



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:09 AM UTC

PDB ID : 6Z9N / pdb_00006z9n
Title : Copper transporter OprC
Authors : Bhamidimarri, S.P.; van den Berg, B.
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 ⓘ 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

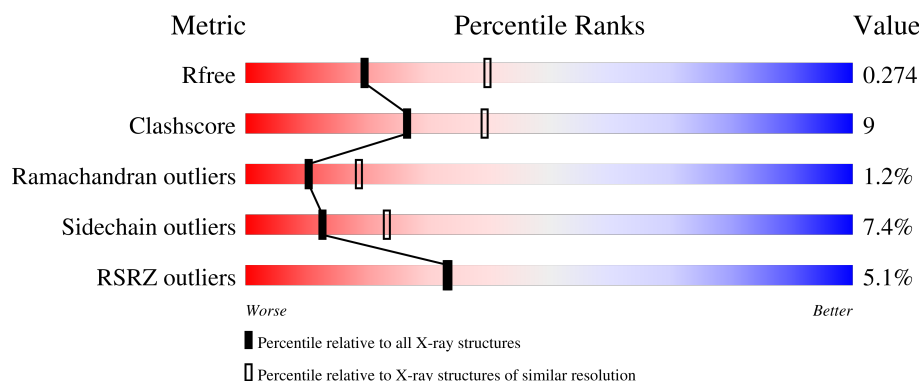
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (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 $\leq 5\%$. 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% 70% 18% • 10%
1	B	723	3% 67% 22% • 9%
1	C	723	6% 62% 24% • 11%
1	D	723	5% 68% 21% • 9%

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	4	1	0
			5028	3156	885	970	17			
1	B	657	Total	C	N	O	S	0	1	0
			5092	3194	899	980	19			
1	C	644	Total	C	N	O	S	4	1	0
			5001	3141	882	963	15			
1	D	658	Total	C	N	O	S	4	1	0
			5100	3200	900	981	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	HIS	engineered mutation	UNP G3XD89
B	323	ALA	HIS	engineered mutation	UNP G3XD89
C	323	ALA	HIS	engineered mutation	UNP G3XD89
D	323	ALA	HIS	engineered mutation	UNP G3XD89

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		

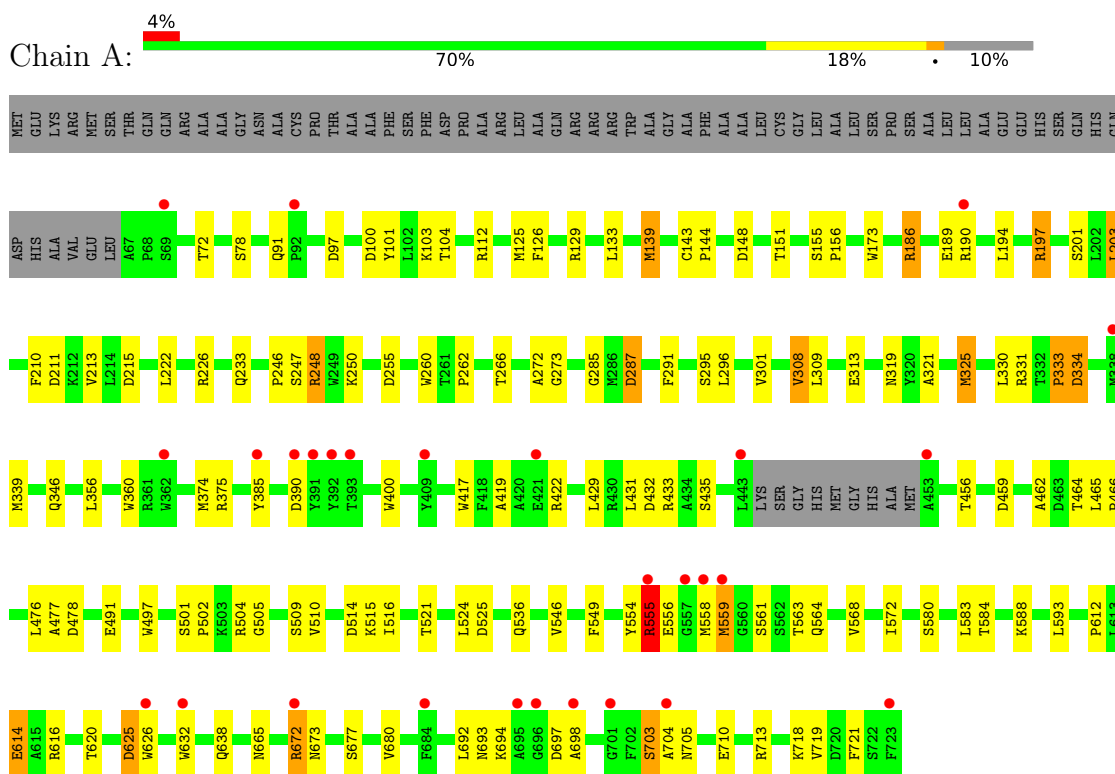
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	13	Total 13	O 13	0	0
3	C	17	Total 17	O 17	0	0
3	D	9	Total 9	O 9	0	0

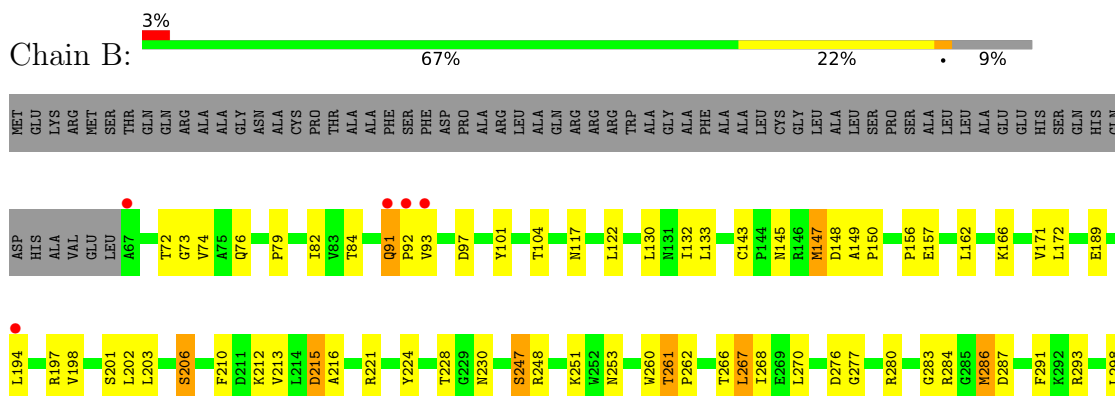
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Putative copper transport outer membrane porin OprC

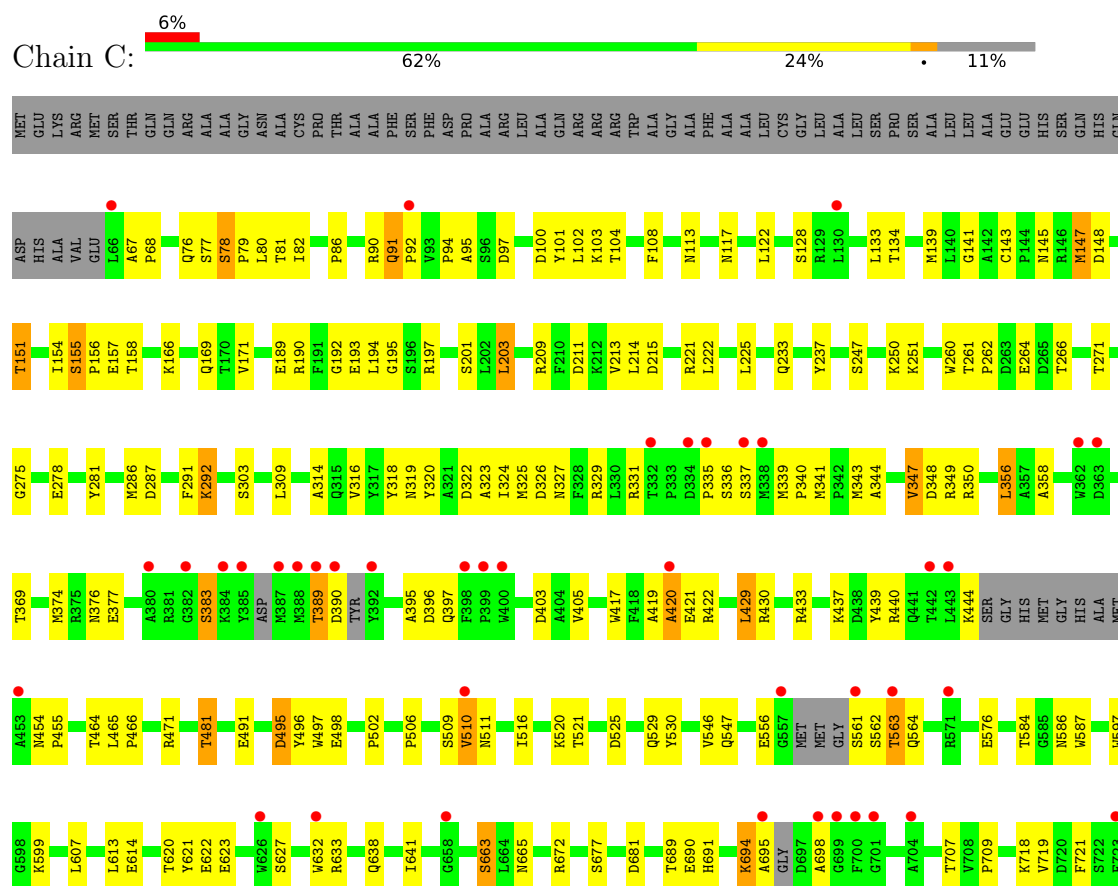


• Molecule 1: Putative copper transport outer membrane porin OprC

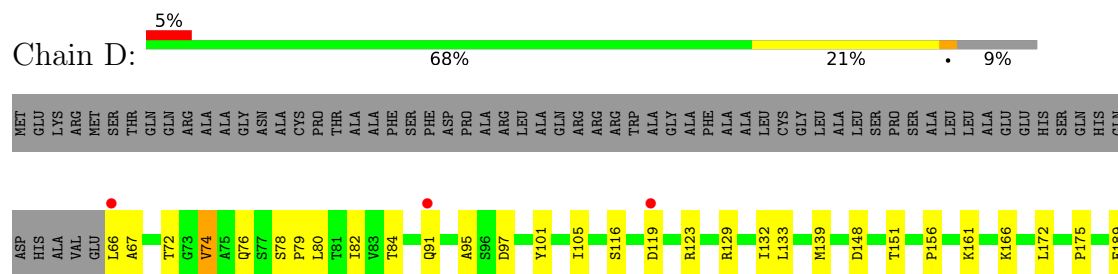


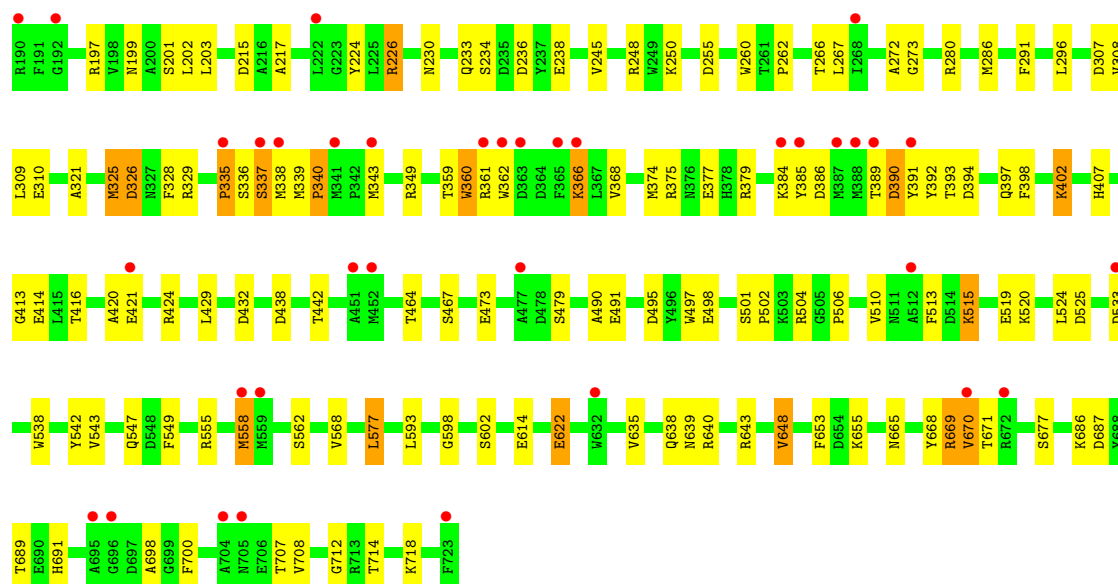


• Molecule 1: Putative copper transport outer membrane porin OprC



• Molecule 1: Putative copper transport outer membrane porin OprC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.33Å 197.27Å 172.12Å 90.00° 91.42° 90.00°	Depositor
Resolution (Å)	67.30 – 2.73 67.30 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.3 (67.30-2.73) 100.0 (67.30-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.216 , 0.267 0.225 , 0.274	Depositor DCC
R_{free} test set	5948 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)	0.30 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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

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	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/5155	0.70	0/6990
1	B	0.44	0/5222	0.65	1/7079 (0.0%)
1	C	0.45	0/5123	0.69	2/6941 (0.0%)
1	D	0.42	0/5230	0.64	0/7090
All	All	0.44	0/20730	0.67	3/28100 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	MET	CB-CG-SD	7.13	134.09	112.70
1	B	147	MET	CB-CG-SD	6.08	130.93	112.70
1	C	92	PRO	N-CA-C	-5.19	101.79	112.47

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	5028	0	4808	76	1
1	B	5092	0	4870	93	1
1	C	5001	0	4791	109	0
1	D	5100	0	4881	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	0	2	0
3	B	13	0	0	0	0
3	C	17	0	0	1	0
3	D	9	0	0	1	0
All	All	20292	0	19350	369	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 (369) 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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:MET:SD	1:B:343:MET:HE2	2.37	0.64
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:C:689:THR:OG1	1:C:707:THR:OG1	2.18	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:C:264:GLU:CD	1:C:264:GLU:H	2.10	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
1:C:335:PRO:HB3	1:C:340:PRO:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:339:MET:HE3	1:D:343:MET:HE2	1.86	0.57
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:B:145:ASN:HB2	1:B:147:MET:HE2	1.86	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:286:MET:HG2	1:B:326:ASP:C	2.33	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:D:698:ALA:C	1:D:700:PHE:H	2.17	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:C:491:GLU:CD	1:C:520:LYS:HD3	2.34	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:C:324:ILE:C	1:C:325:MET:HG3	2.33	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: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:D:286:MET:HE2	1:D:325:MET:HB2	1.92	0.51
1:C:287:ASP:CG	1:C:331:ARG:HE	2.19	0.51
1:A:333:PRO:O	1:A:334:ASP:HB3	2.10	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:D:236:ASP:HB3	1:D:245:VAL:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:703:SER:C	1:A:705:ASN:H	2.19	0.49
1:D:132:ILE:C	1:D:133:LEU:HD23	2.37	0.49
1:D:139:MET:CE	1:D:321:ALA:HB2	2.42	0.49
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:286:MET:SD	1:D:339:MET:HE1	2.53	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:B:491:GLU:CD	1:B:520:LYS:HD3	2.39	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:286:MET:HG3	1:D:339:MET:HE1	1.96	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
1:B:79:PRO:HB3	1:B:484:TYR:CD2	2.50	0.47
1:B:386:ASP:CG	1:B:389:THR:HG22	2.39	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:D:361:ARG:C	1:D:362:TRP:HE3	2.23	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:B:287:ASP:CG	1:B:331:ARG:HE	2.22	0.46
1:C:320:TYR:CE1	1:C:348:ASP:HB2	2.50	0.46
1:A:143:CYS:HB2	1:A:325:MET:HE1	1.96	0.46
1:A:374:MET:HE3	1:A:374:MET:HB3	1.62	0.46
1:B:198:VAL:HG23	1:B:216:ALA:HB2	1.96	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:B:325:MET:HE3	1:B:325:MET:HB3	1.61	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:C:621:TYR:OH	1:C:623:GLU:OE2	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:145:ASN:HB2	1:C:147:MET:HE2	1.99	0.45
1:D:76:GLN:HB2	1:D:538:TRP:CD2	2.51	0.45
1:B:416:THR:HG23	1:B:426:ILE:HG13	1.99	0.45
1:C:395:ALA:C	1:C:397:GLN:H	2.24	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:326:ASP:OD1	1:B:329:ARG:HB2	2.16	0.44
1:C:633:ARG:HH22	1:C:690:GLU:CD	2.24	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:A:558:MET:HE2	1:A:559:MET:HE2	1.99	0.44
1:C:496:TYR:CD1	1:C:496:TYR:C	2.96	0.44
1:D:74:VAL:HG11	1:D:84:THR:HB	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:125:MET:HE1	1:A:572:ILE:HG21	2.00	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:D:374:MET:HE3	1:D:374:MET:HB3	1.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:ARG:NH1	1:D:473:GLU:OE1	2.51	0.44
1:A:325:MET:HB3	1:A:325:MET:HE2	1.76	0.43
1:B:84:THR:HG23	1:B:162:LEU:HB3	2.00	0.43
1:D:286:MET:CG	1:D:339:MET:HE1	2.49	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:392:TYR:OH	1:B:394:ASP:OD1	2.33	0.43
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:166:LYS:NZ	1:C:576:GLU:OE1	2.36	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:B:206:SER:HG	1:B:715:PHE:H	1.63	0.42
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:139:MET:HE3	1:A:321:ALA:HB2	2.00	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:C:286:MET:HE1	1:C:325:MET:O	2.19	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:261:THR:HG22	1:B:266:THR:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:132:ILE:C	1:B:133:LEU:HD23	2.45	0.41
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
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:B:300:PHE:CD1	1:B:300:PHE:C	2.98	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:D:175:PRO:HB3	1:D:432:ASP:CG	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:325:MET:HE3	1:C:325:MET:HB2	1.69	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	Percentiles	
1	A	645/723 (89%)	601 (93%)	34 (5%)	10 (2%)	7	13
1	B	656/723 (91%)	624 (95%)	27 (4%)	5 (1%)	16	29
1	C	633/723 (88%)	578 (91%)	47 (7%)	8 (1%)	9	16
1	D	657/723 (91%)	605 (92%)	44 (7%)	8 (1%)	10	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2591/2892 (90%)	2408 (93%)	152 (6%)	31 (1%)	10 19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	ASP
1	A	555	ARG
1	A	625	ASP
1	C	336	SER
1	C	389	THR
1	C	495	ASP
1	D	337	SER
1	D	390	ASP
1	D	558	MET
1	D	671	THR
1	A	559	MET
1	A	698	ALA
1	A	704	ALA
1	B	624	GLY
1	C	698	ALA
1	A	583	LEU
1	B	583	LEU
1	C	247	SER
1	C	421	GLU
1	A	247	SER
1	A	334	ASP
1	B	561	SER
1	B	704	ALA
1	D	340	PRO
1	D	421	GLU
1	C	511	ASN
1	D	335	PRO
1	D	420	ALA
1	B	247	SER
1	C	420	ALA
1	A	246	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	519/572 (91%)	480 (92%)	39 (8%)	12	23
1	B	525/572 (92%)	489 (93%)	36 (7%)	14	26
1	C	517/572 (90%)	475 (92%)	42 (8%)	11	20
1	D	526/572 (92%)	489 (93%)	37 (7%)	14	26
All	All	2087/2288 (91%)	1933 (93%)	154 (7%)	13	23

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	78	SER
1	A	97	ASP
1	A	104	THR
1	A	139	MET
1	A	151	THR
1	A	155	SER
1	A	186	ARG
1	A	190	ARG
1	A	197	ARG
1	A	203	LEU
1	A	222	LEU
1	A	248	ARG
1	A	287	ASP
1	A	308	VAL
1	A	309	LEU
1	A	325	MET
1	A	330	LEU
1	A	333	PRO
1	A	339	MET
1	A	356	LEU
1	A	510	VAL
1	A	524	LEU
1	A	525	ASP
1	A	555	ARG
1	A	561	SER
1	A	563	THR
1	A	580	SER
1	A	584	THR
1	A	593	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	614	GLU
1	A	620	THR
1	A	632	TRP
1	A	672	ARG
1	A	677	SER
1	A	680	VAL
1	A	694	LYS
1	A	703	SER
1	A	719	VAL
1	B	91	GLN
1	B	93	VAL
1	B	97	ASP
1	B	194	LEU
1	B	206	SER
1	B	212	LYS
1	B	215	ASP
1	B	221	ARG
1	B	247	SER
1	B	261	THR
1	B	267	LEU
1	B	284	ARG
1	B	286	MET
1	B	303	SER
1	B	309	LEU
1	B	313	GLU
1	B	325	MET
1	B	338	MET
1	B	355	ARG
1	B	388	MET
1	B	442	THR
1	B	495	ASP
1	B	510	VAL
1	B	534	LYS
1	B	556	GLU
1	B	558	MET
1	B	561	SER
1	B	562	SER
1	B	577	LEU
1	B	630	SER
1	B	634	VAL
1	B	635	VAL
1	B	673	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	677	SER
1	B	705	ASN
1	B	719	VAL
1	C	77	SER
1	C	78	SER
1	C	91	GLN
1	C	97	ASP
1	C	104	THR
1	C	133	LEU
1	C	134	THR
1	C	151	THR
1	C	155	SER
1	C	193	GLU
1	C	203	LEU
1	C	222	LEU
1	C	271	THR
1	C	278	GLU
1	C	292	LYS
1	C	303	SER
1	C	316	VAL
1	C	337	SER
1	C	341	MET
1	C	347	VAL
1	C	356	LEU
1	C	369	THR
1	C	383	SER
1	C	396	ASP
1	C	429	LEU
1	C	444	LYS
1	C	481	THR
1	C	510	VAL
1	C	516	ILE
1	C	529	GLN
1	C	562	SER
1	C	563	THR
1	C	564	GLN
1	C	620	THR
1	C	632	TRP
1	C	641	ILE
1	C	663	SER
1	C	672	ARG
1	C	677	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	694	LYS
1	C	719	VAL
1	C	721	PHE
1	D	66	LEU
1	D	74	VAL
1	D	116	SER
1	D	119	ASP
1	D	161	LYS
1	D	201	SER
1	D	202	LEU
1	D	226	ARG
1	D	230	ASN
1	D	234	SER
1	D	238	GLU
1	D	267	LEU
1	D	307	ASP
1	D	310	GLU
1	D	325	MET
1	D	326	ASP
1	D	360	TRP
1	D	366	LYS
1	D	386	ASP
1	D	393	THR
1	D	397	GLN
1	D	402	LYS
1	D	442	THR
1	D	479	SER
1	D	510	VAL
1	D	515	LYS
1	D	525	ASP
1	D	543	VAL
1	D	558	MET
1	D	562	SER
1	D	577	LEU
1	D	622	GLU
1	D	648	VAL
1	D	669	ARG
1	D	670	VAL
1	D	677	SER
1	D	707	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	304	ASN
1	A	441	GLN
1	A	529	GLN
1	A	645	GLN
1	B	76	GLN
1	B	199	ASN
1	B	408	ASN
1	B	665	ASN
1	B	691	HIS
1	C	458	ASN
1	C	547	GLN
1	C	639	ASN
1	C	645	GLN
1	D	76	GLN
1	D	231	HIS
1	D	376	ASN
1	D	547	GLN
1	D	673	ASN
1	D	705	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

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	648/723 (89%)	0.26	28 (4%)	40	38	37, 56, 86, 125	1 (0%)
1	B	657/723 (90%)	0.38	25 (3%)	44	42	33, 60, 96, 124	1 (0%)
1	C	644/723 (89%)	0.46	41 (6%)	25	25	36, 61, 100, 130	1 (0%)
1	D	658/723 (91%)	0.45	39 (5%)	28	28	34, 62, 100, 135	1 (0%)
All	All	2607/2892 (90%)	0.39	133 (5%)	33	33	33, 60, 96, 135	4 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	66	LEU	6.3
1	D	66	LEU	5.4
1	B	362	TRP	5.3
1	C	695	ALA	5.0
1	C	385	TYR	4.8
1	A	696	GLY	4.6
1	A	453	ALA	4.4
1	B	91	GLN	4.4
1	A	443	LEU	4.2
1	D	91	GLN	4.0
1	D	558	MET	4.0
1	C	557	GLY	3.8
1	D	723	PHE	3.7
1	A	704	ALA	3.7
1	A	392	TYR	3.7
1	B	723	PHE	3.6
1	D	695	ALA	3.6
1	C	698	ALA	3.6
1	B	442	THR	3.5
1	C	704	ALA	3.4
1	D	361	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	392	TYR	3.4
1	B	92	PRO	3.4
1	A	558	MET	3.4
1	D	362	TRP	3.4
1	C	723	PHE	3.4
1	C	389	THR	3.3
1	C	443	LEU	3.3
1	B	398	PHE	3.3
1	B	361	ARG	3.3
1	B	387	MET	3.2
1	C	332	THR	3.2
1	A	701	GLY	3.2
1	B	67	ALA	3.2
1	D	705	ASN	3.2
1	D	335	PRO	3.2
1	D	632	TRP	3.1
1	D	421	GLU	3.1
1	C	626	TRP	3.0
1	A	391	TYR	3.0
1	C	334	ASP	3.0
1	B	558	MET	3.0
1	C	382	GLY	3.0
1	D	119	ASP	3.0
1	D	338	MET	2.9
1	C	442	THR	2.9
1	C	510	VAL	2.9
1	A	338	MET	2.9
1	C	388	MET	2.9
1	C	658	GLY	2.9
1	C	398	PHE	2.9
1	C	699	GLY	2.9
1	D	389	THR	2.9
1	C	337	SER	2.8
1	D	704	ALA	2.8
1	B	700	PHE	2.8
1	C	387	MET	2.8
1	C	92	PRO	2.8
1	B	385	TYR	2.8
1	D	337	SER	2.7
1	D	190	ARG	2.7
1	C	399	PRO	2.7
1	D	384	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	559	MET	2.7
1	B	300	PHE	2.7
1	D	672	ARG	2.7
1	B	391	TYR	2.6
1	D	391	TYR	2.6
1	A	92	PRO	2.6
1	A	557	GLY	2.6
1	D	192	GLY	2.6
1	C	561	SER	2.6
1	C	380	ALA	2.6
1	D	477	ALA	2.6
1	A	385	TYR	2.5
1	C	701	GLY	2.5
1	A	555	ARG	2.5
1	A	362	TRP	2.5
1	C	363	ASP	2.5
1	C	335	PRO	2.5
1	C	420	ALA	2.5
1	C	632	TRP	2.4
1	B	194	LEU	2.4
1	D	343	MET	2.4
1	B	696	GLY	2.4
1	D	670	VAL	2.4
1	B	509	SER	2.3
1	D	387	MET	2.3
1	D	559	MET	2.3
1	A	695	ALA	2.3
1	D	365	PHE	2.3
1	D	451	ALA	2.3
1	B	563	THR	2.3
1	D	341	MET	2.3
1	A	390	ASP	2.3
1	D	512	ALA	2.3
1	B	341	MET	2.3
1	C	338	MET	2.3
1	C	453	ALA	2.3
1	D	268	ILE	2.3
1	B	389	THR	2.3
1	D	363	ASP	2.3
1	D	533	ASP	2.3
1	C	384	LYS	2.2
1	D	388	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	626	TRP	2.2
1	C	700	PHE	2.2
1	D	385	TYR	2.2
1	D	222	LEU	2.2
1	D	366	LYS	2.2
1	A	559	MET	2.2
1	B	704	ALA	2.2
1	C	571	ARG	2.2
1	B	503	LYS	2.2
1	C	390	ASP	2.2
1	C	400	TRP	2.1
1	A	190	ARG	2.1
1	B	703	SER	2.1
1	A	421	GLU	2.1
1	A	632	TRP	2.1
1	C	362	TRP	2.1
1	D	452	MET	2.1
1	A	409	TYR	2.1
1	D	696	GLY	2.1
1	B	93	VAL	2.1
1	A	698	ALA	2.1
1	C	130	LEU	2.1
1	A	723	PHE	2.1
1	A	393	THR	2.0
1	A	672	ARG	2.0
1	A	684	PHE	2.0
1	A	69	SER	2.0
1	C	563	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CU	D	801	1/1	0.93	0.09	97,97,97,97	0
2	CU	A	801	1/1	0.95	0.07	83,83,83,83	0
2	CU	C	801	1/1	0.96	0.06	95,95,95,95	0
2	CU	B	801	1/1	0.96	0.07	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.