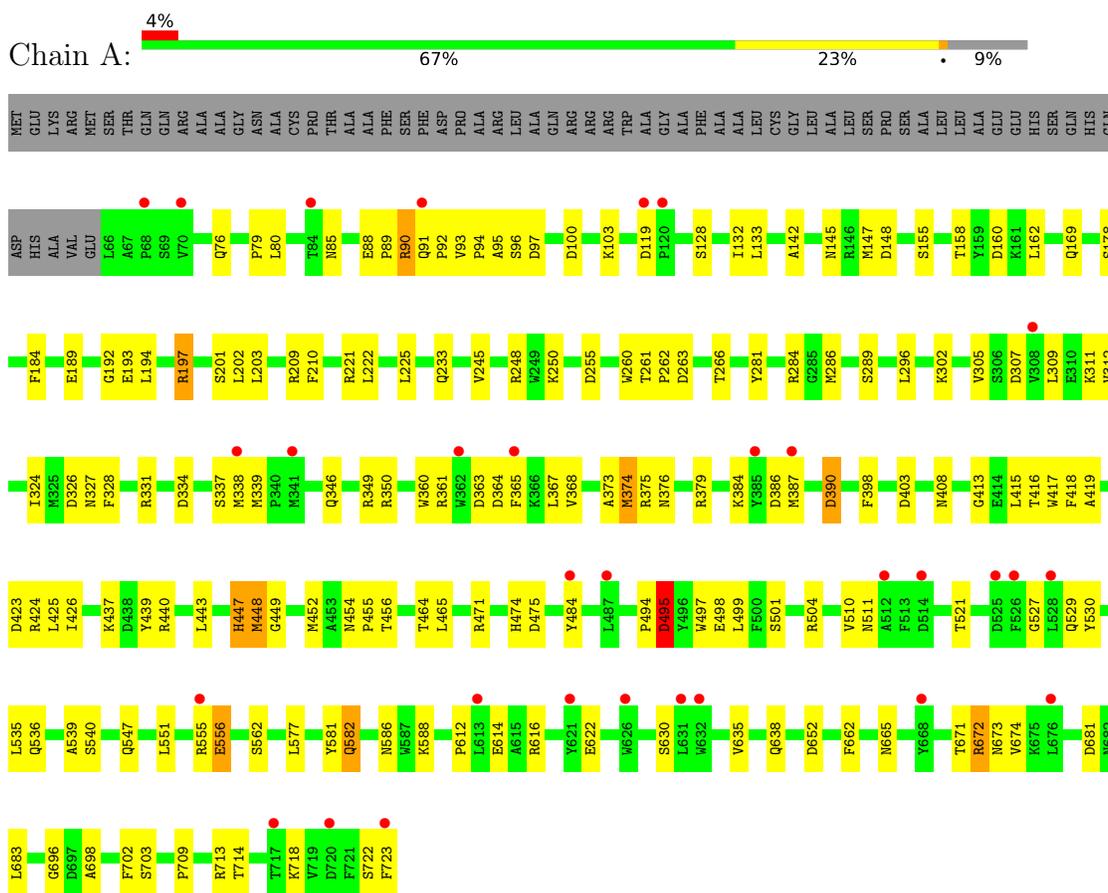
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	11	Total	O	0	0
			11	11		

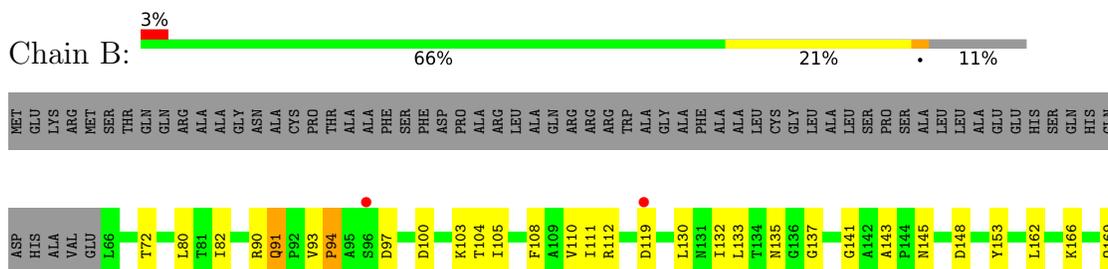
3 Residue-property plots [i](#)

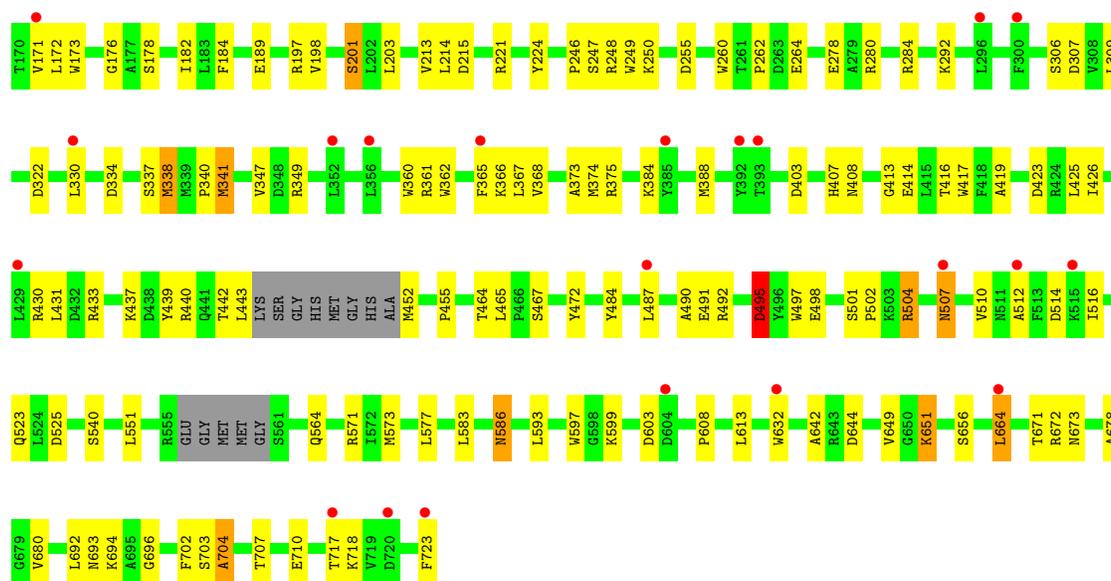
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.03Å 170.74Å 198.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.03 – 2.78 129.32 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.03-2.78) 100.0 (129.32-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.210 , 0.266 0.213 , 0.269	Depositor DCC
R_{free} test set	2893 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10142	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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](#)

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	0/5235	0.66	0/7097
1	B	0.47	0/5142	0.69	1/6973 (0.0%)
All	All	0.47	0/10377	0.68	1/14070 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	LEU	CB-CG-CD1	-5.03	102.46	111.00

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	5104	0	4884	102	0
1	B	5015	0	4800	91	0
2	A	12	0	0	0	0
2	B	11	0	0	0	0
All	All	10142	0	9684	192	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 10.

All (192) 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:88:GLU:O	1:A:90:ARG:NH2	1.65	1.28
1:B:172:LEU:HD13	1:B:414:GLU:OE2	1.75	0.84
1:A:504:ARG:HH12	1:A:562:SER:HB3	1.43	0.84
1:A:289:SER:OG	1:A:326:ASP:OD2	1.95	0.84
1:A:614:GLU:HG3	1:A:635:VAL:HG12	1.64	0.78
1:B:423:ASP:OD2	1:B:472:TYR:OH	2.01	0.78
1:B:671:THR:HG23	1:B:673:ASN:H	1.49	0.78
1:A:324:ILE:HG12	1:A:346:GLN:HG3	1.65	0.76
1:A:681:ASP:HB2	1:A:714:THR:HB	1.69	0.74
1:A:671:THR:HG22	1:A:674:VAL:HG12	1.72	0.71
1:B:361:ARG:HH11	1:B:361:ARG:HG2	1.60	0.66
1:A:334:ASP:HB3	1:A:337:SER:HB2	1.78	0.66
1:A:437:LYS:HD3	1:A:439:TYR:CZ	2.32	0.64
1:B:172:LEU:HD11	1:B:414:GLU:HB2	1.79	0.64
1:B:403:ASP:HB2	1:B:440:ARG:HG2	1.78	0.64
1:A:423:ASP:OD1	1:A:474:HIS:ND1	2.26	0.64
1:A:671:THR:HG23	1:A:673:ASN:H	1.63	0.63
1:B:593:LEU:HD11	1:B:613:LEU:HD11	1.79	0.63
1:A:586:ASN:HB2	1:A:622:GLU:O	1.99	0.63
1:A:403:ASP:HB2	1:A:440:ARG:HG2	1.81	0.62
1:A:203:LEU:HD12	1:A:718:LYS:HD3	1.82	0.62
1:A:350:ARG:HH12	1:A:379:ARG:NH2	1.98	0.62
1:B:703:SER:OG	1:B:704:ALA:N	2.33	0.61
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.82	0.60
1:A:91:GLN:OE1	1:A:665:ASN:HB3	2.02	0.60
1:B:417:TRP:CE2	1:B:419:ALA:HB2	2.36	0.60
1:A:417:TRP:CE2	1:A:419:ALA:HB2	2.37	0.60
1:B:82:ILE:HD11	1:B:166:LYS:HE2	1.84	0.60
1:A:555:ARG:HG2	1:A:556:GLU:N	2.18	0.59
1:B:608:PRO:HB3	1:B:642:ALA:HB3	1.83	0.59
1:A:103:LYS:O	1:A:616:ARG:NH2	2.35	0.59
1:A:443:LEU:HG	1:A:454:ASN:HB2	1.85	0.59
1:B:306:SER:HB3	1:B:309:LEU:HB3	1.83	0.59
1:A:309:LEU:HD12	1:A:360:TRP:CZ3	2.38	0.59
1:B:497:TRP:O	1:B:501:SER:HB2	2.03	0.59
1:B:80:LEU:HD13	1:B:169:GLN:HG3	1.85	0.58
1:A:169:GLN:HB3	1:A:471:ARG:NH1	2.18	0.58
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.39	0.57
1:A:456:THR:OG1	1:A:511:ASN:ND2	2.35	0.57
1:A:547:GLN:HG3	1:B:433:ARG:HH12	1.68	0.57
1:A:364:ASP:HB3	1:A:418:PHE:HB2	1.87	0.57
1:B:141:GLY:O	1:B:349:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HB2	1:A:415:LEU:HD12	1.87	0.56
1:B:172:LEU:HD13	1:B:414:GLU:CD	2.26	0.56
1:B:90:ARG:HG2	1:B:104:THR:HG21	1.88	0.56
1:A:582:GLN:HG3	1:A:588:LYS:HG3	1.87	0.55
1:B:442:THR:HG22	1:B:443:LEU:H	1.71	0.55
1:A:202:LEU:HD11	1:A:210:PHE:CZ	2.43	0.54
1:A:447:HIS:C	1:A:449:GLY:H	2.10	0.54
1:A:305:VAL:HB	1:A:309:LEU:HD22	1.89	0.54
1:B:112:ARG:NE	1:B:710:GLU:OE1	2.29	0.54
1:A:80:LEU:HD13	1:A:169:GLN:HG3	1.90	0.54
1:A:671:THR:HG22	1:A:674:VAL:CG1	2.38	0.54
1:B:148:ASP:HB2	1:B:153:TYR:CE2	2.43	0.54
1:A:671:THR:OG1	1:A:672:ARG:NH1	2.42	0.53
1:B:361:ARG:HG3	1:B:365:PHE:O	2.08	0.53
1:A:504:ARG:NH1	1:A:562:SER:HB3	2.18	0.53
1:A:94:PRO:O	1:A:209:ARG:NH2	2.41	0.53
1:B:111:ILE:HG12	1:B:692:LEU:HB3	1.91	0.52
1:B:306:SER:OG	1:B:307:ASP:N	2.43	0.52
1:A:696:GLY:HA3	1:A:702:PHE:CG	2.44	0.52
1:B:280:ARG:NH1	1:B:330:LEU:O	2.43	0.52
1:B:189:GLU:OE1	1:B:197:ARG:NH2	2.39	0.52
1:A:91:GLN:HB3	1:A:92:PRO:HD3	1.92	0.52
1:B:145:ASN:HB2	1:B:284:ARG:HH12	1.75	0.52
1:A:169:GLN:HB3	1:A:471:ARG:HH12	1.74	0.51
1:B:416:THR:HG23	1:B:426:ILE:CD1	2.40	0.51
1:A:328:PHE:HA	1:A:331:ARG:O	2.10	0.51
1:A:368:VAL:O	1:A:413:GLY:HA2	2.11	0.51
1:B:214:LEU:HD12	1:B:215:ASP:H	1.75	0.51
1:A:497:TRP:O	1:A:501:SER:HB2	2.11	0.51
1:B:292:LYS:HB3	1:B:322:ASP:HB3	1.92	0.51
1:A:266:THR:OG1	1:A:302:LYS:HE2	2.11	0.51
1:A:455:PRO:HG2	1:A:510:VAL:HG12	1.93	0.51
1:B:201:SER:HB3	1:B:213:VAL:CG1	2.40	0.51
1:A:189:GLU:OE2	1:A:197:ARG:NH2	2.44	0.51
1:A:527:GLY:HA3	1:A:539:ALA:O	2.11	0.50
1:A:337:SER:OG	1:A:338:MET:N	2.43	0.50
1:B:368:VAL:O	1:B:413:GLY:HA2	2.11	0.50
1:B:375:ARG:HG3	1:B:407:HIS:CD2	2.45	0.50
1:A:76:GLN:HE21	1:A:529:GLN:NE2	2.09	0.50
1:A:374:MET:HG2	1:A:375:ARG:N	2.27	0.50
1:B:696:GLY:HA3	1:B:702:PHE:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD21	1:A:312:VAL:HG23	1.94	0.49
1:A:683:LEU:O	1:A:713:ARG:HD3	2.13	0.49
1:B:214:LEU:HD12	1:B:215:ASP:N	2.26	0.49
1:A:672:ARG:HH21	1:A:672:ARG:HG3	1.77	0.49
1:B:649:VAL:O	1:B:694:LYS:HE2	2.13	0.49
1:A:334:ASP:CB	1:A:337:SER:HB2	2.42	0.48
1:A:386:ASP:OD2	1:A:387:MET:N	2.47	0.48
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.48	0.48
1:A:193:GLU:HG3	1:A:194:LEU:H	1.78	0.48
1:B:437:LYS:HD3	1:B:439:TYR:CZ	2.47	0.48
1:B:133:LEU:HD22	1:B:173:TRP:HB3	1.96	0.48
1:B:361:ARG:HH11	1:B:361:ARG:CG	2.26	0.48
1:B:417:TRP:CZ2	1:B:419:ALA:HB2	2.49	0.48
1:A:147:MET:HE3	1:A:281:TYR:CE2	2.49	0.48
1:B:132:ILE:HG12	1:B:182:ILE:HD12	1.95	0.48
1:B:133:LEU:CD2	1:B:173:TRP:HB3	2.43	0.48
1:A:373:ALA:HA	1:A:408:ASN:O	2.14	0.48
1:A:85:ASN:O	1:A:90:ARG:NH1	2.47	0.47
1:B:495:ASP:HB3	1:B:498:GLU:H	1.77	0.47
1:B:455:PRO:HB2	1:B:510:VAL:HG21	1.97	0.47
1:A:307:ASP:OD1	1:A:307:ASP:N	2.47	0.47
1:A:424:ARG:NH2	1:A:475:ASP:OD1	2.48	0.47
1:B:309:LEU:HD13	1:B:360:TRP:CE3	2.50	0.47
1:A:309:LEU:HD21	1:A:312:VAL:CG2	2.44	0.47
1:B:248:ARG:HG2	1:B:249:TRP:N	2.28	0.46
1:B:467:SER:HB3	1:B:490:ALA:HA	1.97	0.46
1:B:100:ASP:HA	1:B:103:LYS:HG3	1.97	0.46
1:A:535:LEU:HD12	1:A:536:GLN:N	2.31	0.46
1:B:644:ASP:OD1	1:B:651:LYS:NZ	2.42	0.45
1:B:130:LEU:HD23	1:B:182:ILE:HD11	1.97	0.45
1:B:176:GLY:HA3	1:B:492:ARG:HG3	1.98	0.45
1:B:189:GLU:HB2	1:B:224:TYR:CD2	2.51	0.45
1:B:586:ASN:OD1	1:B:586:ASN:N	2.48	0.45
1:A:178:SER:HB3	1:A:521:THR:HG21	1.98	0.45
1:A:464:THR:C	1:A:465:LEU:HG	2.36	0.45
1:B:162:LEU:HD13	1:B:184:PHE:CE2	2.53	0.45
1:B:246:PRO:HB3	1:B:280:ARG:HD2	1.98	0.44
1:B:203:LEU:HD12	1:B:718:LYS:HB2	2.00	0.44
1:A:147:MET:HE3	1:A:281:TYR:HE2	1.83	0.44
1:B:334:ASP:HB2	1:B:337:SER:HB2	1.98	0.44
1:B:338:MET:C	1:B:340:PRO:HD3	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:PRO:HB2	1:A:499:LEU:HG	2.00	0.44
1:A:222:LEU:HA	1:A:261:THR:HG23	2.00	0.44
1:A:79:PRO:HB3	1:A:484:TYR:CD1	2.52	0.44
1:B:373:ALA:HA	1:B:408:ASN:O	2.18	0.44
1:B:465:LEU:HB3	1:B:491:GLU:HB2	2.00	0.44
1:A:447:HIS:CG	1:A:448:MET:H	2.34	0.43
1:B:250:LYS:HB3	1:B:278:GLU:HG2	1.98	0.43
1:A:76:GLN:OE1	1:A:540:SER:HB2	2.18	0.43
1:A:96:SER:O	1:A:96:SER:OG	2.28	0.43
1:A:302:LYS:O	1:A:311:LYS:HA	2.18	0.43
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.80	0.43
1:A:197:ARG:CZ	1:A:197:ARG:HB2	2.47	0.43
1:B:367:LEU:HD12	1:B:414:GLU:O	2.19	0.43
1:B:523:GLN:NE2	1:B:525:ASP:OD2	2.48	0.43
1:B:678:ALA:HB2	1:B:717[B]:THR:HG22	2.00	0.43
1:A:286:MET:HG2	1:A:327:ASN:HB3	1.99	0.43
1:A:132:ILE:O	1:A:133:LEU:HD23	2.18	0.43
1:A:495:ASP:HB3	1:A:498:GLU:H	1.84	0.43
1:A:95:ALA:O	1:A:97:ASP:N	2.49	0.43
1:A:504:ARG:HH22	1:A:555:ARG:HB3	1.84	0.43
1:B:693:ASN:HB2	1:B:707:THR:HG22	2.01	0.43
1:A:76:GLN:HE21	1:A:529:GLN:HE22	1.67	0.43
1:B:105:ILE:HB	1:B:108:PHE:HD2	1.84	0.43
1:B:340:PRO:HD2	1:B:341:MET:SD	2.59	0.43
1:B:143:ALA:HA	1:B:347:VAL:HG21	2.00	0.42
1:B:145:ASN:HB2	1:B:284:ARG:NH1	2.34	0.42
1:B:384:LYS:HE3	1:B:384:LYS:HB2	1.67	0.42
1:A:233:GLN:HB3	1:A:250:LYS:HG3	2.02	0.42
1:A:417:TRP:CZ2	1:A:419:ALA:HB2	2.55	0.42
1:A:145:ASN:HD22	1:A:284:ARG:HH11	1.67	0.42
1:A:142:ALA:H	1:A:148:ASP:CG	2.22	0.42
1:A:384:LYS:HD3	1:A:398:PHE:CE1	2.54	0.42
1:A:424:ARG:HH22	1:A:475:ASP:CG	2.23	0.42
1:B:93:VAL:HA	1:B:94:PRO:HD3	1.93	0.42
1:B:375:ARG:HG3	1:B:407:HIS:NE2	2.35	0.42
1:A:296:LEU:HA	1:A:296:LEU:HD23	1.85	0.42
1:B:171:VAL:HG22	1:B:414:GLU:HG3	2.02	0.42
1:B:431:LEU:HD11	1:B:464:THR:HG22	2.02	0.42
1:A:386:ASP:O	1:A:390:ASP:HA	2.20	0.41
1:B:664:LEU:HB2	1:B:680:VAL:HG12	2.02	0.41
1:A:350:ARG:O	1:A:376:ASN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:O	1:A:158:THR:OG1	2.38	0.41
1:A:403:ASP:HB2	1:A:440:ARG:CG	2.50	0.41
1:B:484:TYR:OH	1:B:540:SER:HB2	2.20	0.41
1:B:502:PRO:HG2	1:B:512:ALA:CB	2.50	0.41
1:A:93:VAL:HA	1:A:94:PRO:HD3	1.87	0.41
1:B:93:VAL:O	1:B:93:VAL:HG13	2.21	0.41
1:B:360:TRP:HB2	1:B:362:TRP:HZ3	1.85	0.41
1:A:416:THR:HG23	1:A:426:ILE:HG13	2.02	0.41
1:B:103:LYS:HE2	1:B:110:VAL:HG21	2.02	0.41
1:B:571:ARG:HH22	1:B:573:MET:CE	2.34	0.41
1:A:160:ASP:N	1:A:160:ASP:OD1	2.53	0.41
1:A:447:HIS:C	1:A:449:GLY:N	2.74	0.41
1:B:516:ILE:HD13	1:B:516:ILE:HA	1.85	0.41
1:B:597:TRP:CH2	1:B:599:LYS:HB2	2.55	0.41
1:B:72:THR:HG22	1:B:91:GLN:HB3	2.02	0.41
1:B:361:ARG:CG	1:B:361:ARG:NH1	2.84	0.41
1:A:245:VAL:HG21	1:A:709:PRO:HG2	2.03	0.40
1:B:135:ASN:C	1:B:137:GLY:H	2.24	0.40
1:B:360:TRP:O	1:B:366:LYS:HA	2.22	0.40
1:A:89:PRO:HB3	1:A:718:LYS:HE3	2.02	0.40
1:A:361:ARG:HA	1:A:365:PHE:O	2.21	0.40
1:A:162:LEU:HD13	1:A:184:PHE:CE1	2.56	0.40
1:A:630:SER:HB2	1:A:662:PHE:CE1	2.56	0.40
1:B:504:ARG:HH21	1:B:564:GLN:HB2	1.87	0.40
1:A:530:TYR:O	1:A:536:GLN:HA	2.22	0.40
1:B:171:VAL:O	1:B:430:ARG:NH1	2.55	0.40
1:B:198:VAL:HG13	1:B:214:LEU:HD11	2.02	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	657/723 (91%)	591 (90%)	58 (9%)	8 (1%)	13	36
1	B	640/723 (88%)	591 (92%)	42 (7%)	7 (1%)	14	38
All	All	1297/1446 (90%)	1182 (91%)	100 (8%)	15 (1%)	13	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	495	ASP
1	B	388	MET
1	A	698	ALA
1	B	495	ASP
1	B	507	ASN
1	B	514	ASP
1	A	703	SER
1	B	704	ALA
1	A	248	ARG
1	A	447	HIS
1	A	448	MET
1	B	247	SER
1	B	583	LEU
1	A	192	GLY
1	A	339	MET

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	526/572 (92%)	501 (95%)	25 (5%)	25	55
1	B	518/572 (91%)	491 (95%)	27 (5%)	23	52
All	All	1044/1144 (91%)	992 (95%)	52 (5%)	24	53

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG

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Mol	Chain	Res	Type
1	A	100	ASP
1	A	119	ASP
1	A	128	SER
1	A	197	ARG
1	A	201	SER
1	A	221	ARG
1	A	225	LEU
1	A	255	ASP
1	A	263	ASP
1	A	349	ARG
1	A	363	ASP
1	A	374	MET
1	A	390	ASP
1	A	452	MET
1	A	495	ASP
1	A	551	LEU
1	A	556	GLU
1	A	577	LEU
1	A	581	TYR
1	A	582	GLN
1	A	652	ASP
1	A	672	ARG
1	A	722	SER
1	A	723	PHE
1	B	91	GLN
1	B	94	PRO
1	B	97	ASP
1	B	119	ASP
1	B	178	SER
1	B	201	SER
1	B	221	ARG
1	B	255	ASP
1	B	264	GLU
1	B	338	MET
1	B	341	MET
1	B	374	MET
1	B	425	LEU
1	B	452	MET
1	B	487	LEU
1	B	495	ASP
1	B	504	ARG
1	B	507	ASN

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Mol	Chain	Res	Type
1	B	551	LEU
1	B	577	LEU
1	B	586	ASN
1	B	603	ASP
1	B	632	TRP
1	B	651	LYS
1	B	656	SER
1	B	672	ARG
1	B	723	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	529	GLN
1	B	230	ASN
1	B	253	ASN
1	B	529	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 monosaccharides 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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%)	0.62	31 (4%) 31 25	42, 67, 107, 142	0
1	B	645/723 (89%)	0.60	23 (3%) 42 37	43, 66, 96, 124	0
All	All	1303/1446 (90%)	0.61	54 (4%) 37 32	42, 67, 102, 142	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	723	PHE	7.6
1	B	723	PHE	6.7
1	A	387	MET	4.3
1	B	507	ASN	3.6
1	A	362	TRP	3.3
1	B	717[A]	THR	3.3
1	A	91	GLN	3.1
1	B	393	THR	3.0
1	B	96	SER	3.0
1	B	392	TYR	2.9
1	A	668	TYR	2.8
1	B	385	TYR	2.7
1	A	308	VAL	2.6
1	A	525	ASP	2.6
1	B	330	LEU	2.6
1	B	352	LEU	2.6
1	A	341	MET	2.6
1	A	626	TRP	2.5
1	B	487	LEU	2.5
1	A	119	ASP	2.5
1	A	514	ASP	2.5
1	B	365	PHE	2.5
1	B	604	ASP	2.5
1	A	512	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	613	LEU	2.4
1	A	338	MET	2.4
1	B	296	LEU	2.4
1	A	632	TRP	2.4
1	A	720	ASP	2.4
1	B	356	LEU	2.4
1	A	631	LEU	2.4
1	A	84	THR	2.3
1	B	171	VAL	2.3
1	A	68	PRO	2.3
1	B	632	TRP	2.3
1	A	528	LEU	2.3
1	A	385	TYR	2.3
1	B	515	LYS	2.3
1	A	717[A]	THR	2.2
1	A	365	PHE	2.2
1	B	300	PHE	2.2
1	B	119	ASP	2.2
1	A	555	ARG	2.2
1	A	487	LEU	2.2
1	A	120	PRO	2.2
1	A	484	TYR	2.1
1	A	621	TYR	2.1
1	B	720	ASP	2.1
1	A	70	VAL	2.1
1	A	526	PHE	2.1
1	B	429	LEU	2.1
1	B	512	ALA	2.1
1	B	664	LEU	2.0
1	A	676	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.