

Full wwPDB X-ray Structure Validation Report (i)

Nov 24, 2021 – 06:14 pm GMT

PDB ID	:	6Z9N
Title	:	Copper transporter OprC
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Deposited on	:	2020-06-04
Resolution	:	2.73 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 (i) symbol.

The following versions of software and data (see references (1)) 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.73 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	$1271 \ (2.76-2.72)$
Clashscore	141614	$1322 \ (2.76-2.72)$
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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% 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	А	723	70%	18%	• 10%
1	В	723	.% 68%	21%	• 9%
1	С	723	.% 63%	23%	• 11%
1	D	723	67%	21%	• 9%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20292 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	648	Total	С	Ν	0	\mathbf{S}	4	1	0
	A	048	5028	3156	885	970	17	4		0
1	р	657	Total	С	Ν	0	S	0	1	0
	I D	057	5092	3194	899	980	19			
1	C	C 4 4	Total	С	Ν	0	S	4	1	0
	044	5001	3141	882	963	15	4		0	
1	1 D	CEO	Total	С	Ν	0	S	4	1	0
	058	5100	3200	900	981	19	4		0	

• Molecule 1 is a protein called Putative copper transport outer membrane porin OprC.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	323	ALA	HIS	engineered mutation	UNP G3XD89
В	323	ALA	HIS	engineered mutation	UNP G3XD89
С	323	ALA	HIS	engineered mutation	UNP G3XD89
D	323	ALA	HIS	engineered mutation	UNP G3XD89

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Cu 1 1	0	0
2	В	1	Total Cu 1 1	0	0
2	С	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	28	TotalO2828	0	0
3	В	13	Total O 13 13	0	0
3	С	17	Total O 17 17	0	0
3	D	9	Total O 9 9	0	0



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.





1426 1426 1426 1426 1426 1426 14465 14465 14465 14465 14465 14465 14465 14465 14465 14465 14465 14465 1441 1441 1441 1441 1441 1441 1446 1446 1446 1441 1441 1441 1441 1446 1446 1441 1441 1446 1446 1446 1446 1446 1446 1446 1446 1454 1456 1556 1556 1556 1568 1568



VTO8 SSG2 L429 (712 V666 P438 K718 V566 P438 K588 V569 P478 K588 P478 P496 K588 F479 P496 K640 K640 F491 K640 K640 F691 K640 K640 K641 K640 K640 K641 K640 K640 K641 K640 K640 K641 K640 K640 K643 K640 K643 K643



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	67.33Å 197.27Å 172.12Å	Deneiten
a, b, c, α , β , γ	90.00° 91.42° 90.00°	Depositor
D ecolution $(\hat{\lambda})$	67.30 - 2.73	Depositor
Resolution (A)	172.07 - 2.73	EDS
% Data completeness	98.3 (67.30-2.73)	Depositor
(in resolution range)	92.9(172.07-2.73)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 2.73 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
D D	0.216 , 0.267	Depositor
Λ, Λ_{free}	0.216 , 0.267	DCC
R_{free} test set	5947 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	67.3	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.226 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20292	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 6.98% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.53	1/5155~(0.0%)	0.71	1/6990~(0.0%)	
1	В	0.50	0/5222	0.67	1/7079~(0.0%)	
1	С	0.51	0/5123	0.69	2/6941~(0.0%)	
1	D	0.48	0/5230	0.68	1/7090~(0.0%)	
All	All	0.50	1/20730~(0.0%)	0.69	5/28100~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	ARG	CG-CD	5.06	1.64	1.51

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	С	147	MET	CB-CG-SD	7.23	134.09	112.40
1	В	147	MET	CB-CG-SD	6.18	130.93	112.40
1	D	147	MET	CG-SD-CE	5.41	108.86	100.20
1	С	147	MET	CG-SD-CE	5.08	108.33	100.20
1	А	348	ASP	CB-CG-OD1	5.00	122.81	118.30

All (5) bond angle outliers are listed below:

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	А	5028	0	4808	71	1
1	В	5092	0	4870	89	1
1	С	5001	0	4791	102	0
1	D	5100	0	4881	93	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	28	0	0	2	0
3	В	13	0	0	0	0
3	C	17	0	0	1	0
3	D	9	0	0	1	0
All	All	20292	0	19350	347	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 9.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:385:TYR:OH	1:A:390:ASP:OD1	1.88	0.91
1:A:509:SER:HB3	1:A:515:LYS:HG3	1.62	0.81
1:B:202:LEU:HD12	1:C:225:LEU:HD22	1.63	0.80
1:C:94:PRO:O	1:C:209:ARG:NH2	2.13	0.80
1:A:672:ARG:H	1:A:672:ARG:HD2	1.49	0.77
1:A:433:ARG:HH12	1:B:547:GLN:HG3	1.51	0.76
1:B:283:GLY:HA2	1:B:696:GLY:HA2	1.67	0.76
1:C:584:THR:HG23	1:C:586:ASN:H	1.51	0.75
1:B:215:ASP:HB2	1:B:228:THR:HG23	1.69	0.74
1:A:504:ARG:HH21	1:A:555:ARG:HH12	1.35	0.74
1:C:433:ARG:NH1	1:D:547:GLN:OE1	2.19	0.74
1:D:359:THR:HG23	1:D:368:VAL:HG22	1.69	0.73
1:C:91:GLN:OE1	1:C:663:SER:HB2	1.89	0.73
1:D:384:LYS:HG3	1:D:398:PHE:CZ	2.24	0.72
1:B:122:LEU:HB3	1:B:130:LEU:HD21	1.72	0.71
1:C:344:ALA:H	1:C:383:SER:HB3	1.54	0.71
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.26	0.71
1:A:301:VAL:HG22	1:A:313:GLU:HG2	1.72	0.70
1:D:360:TRP:HB2	1:D:362:TRP:CZ3	2.27	0.70
1:B:143:CYS:SG	1:B:147:MET:HB2	2.32	0.70
1:C:143:CYS:SG	1:C:147:MET:HB2	2.32	0.69
1:C:663:SER:HB3	1:C:681:ASP:HA	1.73	0.69



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:82:ILE:HD11	1:B:166:LYS:HE2	1.73	0.69	
1:C:203:LEU:HD12	1:C:718:LYS:HB2	1.74	0.69	
1:D:495:ASP:HB3	1:D:498:GLU:H	1.58	0.68	
1:B:339:MET:HG2	1:B:343:MET:HE3	1.76	0.68	
1:A:133:LEU:HD11	1:A:173:TRP:HB3	1.74	0.68	
1:A:521:THR:HG23	1:A:546:VAL:HG22	1.76	0.67	
1:A:536:GLN:NE2	3:A:901:HOH:O	2.27	0.67	
1:B:359:THR:HG23	1:B:368:VAL:HG22	1.75	0.67	
1:A:703:SER:O	1:A:703:SER:OG	2.13	0.66	
1:D:375:ARG:NH2	1:D:377:GLU:OE1	2.29	0.66	
1:C:113:ASN:HB3	1:C:281:TYR:HD1	1.61	0.65	
1:C:389:THR:OG1	1:C:390:ASP:N	2.28	0.65	
1:B:76:GLN:HE21	1:B:166:LYS:NZ	1.93	0.65	
1:C:262:PRO:HD2	1:C:266:THR:HB	1.79	0.65	
1:C:506:PRO:O	1:C:509:SER:OG	2.13	0.65	
1:B:504:ARG:HH12	1:B:562:SER:HB3	1.61	0.64	
1:C:464:THR:OG1	1:D:547:GLN:NE2	2.31	0.64	
1:C:292:LYS:HB3	1:C:322:ASP:HB3	1.80	0.63	
1:A:262:PRO:HD2	1:A:266:THR:HB	1.81	0.63	
1:B:261:THR:HG23	1:B:267:LEU:HD23	1.79	0.62	
1:C:465:LEU:HB3	1:C:491:GLU:HB2	1.80	0.62	
1:A:554:TYR:O	1:A:556:GLU:N	2.31	0.62	
1:A:203:LEU:HD12	1:A:718:LYS:HB2	1.80	0.62	
1:C:233:GLN:HB3	1:C:250:LYS:HG3	1.81	0.62	
1:D:67:ALA:HB3	1:D:622:GLU:HG2	1.81	0.62	
1:C:613:LEU:HD12	1:C:614:GLU:H	1.64	0.62	
1:B:504:ARG:HH22	1:B:562:SER:HB3	1.65	0.61	
1:D:392:TYR:OH	1:D:394:ASP:OD1	2.15	0.61	
1:B:506:PRO:HG2	1:B:515:LYS:HD3	1.82	0.61	
1:A:148:ASP:HB3	1:A:291:PHE:CE1	2.34	0.61	
1:A:509:SER:CB	1:A:515:LYS:HG3	2.31	0.61	
1:B:379:ARG:HG2	1:B:402:LYS:HB2	1.82	0.61	
1:D:262:PRO:HD2	1:D:266:THR:HB	1.83	0.61	
1:A:197:ARG:NH2	1:A:215:ASP:OD1	2.35	0.60	
1:A:672:ARG:HD2	1:A:672:ARG:N	2.16	0.60	
1:D:203:LEU:HD12	1:D:718:LYS:HB2	1.84	0.59	
1:C:117:ASN:OD1	1:C:251:LYS:NZ	2.36	0.59	
1:C:171:VAL:HB	1:C:430:ARG:HG3	1.84	0.59	
1:C:201:SER:HB2	1:C:213:VAL:HB	1.85	0.58	
1:C:339:MET:HG2	1:C:343:MET:HG3	1.85	0.58	
1:C:237:TYR:OH	1:C:709:PRO:O	2.16	0.58	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:335:PRO:HB3	1:C:340:PRO:HB3	1.85	0.58	
1:C:638:GLN:HG2	1:C:691:HIS:CD2	2.39	0.58	
1:D:82:ILE:HD11	1:D:166:LYS:HE2	1.84	0.58	
1:C:403:ASP:HB2	1:C:440:ARG:HG3	1.85	0.58	
1:C:420:ALA:O	1:C:422:ARG:N	2.33	0.58	
1:B:143:CYS:HA	1:B:347:VAL:HG21	1.87	0.57	
1:C:429:LEU:HD21	1:D:429:LEU:HD21	1.84	0.57	
1:D:172:LEU:HD21	1:D:414:GLU:HB2	1.87	0.57	
1:B:101:TYR:OH	1:B:157:GLU:HG3	2.04	0.57	
1:C:203:LEU:HB3	1:C:211:ASP:HB2	1.87	0.57	
1:A:287:ASP:OD2	1:A:331:ARG:HG2	2.05	0.57	
1:B:616:ARG:HH21	1:B:633:ARG:HE	1.53	0.57	
1:C:76:GLN:HG2	1:C:78:SER:O	2.05	0.56	
1:B:91:GLN:HB3	1:B:92:PRO:HD3	1.85	0.56	
1:B:117:ASN:OD1	1:B:251:LYS:NZ	2.37	0.56	
1:C:68:PRO:O	1:C:627:SER:HB3	2.05	0.56	
1:D:533:ASP:N	1:D:533:ASP:OD1	2.38	0.56	
1:B:670:VAL:HG12	1:B:671:THR:HG23	1.87	0.56	
1:C:151:THR:HA	1:C:154:ILE:HD12	1.87	0.56	
1:C:79:PRO:O	1:C:81:THR:HG23	2.06	0.56	
1:C:148:ASP:HB3	1:C:291:PHE:CE1	2.41	0.56	
1:A:100:ASP:HA	1:A:103:LYS:HD2	1.88	0.56	
1:C:323:ALA:HB3	1:C:347:VAL:HG23	1.88	0.56	
1:D:379:ARG:HA	1:D:402:LYS:HA	1.89	0.55	
1:C:264:GLU:CD	1:C:264:GLU:H	2.10	0.55	
1:D:91:GLN:OE1	1:D:665:ASN:HB3	2.07	0.55	
1:C:221:ARG:O	1:C:261:THR:HG23	2.06	0.55	
1:D:385:TYR:CE1	1:D:390:ASP:HB2	2.41	0.55	
1:B:248:ARG:HG2	1:B:280:ARG:HG3	1.88	0.55	
1:A:703:SER:O	1:A:705:ASN:N	2.39	0.55	
1:B:203:LEU:HB2	1:B:718:LYS:HG3	1.90	0.54	
1:B:476:LEU:HD12	1:B:481:THR:HB	1.88	0.54	
1:A:625:ASP:HB3	1:A:626:TRP:HD1	1.73	0.54	
1:B:287:ASP:OD1	1:B:331:ARG:NE	2.35	0.54	
1:B:502:PRO:HA	1:B:563:THR:HG23	1.90	0.54	
1:D:568:VAL:HB	1:D:602:SER:HB2	1.90	0.54	
1:C:497:TRP:O	1:C:502:PRO:HD3	2.07	0.54	
1:D:389:THR:O	1:D:391:TYR:N	2.41	0.54	
1:B:324:ILE:HG12	1:B:346:GLN:HG3	1.90	0.54	
1:C:437:LYS:HD3	1:C:439:TYR:CZ	2.43	0.54	
1:C:122:LEU:HD12	1:C:122:LEU:O	2.08	0.53	



	lo uo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:128:SER:OG	1:C:495:ASP:OD1	2.17	0.53	
1:C:495:ASP:HB2	1:C:498:GLU:HG3	1.90	0.53	
1:C:260:TRP:CE2	1:C:262:PRO:HG3	2.44	0.53	
1:D:326:ASP:OD1	1:D:329:ARG:HB2	2.09	0.53	
1:B:467:SER:OG	1:B:490:ALA:HA	2.08	0.53	
1:B:613:LEU:HD12	1:B:614:GLU:H	1.73	0.53	
1:A:295:SER:HB2	1:A:319:ASN:OD1	2.08	0.53	
1:A:248:ARG:HG3	1:A:248:ARG:HH11	1.74	0.53	
1:C:82:ILE:HD11	1:C:166:LYS:HE2	1.91	0.53	
1:B:504:ARG:HH12	1:B:562:SER:CB	2.21	0.52	
1:C:374:MET:SD	1:C:376:ASN:ND2	2.81	0.52	
1:C:521:THR:HG23	1:C:546:VAL:HG22	1.90	0.52	
1:B:145:ASN:HB2	1:B:147:MET:CE	2.39	0.52	
1:B:384:LYS:HD2	1:B:398:PHE:CE2	2.44	0.52	
1:D:519:GLU:HG3	1:D:549:PHE:HA	1.91	0.52	
1:D:129:ARG:NH2	1:D:519:GLU:OE1	2.41	0.52	
1:A:333:PRO:O	1:A:334:ASP:HB3	2.10	0.52	
1:C:169:GLN:OE1	1:C:471:ARG:HD3	2.09	0.52	
1:A:432:ASP:O	1:A:464:THR:HA	2.10	0.52	
1:B:253:ASN:HB3	1:B:293:ARG:HH21	1.75	0.52	
1:D:326:ASP:OD2	1:D:329:ARG:NE	2.34	0.51	
1:C:95:ALA:HA	1:C:209:ARG:NH2	2.24	0.51	
1:C:197:ARG:NH2	1:C:215:ASP:OD1	2.43	0.51	
1:A:133:LEU:CD1	1:A:173:TRP:HB3	2.39	0.51	
1:C:101:TYR:OH	1:C:157:GLU:HG2	2.11	0.51	
1:D:712:GLY:O	1:D:714:THR:HG23	2.11	0.51	
1:C:694:LYS:HE3	1:C:695:ALA:H	1.76	0.51	
1:B:276:ASP:OD1	1:B:277:GLY:N	2.42	0.51	
1:D:337:SER:OG	1:D:338:MET:O	2.29	0.51	
1:D:639:ASN:HA	1:D:655:LYS:HD3	1.94	0.50	
1:C:113:ASN:HB3	1:C:281:TYR:CD1	2.43	0.50	
1:D:148:ASP:HB3	1:D:291:PHE:CE1	2.46	0.50	
1:B:189:GLU:OE1	1:B:197:ARG:NH2	2.44	0.50	
1:D:577:LEU:CD2	1:D:593:LEU:HB3	2.40	0.50	
1:C:286:MET:HE1	1:C:325:MET:O	2.12	0.50	
1:D:236:ASP:HB3	1:D:245:VAL:O	2.12	0.50	
1:C:141:GLY:O	1:C:349:ARG:HD3	2.12	0.50	
1:C:455:PRO:HG2	1:C:510:VAL:HG23	1.93	0.50	
1:D:491:GLU:OE2	1:D:520:LYS:HD3	2.12	0.50	
1:A:509:SER:HA	1:A:515:LYS:NZ	2.27	0.49	
1:D:139:MET:CE	1:D:321:ALA:HB2	2.42	0.49	



	i ageni	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:91:GLN:HG3	1:C:665:ASN:OD1	2.12	0.49	
1:D:375:ARG:HG3	1:D:407:HIS:CD2	2.47	0.49	
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.48	0.49	
1:B:675:LYS:HG2	1:B:720:ASP:HB2	1.94	0.49	
1:D:255:ASP:OD1	1:D:273:GLY:HA3	2.12	0.49	
1:A:189:GLU:OE2	1:A:197:ARG:NH1	2.46	0.49	
1:A:673:ASN:O	1:A:721:PHE:HA	2.13	0.49	
1:B:616:ARG:HH21	1:B:633:ARG:NE	2.11	0.49	
1:D:217:ALA:HB2	1:D:226:ARG:HB2	1.93	0.49	
1:D:335:PRO:O	1:D:340:PRO:HB3	2.12	0.49	
1:D:339:MET:N	1:D:340:PRO:HD3	2.28	0.49	
1:B:267:LEU:HD22	1:B:268:ILE:N	2.28	0.49	
1:A:272:ALA:HB2	1:A:296:LEU:HD23	1.95	0.48	
1:A:91:GLN:OE1	1:A:665:ASN:ND2	2.40	0.48	
1:B:586:ASN:HB3	1:B:621:TYR:CE1	2.48	0.48	
1:B:661:VAL:HG13	1:B:682:ASN:HA	1.95	0.48	
1:D:260:TRP:CE2	1:D:262:PRO:HG3	2.48	0.48	
1:D:577:LEU:HD21	1:D:593:LEU:HB3	1.95	0.48	
1:C:194:LEU:HG	1:C:195:GLY:N	2.29	0.48	
1:C:466:PRO:O	1:C:491:GLU:HG3	2.12	0.48	
1:D:669:ARG:HG2	1:D:669:ARG:HH11	1.78	0.48	
1:A:417:TRP:CE2	1:A:419:ALA:HB2	2.48	0.48	
1:D:438:ASP:HB2	1:D:513:PHE:CE1	2.49	0.48	
1:B:286:MET:HG2	1:B:326:ASP:C	2.33	0.48	
1:C:275:GLY:O	1:C:292:LYS:HD2	2.12	0.48	
1:D:233:GLN:HB3	1:D:250:LYS:HG3	1.94	0.48	
1:D:698:ALA:C	1:D:700:PHE:H	2.17	0.48	
1:A:423:ASP:OD1	1:A:472:TYR:OH	2.27	0.48	
1:C:491:GLU:CD	1:C:520:LYS:HD3	2.34	0.48	
1:B:313:GLU:HG3	1:B:357:ALA:HB3	1.94	0.48	
1:D:309:LEU:HD12	1:D:360:TRP:CZ3	2.49	0.48	
1:B:456:THR:OG1	1:B:511:ASN:ND2	2.30	0.48	
1:D:76:GLN:HE21	1:D:166:LYS:NZ	2.12	0.48	
1:D:349:ARG:NH2	3:D:901:HOH:O	2.31	0.48	
1:C:326:ASP:OD1	1:C:329:ARG:HB2	2.14	0.48	
1:C:417:TRP:CE2	1:C:419:ALA:HB2	2.49	0.48	
1:C:100:ASP:OD1	1:C:103:LYS:HE3	2.13	0.47	
1:C:377:GLU:HG3	1:C:405:VAL:HG22	1.95	0.47	
1:C:324:ILE:C	1:C:325:MET:HG3	2.33	0.47	
1:C:318:TYR:HE1	1:C:350:ARG:HG2	1.79	0.47	
1:A:501:SER:N	1:A:502:PRO:HD2	2.30	0.47	



	io ao pagoini	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:79:PRO:HB3	1:B:484:TYR:CD2	2.50	0.47	
1:C:287:ASP:OD2	1:C:331:ARG:HG2	2.14	0.47	
1:C:481:THR:HG22	1:C:530:TYR:HD1	1.79	0.47	
1:C:495:ASP:HB2	1:C:498:GLU:CG	2.45	0.47	
1:D:189:GLU:HB2	1:D:224:TYR:CD2	2.49	0.47	
1:B:143:CYS:HB3	1:B:148:ASP:OD1	2.14	0.47	
1:D:123:ARG:HB3	1:D:542:TYR:OH	2.15	0.47	
1:D:495:ASP:HB2	1:D:498:GLU:OE1	2.14	0.47	
1:B:76:GLN:HE21	1:B:166:LYS:HZ2	1.60	0.47	
1:B:341:MET:HB2	1:B:385:TYR:CD1	2.50	0.46	
1:C:214:LEU:HD12	1:C:215:ASP:H	1.79	0.46	
1:B:210:PHE:CD1	1:C:194:LEU:HD11	2.51	0.46	
1:C:320:TYR:CE1	1:C:348:ASP:HB2	2.50	0.46	
1:B:198:VAL:HG23	1:B:216:ALA:HB2	1.96	0.46	
1:C:287:ASP:CG	1:C:331:ARG:HE	2.19	0.46	
1:B:340:PRO:HD2	1:B:341:MET:SD	2.55	0.46	
1:A:465:LEU:HB3	1:A:491:GLU:HB2	1.97	0.46	
1:C:139:MET:SD	1:C:319:ASN:HB3	2.55	0.46	
1:C:286:MET:HG2	1:C:327:ASN:HB3	1.97	0.46	
1:A:435:SER:HB3	1:A:462:ALA:HB2	1.96	0.46	
1:C:189:GLU:O	1:C:190:ARG:HD3	2.16	0.46	
1:C:292:LYS:HD2	1:C:292:LYS:HA	1.69	0.46	
1:D:366:LYS:HB3	1:D:416:THR:CG2	2.46	0.46	
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.51	0.45	
1:A:285:GLY:HA2	1:A:697:ASP:OD2	2.15	0.45	
1:C:101:TYR:CD1	1:C:156:PRO:HG2	2.50	0.45	
1:A:514:ASP:HB3	1:A:515:LYS:HG2	1.99	0.45	
1:D:337:SER:OG	1:D:338:MET:N	2.49	0.45	
1:D:95:ALA:O	1:D:97:ASP:N	2.49	0.45	
1:C:192:GLY:O	1:C:221:ARG:HG3	2.16	0.45	
1:C:547:GLN:NE2	1:D:464:THR:OG1	2.49	0.45	
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.52	0.45	
1:B:270:LEU:HD12	1:B:298:LEU:HD13	1.98	0.45	
1:C:584:THR:HG22	1:C:587:TRP:HB2	1.99	0.45	
1:A:139:MET:CE	1:A:321:ALA:HB2	2.46	0.45	
1:A:201:SER:OG	1:A:213:VAL:HB	2.16	0.45	
1:A:703:SER:C	1:A:705:ASN:H	2.19	0.45	
1:D:132:ILE:C	1:D:133:LEU:HD23	2.37	0.45	
1:A:248:ARG:HG3	1:A:248:ARG:NH1	2.32	0.45	
1:B:74:VAL:HG11	1:B:84:THR:HB	1.97	0.45	
1:D:76:GLN:HB2	1:D:538:TRP:CD2	2.51	0.45	



	louo pugom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:416:THR:HG23	1:B:426:ILE:HG13	1.99	0.45	
1:C:481:THR:HG22	1:C:530:TYR:CD1	2.52	0.45	
1:D:203:LEU:HB2	1:D:718:LYS:HG3	1.99	0.45	
1:D:506:PRO:HG2	1:D:515:LYS:HB3	1.99	0.45	
1:B:145:ASN:HB2	1:B:147:MET:HE3	1.99	0.44	
1:B:326:ASP:OD1	1:B:329:ARG:HB2	2.16	0.44	
1:D:78:SER:HB2	1:D:79:PRO:HD2	1.99	0.44	
1:B:213:VAL:HG22	1:B:230:ASN:HB2	1.98	0.44	
1:B:365:PHE:HD2	1:B:415:LEU:HD11	1.82	0.44	
1:C:309:LEU:HD11	1:C:358:ALA:HB1	1.98	0.44	
1:C:314:ALA:HB2	1:C:356:LEU:HD23	2.00	0.44	
1:C:155:SER:O	1:C:158:THR:OG1	2.30	0.44	
1:D:199:ASN:HB3	1:D:215:ASP:HB3	2.00	0.44	
1:A:429:LEU:HD11	1:B:429:LEU:HD21	1.99	0.44	
1:D:74:VAL:HG11	1:D:84:THR:HB	1.99	0.44	
1:D:139:MET:HE3	1:D:321:ALA:HB2	1.99	0.44	
1:C:455:PRO:HB2	1:C:510:VAL:HG21	1.99	0.44	
1:D:123:ARG:HB3	1:D:542:TYR:CZ	2.53	0.44	
1:D:668:TYR:CE2	1:D:670:VAL:HB	2.52	0.44	
1:A:308:VAL:HG23	1:A:360:TRP:HE3	1.83	0.44	
1:B:172:LEU:HD21	1:B:414:GLU:HB2	1.99	0.44	
1:B:495:ASP:HB3	1:B:498:GLU:H	1.83	0.44	
1:B:504:ARG:NH1	1:B:562:SER:HB3	2.29	0.44	
1:A:612:PRO:HB3	1:A:638:GLN:HB2	2.00	0.44	
1:D:82:ILE:HG21	1:D:105:ILE:HD13	2.00	0.44	
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.82	0.44	
1:D:248:ARG:HD3	1:D:280:ARG:CZ	2.47	0.44	
1:D:336:SER:O	1:D:337:SER:HB3	2.18	0.44	
1:D:424:ARG:NH1	1:D:473:GLU:OE1	2.51	0.44	
1:B:84:THR:HG23	1:B:162:LEU:HB3	2.00	0.43	
1:B:206:SER:HG	1:B:715:PHE:H	1.65	0.43	
1:D:328:PHE:CE1	1:D:329:ARG:HG3	2.53	0.43	
1:A:375:ARG:NE	3:A:905:HOH:O	2.49	0.43	
1:A:476:LEU:HD23	1:A:476:LEU:HA	1.77	0.43	
1:B:497:TRP:O	1:B:502:PRO:HD3	2.17	0.43	
1:A:126:PHE:O	1:A:129:ARG:HD2	2.18	0.43	
1:A:233:GLN:HB3	1:A:250:LYS:HG3	1.99	0.43	
1:A:144:PRO:O	1:A:497:TRP:HD1	2.02	0.43	
1:A:186:ARG:HG2	1:A:226:ARG:NH1	2.33	0.43	
1:A:203:LEU:O	1:A:210:PHE:HA	2.18	0.43	
1:B:491:GLU:CD	1:B:520:LYS:HD3	2.39	0.43	



	i agein	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:433:ARG:NH2	3:C:904:HOH:O	2.49	0.43	
1:A:692:LEU:HD23	1:A:692:LEU:HA	1.81	0.43	
1:B:72:THR:HG22	1:B:631:LEU:HD22	2.01	0.43	
1:C:689:THR:OG1	1:C:707:THR:OG1	2.18	0.43	
1:A:422:ARG:CZ	1:A:477:ALA:HB2	2.49	0.43	
1:B:384:LYS:HD2	1:B:398:PHE:CZ	2.53	0.43	
1:A:112:ARG:NE	1:A:710:GLU:OE1	2.38	0.43	
1:C:339:MET:CG	1:C:343:MET:HG3	2.47	0.43	
1:D:80:LEU:HD22	1:D:166:LYS:O	2.18	0.43	
1:D:101:TYR:CD1	1:D:156:PRO:HG2	2.53	0.43	
1:A:614:GLU:OE1	1:A:616:ARG:NH2	2.52	0.43	
1:C:350:ARG:O	1:C:376:ASN:HA	2.19	0.43	
1:D:76:GLN:HE21	1:D:166:LYS:CE	2.32	0.43	
1:D:686:LYS:HD2	1:D:687:ASP:H	1.84	0.43	
1:C:80:LEU:HD21	1:C:525:ASP:HB3	1.99	0.42	
1:C:108:PHE:CZ	1:C:122:LEU:HD13	2.54	0.42	
1:C:607:LEU:HD23	1:C:607:LEU:HA	1.89	0.42	
1:A:505:GLY:O	1:A:564:GLN:HG3	2.19	0.42	
1:C:86:PRO:HA	1:C:90:ARG:NH1	2.34	0.42	
1:A:466:PRO:O	1:A:491:GLU:HG3	2.20	0.42	
1:C:502:PRO:HA	1:C:563:THR:HG23	2.00	0.42	
1:A:417:TRP:CZ2	1:A:419:ALA:HB2	2.54	0.42	
1:B:148:ASP:HB3	1:B:291:PHE:CE1	2.54	0.42	
1:B:386:ASP:CG	1:B:389:THR:HG22	2.39	0.42	
1:B:261:THR:HG22	1:B:266:THR:O	2.20	0.42	
1:D:308:VAL:HG23	1:D:362:TRP:HB3	2.01	0.42	
1:A:112:ARG:H	1:A:693:ASN:HA	1.84	0.42	
1:C:586:ASN:OD1	1:C:586:ASN:N	2.52	0.42	
1:D:197:ARG:NH1	1:D:215:ASP:OD1	2.51	0.42	
1:D:361:ARG:C	1:D:362:TRP:HE3	2.23	0.42	
1:D:497:TRP:HB3	1:D:648:VAL:HG11	2.00	0.42	
1:B:504:ARG:NH2	1:B:562:SER:HB3	2.33	0.42	
1:B:529:GLN:HE21	1:B:529:GLN:HB3	1.65	0.42	
1:C:597:TRP:CH2	1:C:599:LYS:HB2	2.55	0.42	
1:B:455:PRO:HB2	1:B:510:VAL:CG1	2.49	0.42	
1:B:608:PRO:HB3	1:B:642:ALA:HB3	2.01	0.42	
1:D:368:VAL:O	1:D:413:GLY:HA2	2.19	0.42	
1:A:456:THR:HG22	1:A:459:ASP:OD2	2.20	0.42	
1:B:189:GLU:HB2	1:B:224:TYR:CG	2.55	0.41	
1:B:149:ALA:HB1	1:B:150:PRO:HD2	2.02	0.41	
1:B:320:TYR:CE1	1:B:348:ASP:HB2	2.55	0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:342:PRO:HB2	1:B:392:TYR:CD2	2.55	0.41	
1:D:72:THR:HG22	1:D:91:GLN:HB3	2.02	0.41	
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.86	0.41	
1:A:516:ILE:HD13	1:A:516:ILE:HA	1.89	0.41	
1:A:203:LEU:HB3	1:A:211:ASP:HB2	2.01	0.41	
1:A:346:GLN:HG2	1:A:400:TRP:CH2	2.56	0.41	
1:B:465:LEU:HB3	1:B:491:GLU:HB2	2.01	0.41	
1:B:516:ILE:HD13	1:B:516:ILE:HA	1.88	0.41	
1:D:362:TRP:CE3	1:D:362:TRP:N	2.88	0.41	
1:A:255:ASP:OD1	1:A:273:GLY:HA3	2.20	0.41	
1:B:73:GLY:HA2	1:B:104:THR:O	2.21	0.41	
1:C:556:GLU:O	1:C:561:SER:N	2.54	0.41	
1:D:272:ALA:HB2	1:D:296:LEU:HD23	2.01	0.41	
1:D:638:GLN:HG2	1:D:691:HIS:CD2	2.56	0.41	
1:A:549:PHE:N	1:A:568:VAL:O	2.54	0.41	
1:B:201:SER:O	1:B:202:LEU:HD23	2.20	0.41	
1:D:360:TRP:O	1:D:362:TRP:HZ3	2.04	0.41	
1:A:588:LYS:HE3	1:A:588:LYS:HB3	1.82	0.41	
1:B:171:VAL:O	1:B:430:ARG:NH1	2.50	0.41	
1:B:501:SER:N	1:B:502:PRO:HD2	2.36	0.41	
1:B:72:THR:HB	1:B:631:LEU:HD13	2.02	0.40	
1:D:577:LEU:HD21	1:D:593:LEU:HD23	2.03	0.40	
1:D:598:GLY:O	1:D:640:ARG:NH1	2.54	0.40	
1:B:623:GLU:O	1:B:625:ASP:N	2.53	0.40	
1:D:132:ILE:HD13	1:D:151:THR:HG23	2.02	0.40	
1:D:501:SER:N	1:D:502:PRO:HD2	2.36	0.40	
1:D:504:ARG:HH22	1:D:555:ARG:HD3	1.86	0.40	
1:B:582:GLN:NE2	1:B:588:LYS:HE2	2.36	0.40	
1:C:67:ALA:HB3	1:C:622:GLU:HG2	2.04	0.40	
1:D:385:TYR:CZ	1:D:390:ASP:HB2	2.56	0.40	
1:D:689:THR:OG1	1:D:708:VAL:O	2.36	0.40	
1:C:102:LEU:HD13	1:C:108:PHE:CE1	2.57	0.40	
1:C:440:ARG:O	1:C:454:ASN:ND2	2.37	0.40	
1:C:694:LYS:O	1:C:707:THR:HA	2.22	0.40	
1:D:467:SER:OG	1:D:490:ALA:HA	2.20	0.40	
1:D:524:LEU:O	1:D:542:TYR:HA	2.21	0.40	
1:D:614:GLU:HB2	1:D:635:VAL:HG22	2.04	0.40	
1:D:643:ARG:HE	1:D:653:PHE:HE1	1.69	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:713:ARG:NH1	$1:B:623:GLU:OE2[2_646]$	2.16	0.04

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	Perc	entiles
1	А	645/723~(89%)	601 (93%)	34~(5%)	10 (2%)	9	17
1	В	656/723~(91%)	624 (95%)	27 (4%)	5(1%)	19	36
1	С	633/723~(88%)	578 (91%)	47 (7%)	8 (1%)	12	21
1	D	657/723~(91%)	605~(92%)	44 (7%)	8 (1%)	13	24
All	All	2591/2892~(90%)	2408 (93%)	152 (6%)	31 (1%)	13	24

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	478	ASP
1	А	555	ARG
1	А	625	ASP
1	С	336	SER
1	С	389	THR
1	С	495	ASP
1	D	337	SER
1	D	390	ASP
1	D	558	MET
1	D	671	THR
1	А	559	MET
1	А	698	ALA
1	А	704	ALA
1	В	624	GLY
1	С	698	ALA
1	А	583	LEU
1	В	583	LEU



Mol	Chain	Res	Type
1	С	247	SER
1	С	421	GLU
1	А	247	SER
1	А	334	ASP
1	В	561	SER
1	В	704	ALA
1	D	340	PRO
1	D	421	GLU
1	С	511	ASN
1	D	335	PRO
1	D	420	ALA
1	В	247	SER
1	С	420	ALA
1	A	246	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	519/572~(91%)	485~(93%)	34 (7%)	16	29
1	В	525/572~(92%)	487 (93%)	38 (7%)	14	25
1	С	517/572~(90%)	473 (92%)	44 (8%)	10	20
1	D	526/572~(92%)	483 (92%)	43 (8%)	11	21
All	All	2087/2288~(91%)	1928 (92%)	159 (8%)	13	23

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	72	THR
1	А	78	SER
1	А	97	ASP
1	А	104	THR
1	А	139	MET
1	А	151	THR
1	А	155	SER



Mol	Chain	Res	Type
1	А	190	ARG
1	А	197	ARG
1	А	203	LEU
1	А	248	ARG
1	А	300	PHE
1	А	325	MET
1	А	333	PRO
1	А	339	MET
1	А	341	MET
1	А	356	LEU
1	А	363	ASP
1	А	387	MET
1	А	466	PRO
1	А	510	VAL
1	А	515	LYS
1	А	525	ASP
1	А	555	ARG
1	А	561	SER
1	А	563	THR
1	А	577	LEU
1	А	580	SER
1	А	584	THR
1	А	632	TRP
1	А	672	ARG
1	А	677	SER
1	А	694	LYS
1	А	703	SER
1	В	91	GLN
1	В	97	ASP
1	В	152	SER
1	В	194	LEU
1	В	206	SER
1	В	212	LYS
1	B	215	ASP
1	В	221	ARG
1	В	261	THR
1	В	267	LEU
1	В	284	ARG
1	В	286	MET
1	В	292	LYS
1	В	299	ARG
1	В	303	SER



Mol	Chain	Res	Type
1	В	306	SER
1	В	307	ASP
1	В	313	GLU
1	В	325	MET
1	В	338	MET
1	В	341	MET
1	В	355	ARG
1	В	362	TRP
1	В	388	MET
1	В	442	THR
1	В	495	ASP
1	В	510	VAL
1	В	556	GLU
1	В	558	MET
1	В	561	SER
1	В	562	SER
1	В	625	ASP
1	В	634	VAL
1	В	635	VAL
1	В	673	ASN
1	В	677	SER
1	В	694	LYS
1	В	705	ASN
1	С	77	SER
1	С	78	SER
1	С	91	GLN
1	С	97	ASP
1	С	104	THR
1	С	134	THR
1	С	151	THR
1	С	155	SER
1	С	193	GLU
1	С	203	LEU
1	C	209	ARG
1	С	274	LYS
1	C	278	GLU
1	С	303	SER
1	С	306	SER
1	C	337	SER
1	С	341	MET
1	С	347	VAL
1	С	369	THR



Mol	Chain	Res	Type
1	С	383	SER
1	С	396	ASP
1	С	425	LEU
1	С	429	LEU
1	C	430	ARG
1	С	444	LYS
1	С	481	THR
1	С	503	LYS
1	С	510	VAL
1	С	529	GLN
1	С	547	GLN
1	С	562	SER
1	С	564	GLN
1	C	586	ASN
1	C	603	ASP
1	С	616	ARG
1	С	620	THR
1	С	632	TRP
1	С	663	SER
1	С	672	ARG
1	С	677	SER
1	С	700	PHE
1	С	705	ASN
1	С	719	VAL
1	С	721	PHE
1	D	66	LEU
1	D	116	SER
1	D	119	ASP
1	D	139	MET
1	D	155	SER
1	D	197	ARG
1	D	201	SER
1	D	202	LEU
1	D	203	LEU
1	D	226	ARG
1	D	230	ASN
1	D	234	SER
1	D	292	LYS
1	D	293	ARG
1	D	307	ASP
1	D	325	MET
1	D	326	ASP
-			



Mol	Chain	Res	Type
1	D	341	MET
1	D	355	ARG
1	D	360	TRP
1	D	362	TRP
1	D	386	ASP
1	D	393	THR
1	D	397	GLN
1	D	402	LYS
1	D	478	ASP
1	D	479	SER
1	D	510	VAL
1	D	515	LYS
1	D	525	ASP
1	D	558	MET
1	D	562	SER
1	D	577	LEU
1	D	581	TYR
1	D	586	ASN
1	D	588	LYS
1	D	616	ARG
1	D	648	VAL
1	D	669	ARG
1	D	670	VAL
1	D	672	ARG
1	D	677	SER
1	D	707	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	441	GLN
1	А	529	GLN
1	В	76	GLN
1	В	199	ASN
1	В	253	ASN
1	В	665	ASN
1	С	547	GLN
1	D	76	GLN
1	D	408	ASN
1	D	547	GLN
1	D	673	ASN
1	D	705	ASN



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)

Of 4 ligands modelled in this entry, 4 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 (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, 95^{th} 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	А	648/723~(89%)	0.09	2 (0%) 94 96	43, 56, 86, 125	0
1	В	657/723~(90%)	0.24	10 (1%) 73 79	42, 60, 96, 124	0
1	С	644/723~(89%)	0.07	5 (0%) 86 89	42, 61, 100, 130	0
1	D	658/723~(91%)	0.25	15 (2%) 60 67	43, 62, 100, 135	0
All	All	2607/2892~(90%)	0.16	32 (1%) 79 83	42, 60, 96, 135	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	362	TRP	5.3
1	С	510	VAL	4.2
1	А	555	ARG	4.1
1	D	362	TRP	3.9
1	В	387	MET	3.8
1	В	398	PHE	3.3
1	С	443	LEU	3.1
1	В	700	PHE	2.9
1	D	382	GLY	2.8
1	В	300	PHE	2.8
1	С	704	ALA	2.8
1	D	268	ILE	2.7
1	D	119	ASP	2.6
1	D	508	GLY	2.5
1	D	512	ALA	2.5
1	D	384	LYS	2.5
1	С	300	PHE	2.4
1	D	514	ASP	2.4
1	D	389	THR	2.2
1	D	452	MET	2.2
1	А	365	PHE	2.2



	5	1	1 0	
Mol	Chain	Res	Type	RSRZ
1	D	524	LEU	2.2
1	В	558	MET	2.2
1	D	363	ASP	2.1
1	D	509	SER	2.1
1	В	415	LEU	2.1
1	С	556	GLU	2.1
1	В	210	PHE	2.1
1	В	367	LEU	2.1
1	D	409	TYR	2.1
1	D	390	ASP	2.0
1	В	388	MET	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 (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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	CU	D	801	1/1	0.96	0.14	$97,\!97,\!97,\!97$	0
2	CU	А	801	1/1	0.97	0.16	83,83,83,83	0
2	CU	В	801	1/1	0.98	0.13	88,88,88,88	0
2	CU	С	801	1/1	0.99	0.14	$95,\!95,\!95,\!95$	0

6.5 Other polymers (i)

There are no such residues in this entry.

