Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 06:13 pm GMT

PDB ID	:	6Z8Z
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 following versions of software and data (see references ⓘ) were used in the production of this report:

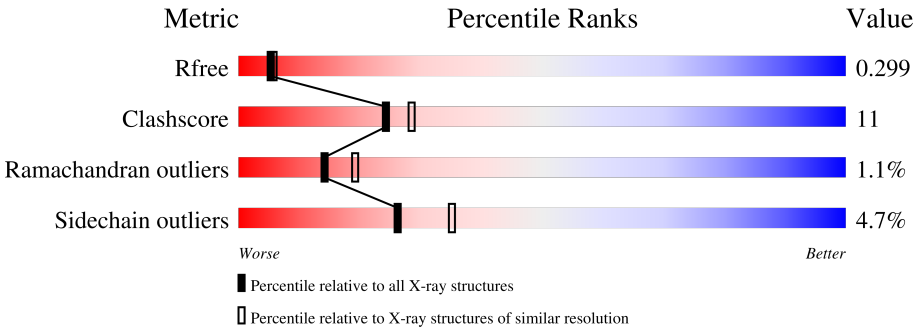
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	723	66% 24% • 9%
1	B	723	62% 26% • 10%

2 Entry composition (i)

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.

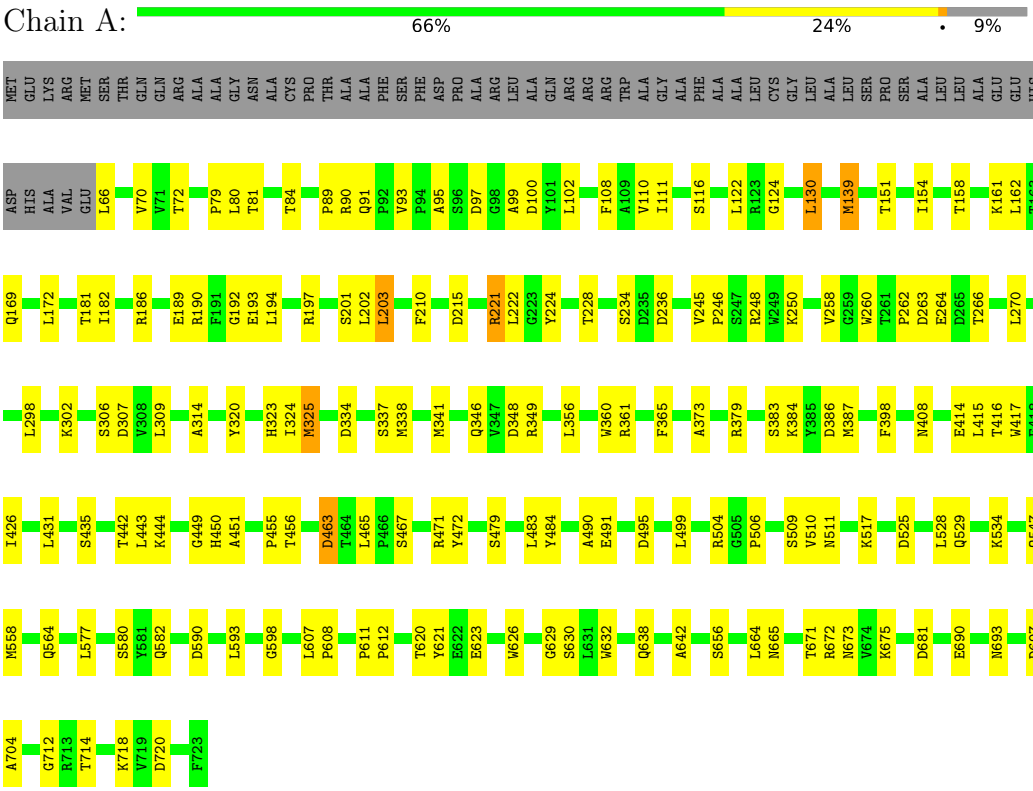
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	19	Total	O	0	0
			19	19		

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. 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. 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.

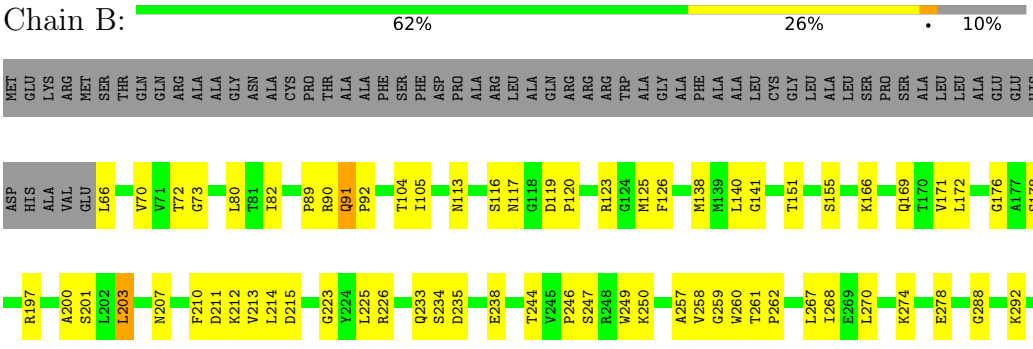
• Molecule 1: Putative copper transport outer membrane porin OprC

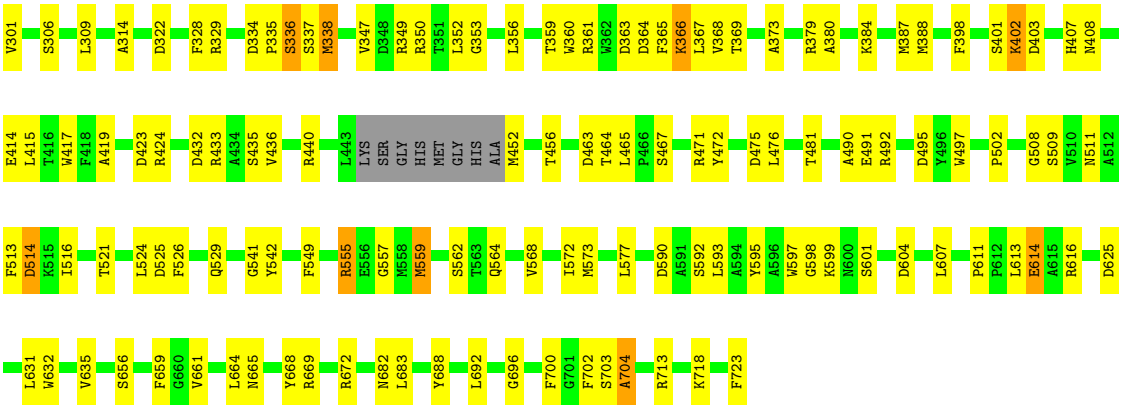
Chain A:



• Molecule 1: Putative copper transport outer membrane porin OprC

Chain B:




V301 S306 L309 A314 D322 F328 R329 D334 P335 S336 S337 M338 V347 D348 R349 R350 T351 L352 G353 L356 T359 W360 R361 W362 D363 D364 F365 K366 L367 V368 T369 A373 R379 A380 K384 M387 M388 F398 S401 K402 D403 H407 N408
E414 L415 T416 W417 F418 A419 D423 R424 D432 R433 A434 S435 V436 R440 L443 LYS SER GLY HIS MET GLY HIS ALA M452 T456 D463 T464 L465 P466 S467 R471 Y472 D475 L476 T481 A490 E491 R492 D495 Y496 W497 P502 G508 S509 V510 N511 A512
F513 D514 K515 I516 T521 L524 D525 F526 Q529 G541 Y542 F549 R555 E556 G557 M558 M559 S562 T563 Q564 V568 I572 M573 L577 D590 A591 S592 L593 A594 Y595 A596 W597 G598 K599 N600 S601 D604 L607 P611 P612 L613 E614 A615 R616 D625
L631 W632 V635 S656 F659 G660 V661 L664 N665 Y668 R669 R672 N682 L683 Y688 L692 G696 F700 G701 F702 S703 A704 R713 K718 F723

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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 85.61 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.02-2.56) 100.0 (85.61-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.238 , 0.295 0.243 , 0.299	Depositor DCC
R_{free} test set	3728 reflections (5.01%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	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.*

[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

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	0.45	0/5228	0.65	0/7087
1	B	0.46	0/5176	0.68	2/7018 (0.0%)
All	All	0.45	0/10404	0.66	2/14105 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	ARG	C-N-CA	6.18	137.16	121.70
1	B	495	ASP	CB-CG-OD1	5.22	123.00	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	5100	0	4877	96	0
1	B	5048	0	4831	125	0
2	A	20	0	0	1	0
2	B	19	0	0	0	0
All	All	10187	0	9708	219	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 11.

All (219) 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:612:PRO:HG3	1:A:638:GLN:HB2	1.62	0.81
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: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:A:250:LYS:NZ	2:A:801:HOH:O	2.27	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:B:66:LEU:O	1:B:669:ARG:NH1	2.25	0.65
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:387:MET:HE2	1:B:388:MET:HG2	1.82	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
1:B:188:PRO:O	1:B:190:ARG:NH1	2.36	0.59
1:B:387:MET:CE	1:B:388:MET:CG	2.81	0.59
1:B:387:MET:HE1	1:B:388:MET:CG	2.33	0.59
1:B:125:MET:HE1	1:B:572:ILE:HG21	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:547:GLN:HE22	1:B:463:ASP:HA	1.71	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:139:MET:CE	1:A:293:ARG:HG3	2.39	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:335:PRO:C	1:B:337:SER:H	2.14	0.51
1:B:593:LEU:HD21	1:B:613:LEU:HD11	1.91	0.51
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: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:A:260:TRP:CD1	1:A:262:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:387:MET:HE1	1:B:388:MET:HG3	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:226:ARG:HB3	1:B:257:ALA:HB3	2.00	0.43
1:B:703:SER:O	1:B:704:ALA:C	2.57	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:138:MET:HE3	1:B:140:LEU:HD21	2.01	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
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: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:B:452:MET:HE3	1:B:452:MET:HB3	1.91	0.41
1:A:110:VAL:HG12	1:A:111:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	656/723 (91%)	610 (93%)	41 (6%)	5 (1%)	19	27
1	B	647/723 (90%)	596 (92%)	42 (6%)	9 (1%)	11	14
All	All	1303/1446 (90%)	1206 (93%)	83 (6%)	14 (1%)	14	19

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

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Mol	Chain	Res	Type
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%)	497 (95%)	28 (5%)	22	30
1	B	521/572 (91%)	500 (96%)	21 (4%)	31	42
All	All	1046/1144 (91%)	997 (95%)	49 (5%)	26	35

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	116	SER
1	A	130	LEU
1	A	139	MET
1	A	201	SER
1	A	203	LEU
1	A	221	ARG
1	A	234	SER
1	A	263	ASP
1	A	264	GLU
1	A	292	LYS
1	A	302	LYS
1	A	325	MET

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Mol	Chain	Res	Type
1	A	338	MET
1	A	341	MET
1	A	349	ARG
1	A	383	SER
1	A	431	LEU
1	A	435	SER
1	A	463	ASP
1	A	479	SER
1	A	495	ASP
1	A	525	ASP
1	A	577	LEU
1	A	593	LEU
1	A	632	TRP
1	A	656	SER
1	A	672	ARG
1	B	116	SER
1	B	155	SER
1	B	190	ARG
1	B	201	SER
1	B	203	LEU
1	B	212	LYS
1	B	274	LYS
1	B	336	SER
1	B	338	MET
1	B	366	LYS
1	B	509	SER
1	B	514	ASP
1	B	555	ARG
1	B	577	LEU
1	B	592	SER
1	B	601	SER
1	B	614	GLU
1	B	632	TRP
1	B	656	SER
1	B	665	ASN
1	B	672	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	A	450	HIS

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Mol	Chain	Res	Type
1	B	91	GLN

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

There are no ligands in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.