



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 PM UTC

PDB ID : 6Z9Y / pdb_00006z9y
Title : Copper transporter OprC
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Deposited on : 2020-06-04
Resolution : 2.95 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

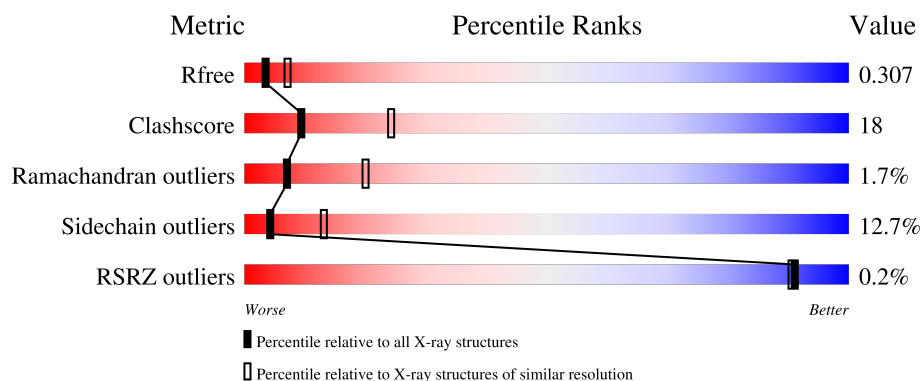
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	
1	B	723	
1	C	723	
1	D	723	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20158 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	657	Total	C	N	O	S	0	0	0
			5092	3195	899	979	19			
1	B	645	Total	C	N	O	S	0	0	0
			5004	3141	882	966	15			
1	C	640	Total	C	N	O	S	0	0	0
			4970	3123	878	955	14			
1	D	656	Total	C	N	O	S	0	1	0
			5088	3194	898	977	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

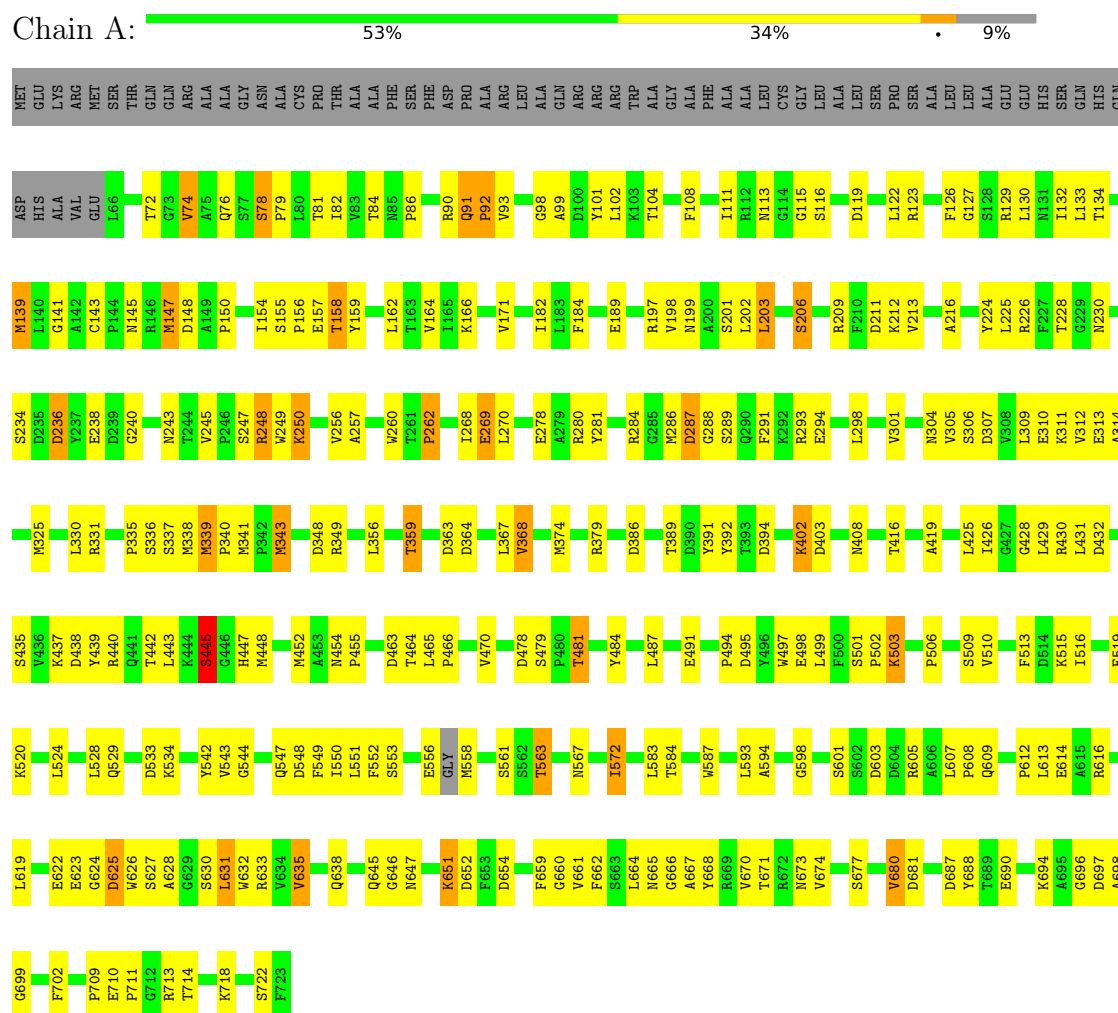
- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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		

3 Residue-property plots

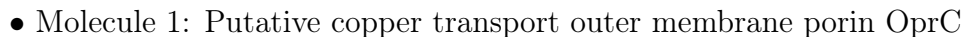
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.34Å 197.67Å 171.75Å 90.00° 88.75° 90.00°	Depositor
Resolution (Å)	85.85 – 2.95 85.85 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (85.85-2.95) 93.7 (85.85-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.242 , 0.302 0.247 , 0.307	Depositor DCC
R_{free} test set	4622 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.238 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20158	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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	0.41	0/5218	0.66	0/7072
1	B	0.44	0/5127	0.69	2/6952 (0.0%)
1	C	0.44	0/5090	0.69	0/6898
1	D	0.38	0/5217	0.64	0/7071
All	All	0.42	0/20652	0.67	2/27993 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	84	THR	CA-C-N	5.62	127.23	122.28
1	B	84	THR	C-N-CA	5.62	127.23	122.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	PRO	Peptide

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	5092	0	4870	176	0
1	B	5004	0	4779	178	0
1	C	4970	0	4759	200	0
1	D	5088	0	4870	162	0
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
All	All	20158	0	19278	709	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 18.

All (709) 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:B:171:VAL:HG22	1:B:414:GLU:HG3	1.51	0.93
1:B:504:ARG:HH12	1:B:555:ARG:HB3	1.37	0.90
1:A:630:SER:HB3	1:A:664:LEU:HD23	1.53	0.88
1:D:253:ASN:HD22	1:D:293:ARG:HH21	1.26	0.84
1:D:324:ILE:HG12	1:D:346:GLN:HG3	1.59	0.84
1:D:476:LEU:HD12	1:D:481:THR:HB	1.59	0.83
1:B:111:ILE:HG22	1:B:692:LEU:HB3	1.60	0.82
1:B:386:ASP:HB3	1:B:389:THR:HG22	1.61	0.82
1:B:374:MET:SD	1:B:376:ASN:ND2	2.53	0.82
1:C:466:PRO:HG2	1:D:466:PRO:HG2	1.62	0.82
1:A:445:SER:HB2	1:A:503:LYS:HE3	1.62	0.81
1:B:129:ARG:NH1	1:B:519:GLU:OE1	2.13	0.81
1:C:614:GLU:OE2	1:C:633:ARG:NE	2.12	0.81
1:C:695:ALA:HB2	1:C:708:VAL:HG23	1.60	0.81
1:A:72:THR:HB	1:A:631:LEU:HD22	1.63	0.81
1:B:671:THR:HG23	1:B:673:ASN:H	1.46	0.80
1:C:300:PHE:HZ	1:C:302:LYS:HD2	1.47	0.80
1:D:548:ASP:HB3	1:D:567:ASN:HD22	1.47	0.80
1:D:172:LEU:HD21	1:D:414:GLU:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ALA:HB3	1:C:707:THR:HA	1.64	0.79
1:B:672:ARG:H	1:B:672:ARG:HD2	1.47	0.78
1:C:274:LYS:HB2	1:C:292:LYS:HZ1	1.46	0.78
1:C:286:MET:HG2	1:C:327:ASN:HB3	1.64	0.78
1:C:147:MET:HB3	1:C:284:ARG:HE	1.48	0.77
1:A:664:LEU:HB2	1:A:680:VAL:HG22	1.65	0.77
1:C:82:ILE:HD11	1:C:166:LYS:HE3	1.64	0.77
1:C:164:VAL:HG22	1:C:182:ILE:HG13	1.66	0.77
1:D:260:TRP:HB3	1:D:268:ILE:HD11	1.66	0.77
1:B:521:THR:HG23	1:B:546:VAL:HG22	1.67	0.76
1:A:466:PRO:HG2	1:B:466:PRO:HG2	1.68	0.76
1:C:612:PRO:HG3	1:C:638:GLN:HB2	1.68	0.76
1:D:176:GLY:HA3	1:D:492:ARG:HG3	1.67	0.75
1:A:499:LEU:HD22	1:A:513:PHE:HA	1.69	0.75
1:C:203:LEU:HB3	1:C:211:ASP:HB3	1.68	0.74
1:A:91:GLN:NE2	1:A:665:ASN:HB3	2.02	0.74
1:A:616:ARG:HE	1:A:633:ARG:HD2	1.52	0.74
1:C:125:MET:HE3	1:C:572:ILE:HD13	1.71	0.73
1:D:671:THR:HG22	1:D:674:VAL:HG12	1.68	0.73
1:B:133:LEU:HD11	1:B:173:TRP:HB3	1.71	0.73
1:C:492:ARG:NH2	1:C:519:GLU:OE2	2.21	0.73
1:B:495:ASP:HB2	1:B:498:GLU:HG3	1.70	0.73
1:A:671:THR:HG22	1:A:674:VAL:HG12	1.70	0.72
1:B:203:LEU:HD12	1:B:718:LYS:HB2	1.71	0.72
1:A:129:ARG:NH1	1:A:519:GLU:OE1	2.23	0.72
1:B:504:ARG:HB3	1:B:564:GLN:HG3	1.71	0.72
1:A:99:ALA:HA	1:A:102:LEU:HD12	1.70	0.71
1:C:125:MET:HE1	1:C:572:ILE:HG21	1.72	0.71
1:A:339:MET:HA	1:A:341:MET:HE2	1.71	0.71
1:B:230:ASN:ND2	1:B:253:ASN:OD1	2.22	0.71
1:A:698:ALA:H	1:A:702:PHE:HB2	1.55	0.70
1:C:467:SER:HB3	1:C:490:ALA:HA	1.73	0.70
1:D:125:MET:HE1	1:D:572:ILE:HG21	1.72	0.70
1:A:91:GLN:HB3	1:A:92:PRO:HD3	1.74	0.70
1:C:653:PHE:HD1	1:C:654:ASP:H	1.38	0.69
1:B:465:LEU:HB3	1:B:491:GLU:HB2	1.74	0.69
1:C:441:GLN:O	1:C:454:ASN:N	2.25	0.69
1:D:584:THR:HG22	1:D:587:TRP:HB2	1.75	0.69
1:C:221:ARG:O	1:C:261:THR:OG1	2.09	0.69
1:C:379:ARG:HA	1:C:402:LYS:HA	1.75	0.69
1:D:643:ARG:HH21	1:D:653:PHE:HE1	1.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LYS:NZ	1:C:157:GLU:O	2.26	0.68
1:D:175:PRO:O	1:D:177:ALA:N	2.23	0.68
1:C:97:ASP:OD2	1:C:117:ASN:N	2.24	0.68
1:D:138:MET:HE3	1:D:140:LEU:HD21	1.75	0.68
1:A:335:PRO:HA	1:A:340:PRO:HB3	1.76	0.68
1:D:163:THR:HB	1:D:183:LEU:HB2	1.75	0.68
1:D:455:PRO:HG3	1:D:510:VAL:HB	1.75	0.68
1:B:495:ASP:HB3	1:B:497:TRP:H	1.59	0.67
1:C:290:GLN:HB3	1:C:324:ILE:HG13	1.77	0.67
1:A:403:ASP:HB2	1:A:440:ARG:HG2	1.75	0.67
1:A:613:LEU:HD12	1:A:614:GLU:H	1.58	0.67
1:C:214:LEU:HD12	1:C:215:ASP:H	1.60	0.67
1:C:465:LEU:HB3	1:C:491:GLU:HB2	1.77	0.67
1:B:84:THR:HG23	1:B:162:LEU:HB3	1.77	0.67
1:C:372:ASP:OD2	1:C:430:ARG:NH2	2.28	0.67
1:D:288:GLY:HA2	1:D:325:MET:HG2	1.77	0.67
1:C:264:GLU:CD	1:C:264:GLU:H	2.03	0.66
1:A:122:LEU:HG	1:A:123:ARG:HG3	1.78	0.66
1:A:583:LEU:HD12	1:A:587:TRP:HB3	1.78	0.66
1:A:338:MET:HE3	1:A:339:MET:H	1.61	0.66
1:A:497:TRP:O	1:A:501:SER:HB2	1.96	0.66
1:D:614:GLU:OE2	1:D:616:ARG:NH2	2.28	0.66
1:C:129:ARG:NH1	1:C:519:GLU:OE2	2.30	0.65
1:B:91:GLN:O	1:B:93:VAL:N	2.29	0.65
1:B:584:THR:HB	1:B:586:ASN:H	1.61	0.65
1:D:125:MET:HE3	1:D:572:ILE:HD13	1.78	0.65
1:A:547:GLN:HG3	1:B:433:ARG:HH12	1.61	0.65
1:C:283:GLY:HA2	1:C:695:ALA:HA	1.77	0.65
1:D:441:GLN:NE2	1:D:458:ASN:OD1	2.29	0.65
1:B:672:ARG:HD2	1:B:672:ARG:N	2.12	0.65
1:C:274:LYS:HB2	1:C:292:LYS:NZ	2.11	0.65
1:D:467:SER:HB2	1:D:490:ALA:HA	1.78	0.65
1:C:584:THR:HB	1:C:586:ASN:H	1.62	0.65
1:C:682:ASN:HD22	1:C:712:GLY:HA2	1.61	0.65
1:D:616:ARG:HE	1:D:633:ARG:HD2	1.62	0.64
1:A:203:LEU:HD12	1:A:718:LYS:HB2	1.79	0.64
1:C:361:ARG:NH2	1:C:363:ASP:O	2.30	0.64
1:D:341:MET:HB3	1:D:385:TYR:HD1	1.62	0.64
1:D:503:LYS:HD3	1:D:562:SER:HB2	1.80	0.64
1:B:638:GLN:HG2	1:B:691:HIS:NE2	2.12	0.64
1:A:587:TRP:HZ3	1:A:619:LEU:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:VAL:HG11	1:B:659:PHE:CZ	2.32	0.64
1:B:83:VAL:HG22	1:B:163:THR:HG23	1.80	0.63
1:C:300:PHE:CZ	1:C:302:LYS:HD2	2.31	0.63
1:D:428:GLY:N	1:D:469:PHE:O	2.30	0.63
1:B:122:LEU:HG	1:B:123:ARG:HD3	1.80	0.63
1:B:484:TYR:OH	1:B:540:SER:HB2	1.98	0.63
1:C:116:SER:OG	1:C:117:ASN:N	2.31	0.62
1:C:546:VAL:HG11	1:C:549:PHE:HD1	1.64	0.62
1:B:157:GLU:OE1	1:B:718:LYS:NZ	2.27	0.62
1:C:689:THR:HG1	1:C:707:THR:HG1	1.47	0.61
1:B:586:ASN:ND2	1:B:622:GLU:O	2.30	0.61
1:A:548:ASP:HB3	1:A:567:ASN:HD22	1.65	0.61
1:B:456:THR:HG21	1:B:511:ASN:HD21	1.65	0.61
1:C:206:SER:HG	1:C:715:PHE:H	1.48	0.61
1:D:465:LEU:HB3	1:D:491:GLU:HB2	1.82	0.61
1:A:437:LYS:HD3	1:A:439:TYR:CZ	2.36	0.61
1:D:262:PRO:HD2	1:D:266:THR:HB	1.82	0.61
1:A:141:GLY:O	1:A:349:ARG:HD3	2.00	0.61
1:D:236:ASP:HB3	1:D:245:VAL:O	2.01	0.61
1:B:693:ASN:OD1	1:B:693:ASN:N	2.25	0.61
1:C:407:HIS:HB2	1:C:435:SER:HB3	1.83	0.61
1:B:111:ILE:HD11	1:B:119:ASP:HB3	1.83	0.60
1:B:128:SER:OG	1:B:495:ASP:OD1	2.19	0.60
1:D:236:ASP:OD2	1:D:280:ARG:NH1	2.34	0.60
1:C:289:SER:OG	1:C:326:ASP:OD2	2.13	0.60
1:B:638:GLN:HG2	1:B:691:HIS:CD2	2.36	0.60
1:C:682:ASN:ND2	1:C:712:GLY:HA2	2.16	0.60
1:C:237:TYR:OH	1:C:709:PRO:O	2.10	0.60
1:C:260:TRP:CE2	1:C:262:PRO:HG3	2.36	0.60
1:C:555:ARG:O	1:C:562:SER:N	2.34	0.60
1:D:129:ARG:NH2	1:D:519:GLU:OE2	2.35	0.60
1:A:608:PRO:HG3	1:A:645:GLN:HB3	1.84	0.60
1:B:311:LYS:HB3	1:B:359:THR:HG22	1.84	0.60
1:A:203:LEU:HB3	1:A:211:ASP:HB2	1.84	0.59
1:D:620:THR:HG22	1:D:629:GLY:HA3	1.84	0.59
1:D:203:LEU:HB3	1:D:211:ASP:HB2	1.84	0.59
1:C:417:TRP:CE2	1:C:419:ALA:HB2	2.37	0.59
1:A:113:ASN:HB3	1:A:281:TYR:HD1	1.68	0.59
1:C:614:GLU:OE2	1:C:616:ARG:NH2	2.35	0.59
1:A:509:SER:OG	1:A:510:VAL:N	2.33	0.59
1:A:551:LEU:HD11	1:A:608:PRO:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:NH1	1:B:576:GLU:OE1	2.35	0.59
1:D:91:GLN:HG2	1:D:665:ASN:HB3	1.85	0.59
1:D:203:LEU:HD12	1:D:718:LYS:HB2	1.84	0.59
1:D:548:ASP:HB3	1:D:567:ASN:ND2	2.17	0.59
1:C:91:GLN:NE2	1:C:681:ASP:OD1	2.34	0.59
1:C:616:ARG:HE	1:C:633:ARG:HD2	1.67	0.59
1:A:416:THR:HG23	1:A:426:ILE:HG13	1.85	0.58
1:A:628:ALA:HA	1:A:666:GLY:HA2	1.85	0.58
1:B:555:ARG:HD2	1:B:556:GLU:H	1.68	0.58
1:D:493:PHE:CD1	1:D:494:PRO:HD2	2.38	0.58
1:D:294:GLU:HB2	1:D:320:TYR:HB3	1.85	0.58
1:B:209:ARG:HD2	1:B:234:SER:HB2	1.85	0.58
1:B:123:ARG:HG2	1:B:542:TYR:CE2	2.39	0.58
1:A:363:ASP:OD1	1:A:364:ASP:N	2.34	0.58
1:B:638:GLN:HE22	1:B:640:ARG:HB2	1.67	0.58
1:A:533:ASP:OD1	1:A:534:LYS:N	2.37	0.58
1:B:688:TYR:CE2	1:B:710:GLU:HG3	2.38	0.58
1:A:189:GLU:OE1	1:A:197:ARG:NH2	2.37	0.57
1:C:573:MET:HG3	1:C:597:TRP:HB3	1.85	0.57
1:B:339:MET:HG2	1:B:343:MET:SD	2.45	0.57
1:A:479:SER:OG	1:A:481:THR:OG1	2.21	0.57
1:C:441:GLN:HG3	1:C:457:ALA:HB1	1.86	0.57
1:D:705:ASN:OD1	1:D:705:ASN:N	2.33	0.57
1:C:394:ASP:O	1:C:396:ASP:N	2.30	0.57
1:A:209:ARG:NH1	1:A:211:ASP:OD2	2.32	0.57
1:A:622:GLU:HB3	1:A:627:SER:HB3	1.86	0.57
1:B:93:VAL:HG12	1:B:681:ASP:OD2	2.05	0.57
1:A:76:GLN:HE21	1:A:529:GLN:NE2	2.03	0.56
1:A:363:ASP:CG	1:A:364:ASP:H	2.12	0.56
1:C:443:LEU:HD23	1:C:454:ASN:N	2.20	0.56
1:D:609:GLN:NE2	1:D:652:ASP:OD1	2.36	0.56
1:A:646:GLY:HA3	1:A:651:LYS:HA	1.86	0.56
1:B:583:LEU:HD12	1:B:587:TRP:HB3	1.87	0.56
1:D:201:SER:HB3	1:D:213:VAL:HB	1.86	0.56
1:D:260:TRP:NE1	1:D:262:PRO:HG3	2.21	0.56
1:B:364:ASP:HB3	1:B:418:PHE:HB2	1.87	0.56
1:A:213:VAL:HG23	1:A:230:ASN:HB3	1.87	0.56
1:B:224:TYR:OH	1:B:269:GLU:OE1	2.19	0.56
1:A:78:SER:O	1:A:529:GLN:NE2	2.38	0.56
1:A:206:SER:HB2	1:A:714:THR:HG23	1.88	0.56
1:B:311:LYS:HB3	1:B:359:THR:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLN:NE2	1:C:458:ASN:OD1	2.39	0.56
1:A:260:TRP:NE1	1:A:262:PRO:HG3	2.21	0.56
1:C:581:TYR:HD2	1:C:582:GLN:H	1.53	0.56
1:C:497:TRP:O	1:C:502:PRO:HD3	2.05	0.56
1:D:494:PRO:HB2	1:D:499:LEU:HD22	1.88	0.56
1:B:238:GLU:HG3	1:B:244:THR:HG22	1.87	0.56
1:D:448:MET:HA	1:D:448:MET:HE2	1.88	0.56
1:C:339:MET:HG3	1:C:340:PRO:HD3	1.87	0.55
1:C:653:PHE:CZ	1:C:707:THR:HG21	2.41	0.55
1:D:608:PRO:HG3	1:D:645:GLN:HB3	1.87	0.55
1:A:616:ARG:HA	1:A:632:TRP:O	2.06	0.55
1:C:85:ASN:O	1:C:87:LYS:N	2.40	0.55
1:C:189:GLU:OE1	1:C:197:ARG:NH2	2.35	0.55
1:A:667:ALA:HB2	1:A:677:SER:HB3	1.89	0.55
1:C:151:THR:HA	1:C:154:ILE:HG13	1.89	0.55
1:B:133:LEU:CD1	1:B:173:TRP:HB3	2.35	0.55
1:B:689:THR:HG22	1:B:709:PRO:HA	1.89	0.55
1:C:140:LEU:HB3	1:C:349:ARG:HD3	1.88	0.55
1:C:521:THR:HG23	1:C:546:VAL:HG22	1.88	0.55
1:D:682:ASN:HD22	1:D:712:GLY:HA2	1.71	0.55
1:B:112:ARG:HB3	1:B:693:ASN:HB3	1.87	0.55
1:C:141:GLY:O	1:C:349:ARG:HD2	2.07	0.55
1:C:498:GLU:HG2	1:C:550:ILE:HG21	1.87	0.55
1:A:698:ALA:HA	1:A:702:PHE:H	1.72	0.55
1:D:91:GLN:HB3	1:D:92:PRO:HD3	1.89	0.55
1:A:598:GLY:HA3	1:A:607:LEU:HD12	1.88	0.54
1:B:85:ASN:O	1:B:87:LYS:N	2.40	0.54
1:C:608:PRO:HB2	1:C:646:GLY:HA2	1.90	0.54
1:A:143:CYS:SG	1:A:147:MET:HG3	2.47	0.54
1:A:491:GLU:OE2	1:A:520:LYS:HE3	2.08	0.54
1:B:432:ASP:O	1:B:464:THR:HA	2.06	0.54
1:B:672:ARG:H	1:B:672:ARG:CD	2.18	0.54
1:C:616:ARG:HH21	1:C:633:ARG:NE	2.06	0.54
1:D:463:ASP:OD1	1:D:464:THR:N	2.40	0.54
1:D:690:GLU:HB2	1:D:693:ASN:OD1	2.07	0.54
1:A:198:VAL:HG23	1:A:216:ALA:HB2	1.88	0.54
1:C:301:VAL:HG22	1:C:313:GLU:HG2	1.89	0.54
1:A:260:TRP:CE2	1:A:262:PRO:HG3	2.43	0.54
1:A:603:ASP:HB3	1:A:605:ARG:HE	1.72	0.54
1:C:360:TRP:HE1	1:C:369:THR:CG2	2.21	0.54
1:D:169:GLN:OE1	1:D:471:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:CYS:SG	1:C:147:MET:HG2	2.47	0.54
1:C:364:ASP:N	1:C:364:ASP:OD1	2.41	0.54
1:A:301:VAL:HA	1:A:312:VAL:O	2.08	0.54
1:A:91:GLN:HE21	1:A:665:ASN:HB3	1.73	0.54
1:B:91:GLN:HG3	1:B:665:ASN:CG	2.33	0.54
1:C:223:GLY:HA2	1:C:261:THR:HG23	1.90	0.54
1:A:442:THR:O	1:A:443:LEU:HD23	2.08	0.53
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.42	0.53
1:D:584:THR:OG1	1:D:585:GLY:N	2.40	0.53
1:D:143:CYS:SG	1:D:147:MET:HG3	2.48	0.53
1:D:359:THR:HG23	1:D:368:VAL:HG12	1.91	0.53
1:D:141:GLY:O	1:D:349:ARG:HD3	2.09	0.53
1:D:171:VAL:HG22	1:D:414:GLU:HG3	1.91	0.53
1:C:583:LEU:HD12	1:C:587:TRP:HB3	1.90	0.53
1:C:547:GLN:NE2	1:D:433:ARG:HE	2.05	0.53
1:B:264:GLU:CD	1:B:264:GLU:H	2.16	0.53
1:C:190:ARG:HE	1:C:190:ARG:HA	1.74	0.53
1:C:286:MET:HE1	1:C:343:MET:HE2	1.90	0.53
1:D:628:ALA:HA	1:D:666:GLY:HA2	1.91	0.53
1:C:74:VAL:CG2	1:C:105:ILE:HG12	2.39	0.53
1:C:682:ASN:HD22	1:C:712:GLY:CA	2.22	0.53
1:D:261:THR:O	1:D:261:THR:OG1	2.24	0.52
1:B:265:ASP:OD1	1:B:304:ASN:ND2	2.42	0.52
1:A:84:THR:HG22	1:A:162:LEU:HB3	1.92	0.52
1:B:171:VAL:HG23	1:B:412:PHE:HB2	1.90	0.52
1:C:385:TYR:CG	1:C:386:ASP:N	2.75	0.52
1:D:671:THR:CG2	1:D:674:VAL:HG12	2.37	0.52
1:A:506:PRO:HB2	1:A:515:LYS:HD3	1.91	0.52
1:C:586:ASN:HB3	1:C:621:TYR:CE2	2.45	0.52
1:C:613:LEU:HD23	1:C:614:GLU:H	1.75	0.52
1:A:108:PHE:HZ	1:A:182:ILE:HD11	1.74	0.52
1:B:326:ASP:HA	1:B:343:MET:O	2.10	0.52
1:B:471:ARG:HD2	1:B:473:GLU:OE2	2.10	0.52
1:C:123:ARG:HB3	1:C:542:TYR:OH	2.10	0.52
1:C:555:ARG:NH2	1:C:562:SER:OG	2.43	0.52
1:C:609:GLN:NE2	1:C:652:ASP:OD1	2.35	0.52
1:D:119:ASP:OD2	1:D:146:ARG:NH1	2.43	0.52
1:D:290:GLN:HB3	1:D:324:ILE:H	1.74	0.52
1:C:475:ASP:N	1:C:475:ASP:OD1	2.42	0.52
1:D:479:SER:OG	1:D:481:THR:OG1	2.14	0.52
1:A:209:ARG:HD2	1:A:234:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:HB2	1:B:224:TYR:CD2	2.45	0.52
1:B:403:ASP:HB2	1:B:440:ARG:HG2	1.92	0.52
1:D:76:GLN:HE21	1:D:166:LYS:HE3	1.74	0.52
1:D:341:MET:HB3	1:D:385:TYR:CD1	2.44	0.52
1:A:613:LEU:HD12	1:A:614:GLU:N	2.25	0.51
1:B:682:ASN:HB3	1:B:712:GLY:O	2.10	0.51
1:C:343:MET:HB2	1:C:383:SER:OG	2.11	0.51
1:B:203:LEU:HB3	1:B:211:ASP:HB2	1.92	0.51
1:C:438:ASP:OD1	1:C:439:TYR:N	2.43	0.51
1:D:348:ASP:OD2	1:D:379:ARG:NH2	2.43	0.51
1:B:103:LYS:HG2	1:B:110:VAL:HG21	1.91	0.51
1:D:91:GLN:CG	1:D:665:ASN:HB3	2.40	0.51
1:C:203:LEU:HD12	1:C:718:LYS:HG3	1.92	0.51
1:C:613:LEU:HD23	1:C:614:GLU:N	2.25	0.51
1:A:202:LEU:HD13	1:C:225:LEU:HD12	1.93	0.51
1:A:287:ASP:CG	1:A:331:ARG:HE	2.19	0.51
1:A:115:GLY:N	1:A:247:SER:HB2	2.26	0.51
1:D:309:LEU:HD12	1:D:360:TRP:CH2	2.46	0.51
1:D:577:LEU:CD2	1:D:593:LEU:HB3	2.41	0.51
1:A:314:ALA:HB2	1:A:356:LEU:HD12	1.93	0.51
1:A:623:GLU:O	1:A:625:ASP:N	2.40	0.51
1:D:614:GLU:OE2	1:D:633:ARG:NE	2.31	0.51
1:A:339:MET:HE3	1:A:343:MET:HG2	1.93	0.51
1:A:671:THR:HG22	1:A:674:VAL:CG1	2.40	0.51
1:A:74:VAL:HG23	1:A:104:THR:O	2.11	0.50
1:B:176:GLY:O	1:B:492:ARG:HD3	2.11	0.50
1:C:138:MET:O	1:C:319:ASN:ND2	2.40	0.50
1:A:126:PHE:CG	1:A:127:GLY:N	2.79	0.50
1:A:386:ASP:HB3	1:A:391:TYR:H	1.75	0.50
1:B:498:GLU:HB3	1:B:550:ILE:HG21	1.92	0.50
1:C:461:ARG:NH1	1:C:513:PHE:O	2.43	0.50
1:C:549:PHE:N	1:C:568:VAL:O	2.35	0.50
1:B:91:GLN:HE22	1:B:663:SER:HB3	1.76	0.50
1:B:172:LEU:HD21	1:B:414:GLU:HB2	1.93	0.50
1:B:260:TRP:CE2	1:B:262:PRO:HG3	2.47	0.50
1:B:586:ASN:ND2	1:B:623:GLU:HB2	2.26	0.50
1:C:463:ASP:OD1	1:C:464:THR:N	2.43	0.50
1:C:84:THR:HG21	1:C:90:ARG:HH12	1.76	0.50
1:D:512:ALA:O	1:D:514:ASP:N	2.45	0.50
1:A:549:PHE:HE2	1:A:551:LEU:HD13	1.75	0.50
1:C:202:LEU:O	1:C:718:LYS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ALA:O	1:C:652:ASP:HB2	2.11	0.50
1:D:97:ASP:HA	1:D:154:ILE:O	2.11	0.50
1:A:671:THR:HG23	1:A:673:ASN:H	1.77	0.50
1:C:171:VAL:HG22	1:C:414:GLU:OE2	2.12	0.50
1:C:287:ASP:OD1	1:C:331:ARG:HD3	2.12	0.50
1:C:379:ARG:HD2	1:C:400:TRP:HB3	1.92	0.50
1:C:618:GLY:HA2	1:C:630:SER:O	2.12	0.50
1:A:379:ARG:HG2	1:A:402:LYS:HB2	1.94	0.49
1:A:544:GLY:O	1:A:572:ILE:HG13	2.11	0.49
1:C:661:VAL:HG21	1:C:688:TYR:CZ	2.47	0.49
1:D:445:SER:O	1:D:445:SER:OG	2.26	0.49
1:D:72:THR:HG22	1:D:631:LEU:HD22	1.92	0.49
1:A:238:GLU:HA	1:A:243:ASN:O	2.11	0.49
1:A:464:THR:C	1:A:465:LEU:HD23	2.36	0.49
1:C:148:ASP:HB3	1:C:291:PHE:CE1	2.47	0.49
1:A:248:ARG:HD3	1:A:280:ARG:NH2	2.27	0.49
1:B:113:ASN:HB3	1:B:281:TYR:CD1	2.47	0.49
1:D:454:ASN:OD1	1:D:456:THR:N	2.43	0.49
1:D:586:ASN:N	1:D:586:ASN:OD1	2.46	0.49
1:B:703:SER:O	1:B:703:SER:OG	2.23	0.49
1:A:633:ARG:NH2	1:A:690:GLU:OE1	2.41	0.49
1:A:697:ASP:C	1:A:699:GLY:H	2.21	0.49
1:A:236:ASP:N	1:A:236:ASP:OD1	2.43	0.49
1:D:84:THR:HG23	1:D:162:LEU:HB3	1.95	0.49
1:D:497:TRP:O	1:D:501:SER:HB2	2.13	0.49
1:D:554:TYR:CD2	1:D:651:LYS:HB3	2.48	0.49
1:A:113:ASN:HB3	1:A:281:TYR:CD1	2.47	0.49
1:B:494:PRO:HA	1:B:498:GLU:OE1	2.12	0.49
1:A:287:ASP:OD2	1:A:331:ARG:HG2	2.13	0.49
1:C:155:SER:HB3	1:C:158:THR:HG23	1.95	0.49
1:C:234:SER:HB3	1:C:249:TRP:CE2	2.48	0.49
1:A:91:GLN:O	1:A:93:VAL:N	2.45	0.48
1:C:70:VAL:HG22	1:C:89:PRO:HB2	1.94	0.48
1:D:513:PHE:HD1	1:D:513:PHE:O	1.96	0.48
1:D:584:THR:HG23	1:D:586:ASN:N	2.28	0.48
1:A:119:ASP:HB3	1:A:126:PHE:HE1	1.77	0.48
1:B:91:GLN:HG2	1:B:716:TRP:HZ2	1.78	0.48
1:D:95:ALA:HB3	1:D:100:ASP:OD2	2.13	0.48
1:D:197:ARG:CZ	1:D:197:ARG:HB2	2.41	0.48
1:A:164:VAL:HG13	1:A:182:ILE:HD13	1.96	0.48
1:A:269:GLU:O	1:A:298:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:166:LYS:HE2	1.96	0.48
1:A:157:GLU:CD	1:A:157:GLU:H	2.21	0.48
1:B:306:SER:OG	1:B:307:ASP:N	2.46	0.48
1:C:203:LEU:HB3	1:C:211:ASP:CB	2.40	0.48
1:C:309:LEU:HD13	1:C:360:TRP:CE3	2.49	0.48
1:A:552:PHE:HB2	1:A:647:ASN:HA	1.95	0.48
1:C:698:ALA:HB2	1:C:702:PHE:HB2	1.96	0.48
1:A:630:SER:HB2	1:A:662:PHE:CZ	2.49	0.48
1:B:475:ASP:OD1	1:B:475:ASP:N	2.46	0.48
1:B:206:SER:HG	1:B:715:PHE:H	1.61	0.48
1:C:162:LEU:HD13	1:C:184:PHE:CE2	2.49	0.48
1:C:578:GLY:HA2	1:C:592:SER:HA	1.94	0.48
1:D:151:THR:HA	1:D:154:ILE:HD12	1.96	0.48
1:D:467:SER:HB2	1:D:489:HIS:O	2.14	0.48
1:A:428:GLY:O	1:A:429:LEU:HD23	2.14	0.48
1:A:668:TYR:HE2	1:A:670:VAL:HG22	1.78	0.48
1:B:280:ARG:HA	1:B:287:ASP:HB3	1.95	0.48
1:C:494:PRO:HB2	1:C:499:LEU:HG	1.95	0.48
1:C:497:TRP:O	1:C:501:SER:HB2	2.14	0.48
1:D:631:LEU:HD12	1:D:632:TRP:N	2.28	0.48
1:A:392:TYR:OH	1:A:394:ASP:OD1	2.28	0.48
1:B:99:ALA:HB1	1:B:110:VAL:HG13	1.94	0.48
1:C:432:ASP:O	1:C:464:THR:HA	2.14	0.48
1:C:515:LYS:NZ	1:D:514:ASP:OD2	2.47	0.48
1:D:298:LEU:O	1:D:315:GLN:HA	2.14	0.48
1:D:584:THR:HG23	1:D:586:ASN:H	1.78	0.48
1:A:445:SER:O	1:A:445:SER:OG	2.27	0.48
1:B:85:ASN:C	1:B:87:LYS:H	2.22	0.48
1:B:363:ASP:CG	1:B:364:ASP:H	2.20	0.48
1:D:101:TYR:CD1	1:D:156:PRO:HG2	2.49	0.48
1:D:197:ARG:HH12	1:D:217:ALA:HB3	1.79	0.48
1:D:577:LEU:HD21	1:D:593:LEU:HB3	1.96	0.48
1:A:79:PRO:HB3	1:A:484:TYR:CD2	2.48	0.47
1:A:495:ASP:HB2	1:A:498:GLU:HG3	1.96	0.47
1:A:694:LYS:HB3	1:A:694:LYS:HE3	1.55	0.47
1:B:584:THR:HG22	1:B:585:GLY:H	1.78	0.47
1:B:635:VAL:HG22	1:B:636:ALA:O	2.14	0.47
1:D:80:LEU:HD22	1:D:166:LYS:O	2.14	0.47
1:B:309:LEU:HD21	1:B:358:ALA:HB1	1.96	0.47
1:B:341:MET:HE2	1:B:343:MET:HG2	1.96	0.47
1:A:91:GLN:HB3	1:A:92:PRO:CD	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:THR:OG1	1:B:85:ASN:N	2.41	0.47
1:B:236:ASP:OD2	1:B:280:ARG:NH1	2.47	0.47
1:B:501:SER:N	1:B:502:PRO:HD2	2.30	0.47
1:C:82:ILE:HG21	1:C:105:ILE:HD13	1.96	0.47
1:C:74:VAL:HG23	1:C:105:ILE:HG12	1.97	0.47
1:C:176:GLY:HA3	1:C:492:ARG:HG3	1.96	0.47
1:C:314:ALA:HB2	1:C:356:LEU:HD12	1.94	0.47
1:C:588:LYS:HB3	1:C:620:THR:OG1	2.15	0.47
1:A:139:MET:HE2	1:A:293:ARG:HG3	1.95	0.47
1:A:432:ASP:O	1:A:464:THR:HA	2.14	0.47
1:A:491:GLU:HA	1:A:519:GLU:O	2.14	0.47
1:D:438:ASP:OD1	1:D:439:TYR:N	2.48	0.47
1:D:334:ASP:N	1:D:334:ASP:OD1	2.47	0.47
1:A:431:LEU:HD13	1:A:466:PRO:HB3	1.97	0.47
1:B:341:MET:HE3	1:B:385:TYR:HB2	1.97	0.47
1:B:635:VAL:HG11	1:B:659:PHE:CE2	2.50	0.47
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.50	0.47
1:C:385:TYR:O	1:C:386:ASP:HB2	2.14	0.47
1:B:143:CYS:SG	1:B:147:MET:HG3	2.55	0.47
1:B:305:VAL:HB	1:B:309:LEU:HB3	1.96	0.47
1:B:350:ARG:HH22	1:B:379:ARG:NH2	2.13	0.47
1:C:91:GLN:O	1:C:93:VAL:N	2.47	0.47
1:D:214:LEU:HD12	1:D:215:ASP:N	2.29	0.47
1:A:681:ASP:O	1:A:713:ARG:HA	2.15	0.47
1:B:213:VAL:HG22	1:B:230:ASN:HB2	1.97	0.47
1:B:221:ARG:NH1	1:B:264:GLU:OE2	2.48	0.47
1:B:517:LYS:HD3	1:B:548:ASP:OD2	2.14	0.47
1:D:108:PHE:HA	1:D:121:VAL:O	2.15	0.47
1:D:463:ASP:HB3	1:D:465:LEU:HD11	1.97	0.47
1:B:84:THR:CG2	1:B:162:LEU:HB3	2.43	0.46
1:B:638:GLN:NE2	1:B:640:ARG:HB2	2.29	0.46
1:C:204:ALA:HA	1:C:209:ARG:O	2.16	0.46
1:A:101:TYR:OH	1:A:157:GLU:HG3	2.14	0.46
1:B:91:GLN:HG3	1:B:665:ASN:OD1	2.16	0.46
1:B:491:GLU:HA	1:B:519:GLU:O	2.15	0.46
1:C:373:ALA:HA	1:C:408:ASN:O	2.15	0.46
1:C:672:ARG:HG2	1:C:672:ARG:HH21	1.80	0.46
1:D:108:PHE:CE1	1:D:122:LEU:HB2	2.49	0.46
1:A:257:ALA:HA	1:A:270:LEU:O	2.15	0.46
1:B:491:GLU:OE1	1:B:520:LYS:HG2	2.16	0.46
1:C:489:HIS:HA	1:C:521:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:HIS:HB2	1:D:435:SER:OG	2.15	0.46
1:C:97:ASP:O	1:C:101:TYR:HD1	1.98	0.46
1:D:86:PRO:C	1:D:88:GLU:H	2.24	0.46
1:D:139:MET:O	1:D:140:LEU:HD23	2.16	0.46
1:A:556:GLU:OE1	1:A:561:SER:HB3	2.15	0.46
1:A:593:LEU:HD21	1:A:613:LEU:HD11	1.98	0.46
1:B:464:THR:C	1:B:465:LEU:HG	2.40	0.46
1:B:626:TRP:HB3	1:B:668:TYR:HD1	1.81	0.46
1:C:266:THR:OG1	1:C:302:LYS:HE3	2.16	0.46
1:C:436:VAL:HG22	1:C:513:PHE:HE2	1.81	0.46
1:C:691:HIS:O	1:C:691:HIS:ND1	2.49	0.46
1:B:91:GLN:NE2	1:B:664:LEU:O	2.49	0.46
1:B:111:ILE:HG12	1:B:119:ASP:O	2.15	0.46
1:B:325:MET:HE3	1:B:325:MET:HB2	1.67	0.46
1:B:638:GLN:NE2	1:B:640:ARG:H	2.13	0.46
1:D:204:ALA:HA	1:D:209:ARG:O	2.15	0.46
1:D:593:LEU:HD12	1:D:615:ALA:HB2	1.98	0.46
1:B:73:GLY:HA2	1:B:104:THR:O	2.14	0.46
1:C:555:ARG:HH12	1:C:564:GLN:HB2	1.81	0.46
1:A:240:GLY:HA3	1:A:687:ASP:HA	1.98	0.46
1:B:93:VAL:HG11	1:B:716:TRP:CD1	2.51	0.46
1:C:555:ARG:HB3	1:C:555:ARG:CZ	2.46	0.46
1:C:672:ARG:HG2	1:C:672:ARG:NH2	2.31	0.46
1:D:267:LEU:HD12	1:D:268:ILE:H	1.81	0.46
1:D:248:ARG:HD3	1:D:280:ARG:NH2	2.31	0.46
1:D:689:THR:HG23	1:D:708:VAL:O	2.16	0.45
1:A:359:THR:HG23	1:A:368:VAL:HG22	1.97	0.45
1:A:623:GLU:HG2	1:A:626:TRP:NE1	2.30	0.45
1:A:667:ALA:CB	1:A:677:SER:HB3	2.45	0.45
1:A:710:GLU:HG3	1:A:711:PRO:HD2	1.97	0.45
1:B:690:GLU:HB2	1:B:693:ASN:OD1	2.17	0.45
1:D:267:LEU:HD12	1:D:268:ILE:N	2.31	0.45
1:B:81:THR:HG22	1:B:165:ILE:HD13	1.99	0.45
1:A:429:LEU:HD21	1:B:429:LEU:HD11	1.99	0.45
1:D:89:PRO:HG3	1:D:718:LYS:HD3	1.99	0.45
1:A:171:VAL:HB	1:A:430:ARG:HB3	1.99	0.45
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.99	0.45
1:B:367:LEU:HD12	1:B:414:GLU:O	2.16	0.45
1:C:535:LEU:C	1:C:535:LEU:HD23	2.42	0.45
1:D:504:ARG:HG3	1:D:564:GLN:HG3	1.98	0.45
1:D:673:ASN:OD1	1:D:673:ASN:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:O	1:B:718:LYS:HA	2.15	0.45
1:D:139:MET:SD	1:D:319:ASN:HB3	2.57	0.45
1:A:158:THR:CG2	1:A:230:ASN:HD22	2.29	0.45
1:B:103:LYS:HG2	1:B:110:VAL:CG2	2.45	0.45
1:B:327:ASN:OD1	1:B:342:PRO:HA	2.17	0.45
1:C:170:THR:HG21	1:C:173:TRP:HD1	1.81	0.45
1:C:694:LYS:HB3	1:C:695:ALA:H	1.69	0.45
1:D:437:LYS:HD3	1:D:439:TYR:CZ	2.52	0.45
1:C:214:LEU:HD12	1:C:215:ASP:N	2.29	0.45
1:C:276:ASP:OD1	1:C:277:GLY:N	2.44	0.45
1:C:437:LYS:HG3	1:C:459:ASP:O	2.17	0.45
1:B:651:LYS:HB3	1:B:651:LYS:HE2	1.55	0.45
1:C:230:ASN:OD1	1:C:253:ASN:ND2	2.47	0.45
1:C:638:GLN:N	1:C:656:SER:OG	2.36	0.45
1:D:198:VAL:CG1	1:D:723:PHE:HB2	2.47	0.45
1:D:472:TYR:CZ	1:D:474:HIS:HB2	2.51	0.45
1:A:250:LYS:HB2	1:A:278:GLU:HG2	1.98	0.44
1:A:661:VAL:HG21	1:A:688:TYR:CE1	2.52	0.44
1:D:438:ASP:OD1	1:D:440:ARG:HG3	2.17	0.44
1:D:515:LYS:O	1:D:516:ILE:HG12	2.17	0.44
1:A:108:PHE:CE2	1:A:122:LEU:HD13	2.53	0.44
1:B:120:PRO:HG3	1:B:151:THR:HG21	1.98	0.44
1:D:158:THR:OG1	1:D:186:ARG:NH2	2.50	0.44
1:A:313:GLU:O	1:A:356:LEU:HA	2.17	0.44
1:B:555:ARG:HD2	1:B:556:GLU:N	2.32	0.44
1:C:181:THR:C	1:C:182:ILE:HD12	2.41	0.44
1:B:359:THR:OG1	1:B:368:VAL:HG22	2.16	0.44
1:C:371:VAL:HA	1:C:411:ALA:HA	1.99	0.44
1:D:343:MET:HA	1:D:392:TYR:HE2	1.81	0.44
1:A:698:ALA:N	1:A:702:PHE:HB2	2.28	0.44
1:C:710:GLU:HB3	1:C:711:PRO:HD2	1.99	0.44
1:A:443:LEU:HG	1:A:454:ASN:HB2	1.98	0.44
1:C:367:LEU:HB2	1:C:415:LEU:HD23	2.00	0.44
1:A:86:PRO:HG2	1:A:159:TYR:O	2.18	0.44
1:B:146:ARG:C	1:B:148:ASP:H	2.25	0.44
1:B:476:LEU:HD23	1:B:476:LEU:HA	1.84	0.44
1:C:113:ASN:HB2	1:C:281:TYR:HD2	1.82	0.44
1:C:374:MET:SD	1:C:376:ASN:ND2	2.89	0.44
1:A:494:PRO:HB2	1:A:499:LEU:HG	1.99	0.44
1:A:609:GLN:H	1:A:652:ASP:CG	2.24	0.44
1:B:481:THR:HA	1:B:529:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ILE:HA	1:B:516:ILE:HD13	1.80	0.44
1:D:350:ARG:HH22	1:D:379:ARG:NH2	2.16	0.44
1:A:189:GLU:HB2	1:A:224:TYR:CD1	2.52	0.44
1:A:661:VAL:HG21	1:A:688:TYR:CZ	2.53	0.44
1:B:304:ASN:OD1	1:B:304:ASN:N	2.50	0.44
1:B:428:GLY:O	1:B:429:LEU:HD23	2.18	0.44
1:B:638:GLN:HE21	1:B:640:ARG:C	2.26	0.44
1:D:84:THR:CG2	1:D:162:LEU:HB3	2.48	0.44
1:D:85:ASN:ND2	1:D:88:GLU:HG2	2.33	0.44
1:D:597:TRP:CH2	1:D:599:LYS:HB2	2.53	0.44
1:D:608:PRO:HB3	1:D:642:ALA:HB3	2.00	0.44
1:A:374:MET:HE3	1:A:408:ASN:HB3	2.00	0.43
1:B:125:MET:HB3	1:B:129:ARG:HD2	2.00	0.43
1:C:133:LEU:HD13	1:C:136:GLY:O	2.17	0.43
1:C:140:LEU:HB3	1:C:349:ARG:CD	2.48	0.43
1:D:76:GLN:HE21	1:D:166:LYS:CE	2.31	0.43
1:B:111:ILE:CG2	1:B:692:LEU:HB3	2.39	0.43
1:B:189:GLU:OE1	1:B:226:ARG:HD2	2.18	0.43
1:C:284:ARG:NH1	1:C:694:LYS:HG3	2.32	0.43
1:C:292:LYS:HB3	1:C:322:ASP:HB3	2.00	0.43
1:C:581:TYR:CD2	1:C:582:GLN:N	2.86	0.43
1:D:326:ASP:OD2	1:D:329:ARG:NE	2.51	0.43
1:A:463:ASP:CG	1:A:465:LEU:HD21	2.44	0.43
1:B:149:ALA:O	1:B:152:SER:N	2.42	0.43
1:C:84:THR:CG2	1:C:90:ARG:HH12	2.31	0.43
1:D:334:ASP:HB2	1:D:335:PRO:HD3	2.00	0.43
1:A:78:SER:HB2	1:A:81:THR:HB	2.01	0.43
1:A:154:ILE:HG21	1:A:184:PHE:CD2	2.54	0.43
1:A:162:LEU:HD13	1:A:184:PHE:CE1	2.52	0.43
1:B:438:ASP:HB2	1:B:513:PHE:CE2	2.53	0.43
1:C:85:ASN:C	1:C:87:LYS:H	2.26	0.43
1:C:116:SER:HG	1:C:117:ASN:H	1.66	0.43
1:C:524:LEU:HD23	1:C:543:VAL:HG22	2.01	0.43
1:A:249:TRP:O	1:A:250:LYS:HG2	2.18	0.43
1:A:288:GLY:HA3	1:A:291:PHE:CZ	2.53	0.43
1:A:438:ASP:HB2	1:A:513:PHE:CE2	2.54	0.43
1:B:577:LEU:HD11	1:B:593:LEU:HD22	2.00	0.43
1:B:324:ILE:HG12	1:B:346:GLN:HG3	2.01	0.43
1:B:334:ASP:O	1:B:337:SER:OG	2.33	0.43
1:B:612:PRO:HG2	1:B:635:VAL:CG2	2.49	0.43
1:C:278:GLU:HA	1:C:288:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:SER:OG	1:D:235:ASP:N	2.51	0.43
1:D:584:THR:HG23	1:D:587:TRP:H	1.83	0.43
1:A:374:MET:HE3	1:A:374:MET:HB3	1.94	0.43
1:C:261:THR:OG1	1:C:261:THR:O	2.36	0.43
1:C:346:GLN:NE2	1:C:381:ARG:HD2	2.33	0.43
1:C:581:TYR:HD2	1:C:582:GLN:N	2.16	0.43
1:A:635:VAL:HG21	1:A:659:PHE:CZ	2.54	0.43
1:B:91:GLN:NE2	1:B:680:VAL:O	2.52	0.43
1:B:248:ARG:HG2	1:B:249:TRP:N	2.34	0.43
1:B:255:ASP:HA	1:B:273:GLY:HA3	2.00	0.43
1:C:199:ASN:HB2	1:C:215:ASP:HB3	2.01	0.43
1:C:515:LYS:HB2	1:C:515:LYS:HE2	1.89	0.43
1:A:143:CYS:HB2	1:A:325:MET:SD	2.59	0.43
1:B:203:LEU:O	1:B:210:PHE:HA	2.19	0.43
1:C:371:VAL:HG12	1:C:411:ALA:HB2	2.01	0.43
1:C:405:VAL:O	1:C:436:VAL:HA	2.17	0.43
1:C:438:ASP:OD1	1:C:438:ASP:C	2.62	0.43
1:C:363:ASP:OD2	1:C:363:ASP:N	2.51	0.43
1:D:334:ASP:HB2	1:D:335:PRO:CD	2.48	0.43
1:A:587:TRP:CZ3	1:A:619:LEU:HD21	2.49	0.42
1:C:203:LEU:HB2	1:C:718:LYS:HG3	2.01	0.42
1:C:672:ARG:N	1:C:672:ARG:HD3	2.34	0.42
1:A:289:SER:HB3	1:A:330:LEU:CD1	2.49	0.42
1:D:189:GLU:HB2	1:D:224:TYR:CZ	2.53	0.42
1:A:341:MET:H	1:A:341:MET:HG2	1.66	0.42
1:A:631:LEU:HD12	1:A:632:TRP:N	2.33	0.42
1:D:443:LEU:O	1:D:452:MET:HB2	2.19	0.42
1:A:93:VAL:HG12	1:A:681:ASP:OD2	2.20	0.42
1:C:673:ASN:OD1	1:C:673:ASN:N	2.52	0.42
1:D:102:LEU:HD22	1:D:108:PHE:CE2	2.54	0.42
1:D:143:CYS:HA	1:D:144:PRO:HD3	1.83	0.42
1:D:489:HIS:HA	1:D:521:THR:O	2.19	0.42
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.54	0.42
1:A:501:SER:N	1:A:502:PRO:HD2	2.34	0.42
1:C:678:ALA:HA	1:C:716:TRP:O	2.20	0.42
1:D:469:PHE:HA	1:D:488:GLY:HA2	2.01	0.42
1:A:145:ASN:O	1:A:284:ARG:NH1	2.49	0.42
1:A:245:VAL:CG2	1:A:709:PRO:HG2	2.50	0.42
1:A:363:ASP:CG	1:A:364:ASP:N	2.77	0.42
1:B:309:LEU:HG	1:B:360:TRP:CZ3	2.55	0.42
1:C:638:GLN:OE1	1:C:640:ARG:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:THR:O	1:D:183:LEU:N	2.51	0.42
1:A:608:PRO:HB3	1:A:645:GLN:O	2.20	0.42
1:C:271:THR:O	1:C:297:GLY:N	2.53	0.42
1:C:333:PRO:O	1:C:335:PRO:HD3	2.20	0.42
1:D:189:GLU:OE1	1:D:197:ARG:NH1	2.52	0.42
1:B:91:GLN:HG3	1:B:665:ASN:HB3	2.01	0.42
1:B:202:LEU:HD23	1:B:721:PHE:HE2	1.85	0.42
1:C:375:ARG:HA	1:C:406:PHE:O	2.20	0.42
1:D:350:ARG:NH2	1:D:379:ARG:NH2	2.68	0.42
1:B:425:LEU:O	1:B:426:ILE:HG13	2.20	0.42
1:B:495:ASP:HB2	1:B:498:GLU:H	1.84	0.42
1:B:540:SER:O	1:B:540:SER:OG	2.38	0.42
1:B:586:ASN:HB3	1:B:621:TYR:CE1	2.55	0.42
1:D:130:LEU:HD23	1:D:179:ALA:HB3	2.01	0.42
1:D:467:SER:CB	1:D:490:ALA:HA	2.48	0.42
1:D:571:ARG:HG3	1:D:601:SER:OG	2.19	0.42
1:B:79:PRO:O	1:B:81:THR:HG23	2.19	0.42
1:B:499:LEU:HD23	1:B:516:ILE:HB	2.01	0.42
1:C:101:TYR:OH	1:C:157:GLU:HG2	2.20	0.42
1:C:381:ARG:NH1	1:C:396:ASP:OD1	2.52	0.42
1:A:98:GLY:HA2	1:A:156:PRO:CG	2.50	0.41
1:A:633:ARG:O	1:A:660:GLY:HA2	2.20	0.41
1:B:628:ALA:HA	1:B:666:GLY:HA2	2.02	0.41
1:C:253:ASN:HB3	1:C:293:ARG:HH12	1.85	0.41
1:C:379:ARG:HG2	1:C:402:LYS:HB3	2.01	0.41
1:D:111:ILE:HG23	1:D:692:LEU:O	2.20	0.41
1:A:225:LEU:HD23	1:A:226:ARG:N	2.34	0.41
1:C:225:LEU:C	1:C:225:LEU:HD23	2.44	0.41
1:D:339:MET:O	1:D:339:MET:HG3	2.19	0.41
1:A:155:SER:HB3	1:A:157:GLU:OE1	2.20	0.41
1:A:553:SER:O	1:A:563:THR:HA	2.19	0.41
1:B:123:ARG:HH11	1:B:576:GLU:CD	2.27	0.41
1:B:571:ARG:NH2	1:B:599:LYS:HD3	2.35	0.41
1:C:598:GLY:O	1:C:607:LEU:HB2	2.21	0.41
1:A:101:TYR:CD2	1:A:156:PRO:HB2	2.55	0.41
1:C:479:SER:OG	1:C:481:THR:HG23	2.19	0.41
1:C:688:TYR:CE1	1:C:710:GLU:HB2	2.55	0.41
1:D:301:VAL:HA	1:D:312:VAL:O	2.21	0.41
1:A:132:ILE:HA	1:A:182:ILE:HB	2.03	0.41
1:A:447:HIS:CE1	1:A:448:MET:HG2	2.55	0.41
1:A:465:LEU:HB3	1:A:491:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:GLY:HA2	1:C:430:ARG:NH2	2.35	0.41
1:C:261:THR:HG22	1:C:267:LEU:HD23	2.03	0.41
1:C:290:GLN:OE1	1:C:292:LYS:HB2	2.21	0.41
1:D:286:MET:HG3	1:D:326:ASP:O	2.20	0.41
1:D:311:LYS:HE2	1:D:313:GLU:HB2	2.01	0.41
1:A:593:LEU:HD23	1:A:594:ALA:N	2.36	0.41
1:B:111:ILE:HD13	1:B:111:ILE:HG21	1.74	0.41
1:C:113:ASN:HB2	1:C:281:TYR:CD2	2.55	0.41
1:C:138:MET:HE3	1:C:138:MET:HB2	1.62	0.41
1:C:689:THR:OG1	1:C:707:THR:OG1	2.25	0.41
1:D:139:MET:C	1:D:140:LEU:HD23	2.46	0.41
1:D:174:GLY:O	1:D:430:ARG:NH1	2.53	0.41
1:A:155:SER:CB	1:A:230:ASN:HD21	2.34	0.41
1:A:524:LEU:O	1:A:542:TYR:HA	2.21	0.41
1:A:668:TYR:CE2	1:A:670:VAL:HG22	2.55	0.41
1:B:328:PHE:CD1	1:B:342:PRO:HB2	2.55	0.41
1:B:455:PRO:HB2	1:B:510:VAL:CG1	2.51	0.41
1:B:583:LEU:HB2	1:B:587:TRP:HB2	2.01	0.41
1:C:362:TRP:CD1	1:C:365:PHE:HB2	2.56	0.41
1:B:103:LYS:CG	1:B:110:VAL:HG21	2.51	0.41
1:B:417:TRP:CE2	1:B:419:ALA:HA	2.55	0.41
1:C:367:LEU:HB2	1:C:415:LEU:CD2	2.51	0.41
1:C:671:THR:OG1	1:C:672:ARG:N	2.53	0.41
1:A:455:PRO:HB2	1:A:510:VAL:CG1	2.50	0.41
1:A:696:GLY:HA3	1:A:702:PHE:CG	2.56	0.41
1:B:261:THR:HG22	1:B:267:LEU:HD13	2.03	0.41
1:B:318:TYR:OH	1:B:350:ARG:HD3	2.20	0.41
1:B:428:GLY:HA3	1:B:469:PHE:CE1	2.56	0.41
1:C:203:LEU:HA	1:C:717:THR:O	2.21	0.41
1:D:82:ILE:HD11	1:D:166:LYS:HE2	2.03	0.41
1:D:90:ARG:HB2	1:D:94:PRO:HD3	2.03	0.41
1:D:182:ILE:O	1:D:183:LEU:HD23	2.21	0.41
1:D:349:ARG:HH12	1:D:496:TYR:HB3	1.85	0.41
1:D:497:TRP:HB3	1:D:648:VAL:HG21	2.03	0.41
1:D:570:ALA:HB1	1:D:607:LEU:HD11	2.03	0.41
1:B:94:PRO:HG2	1:B:101:TYR:CZ	2.56	0.41
1:B:360:TRP:HB2	1:B:362:TRP:HZ3	1.86	0.41
1:B:692:LEU:HD23	1:B:692:LEU:HA	1.79	0.41
1:C:202:LEU:HA	1:C:202:LEU:HD23	1.84	0.41
1:A:134:THR:HG23	1:A:134:THR:O	2.21	0.40
1:A:139:MET:O	1:A:150:PRO:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASN:N	1:A:310:GLU:O	2.50	0.40
1:A:348:ASP:OD2	1:A:379:ARG:NH2	2.46	0.40
1:B:138:MET:SD	1:B:140:LEU:HD11	2.61	0.40
1:B:188:PRO:HG3	1:B:299:ARG:HH22	1.85	0.40
1:B:629:GLY:N	1:B:665:ASN:O	2.49	0.40
1:C:554:TYR:HB2	1:C:644:ASP:O	2.21	0.40
1:C:635:VAL:HG12	1:C:636:ALA:O	2.21	0.40
1:D:79:PRO:O	1:D:81:THR:N	2.54	0.40
1:D:200:ALA:HB3	1:D:721:PHE:HB2	2.03	0.40
1:D:438:ASP:HB2	1:D:513:PHE:CE2	2.56	0.40
1:D:568:VAL:HB	1:D:602:SER:HB2	2.02	0.40
1:B:285:GLY:HA2	1:B:331:ARG:HH12	1.86	0.40
1:B:461:ARG:HE	1:B:461:ARG:HB2	1.65	0.40
1:C:111:ILE:HG23	1:C:692:LEU:O	2.21	0.40
1:C:360:TRP:HE1	1:C:369:THR:HG21	1.84	0.40
1:C:690:GLU:H	1:C:693:ASN:ND2	2.19	0.40
1:D:513:PHE:O	1:D:513:PHE:CD1	2.75	0.40
1:A:339:MET:N	1:A:340:PRO:HD3	2.36	0.40
1:A:454:ASN:HA	1:A:455:PRO:HD3	1.96	0.40
1:B:435:SER:HB3	1:B:462:ALA:HB2	2.03	0.40
1:C:329:ARG:HE	1:C:329:ARG:HB2	1.57	0.40
1:C:503:LYS:HB3	1:C:503:LYS:NZ	2.37	0.40
1:D:81:THR:HA	1:D:164:VAL:O	2.22	0.40
1:D:423:ASP:OD2	1:D:472:TYR:OH	2.28	0.40
1:D:625:ASP:HB3	1:D:626:TRP:HD1	1.85	0.40
1:A:166:LYS:HB2	1:A:166:LYS:HE3	1.84	0.40
1:B:98:GLY:HA3	1:B:151:THR:HB	2.03	0.40
1:B:534:LYS:HB2	1:B:581:TYR:HE1	1.87	0.40
1:A:157:GLU:OE1	1:A:157:GLU:N	2.50	0.40
1:B:135:ASN:HD21	1:B:186:ARG:NH1	2.20	0.40
1:B:515:LYS:HD2	1:B:515:LYS:O	2.22	0.40
1:B:552:PHE:HB2	1:B:647:ASN:HA	2.03	0.40
1:C:673:ASN:O	1:C:722:SER:N	2.51	0.40
1:D:223:GLY:N	1:D:261:THR:HG23	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	653/723 (90%)	577 (88%)	68 (10%)	8 (1%)	10	28
1	B	639/723 (88%)	582 (91%)	50 (8%)	7 (1%)	11	29
1	C	630/723 (87%)	541 (86%)	74 (12%)	15 (2%)	4	13
1	D	653/723 (90%)	578 (88%)	60 (9%)	15 (2%)	5	14
All	All	2575/2892 (89%)	2278 (88%)	252 (10%)	45 (2%)	7	20

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	624	GLY
1	B	583	LEU
1	C	386	ASP
1	C	395	ALA
1	D	175	PRO
1	D	246	PRO
1	D	334	ASP
1	D	513	PHE
1	A	148	ASP
1	A	206	SER
1	B	584	THR
1	C	382	GLY
1	C	624	GLY
1	C	697	ASP
1	D	80	LEU
1	D	447	HIS
1	D	514	ASP
1	A	262	PRO
1	A	419	ALA
1	A	445	SER
1	B	695	ALA
1	D	420	ALA

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Mol	Chain	Res	Type
1	D	516	ILE
1	B	123	ARG
1	C	363	ASP
1	C	694	LYS
1	C	698	ALA
1	D	362	TRP
1	D	388	MET
1	D	704	ALA
1	B	92	PRO
1	C	331	ARG
1	C	333	PRO
1	C	399	PRO
1	C	511	ASN
1	D	262	PRO
1	A	91	GLN
1	B	336	SER
1	C	508	GLY
1	D	176	GLY
1	A	92	PRO
1	B	246	PRO
1	C	149	ALA
1	C	92	PRO
1	D	399	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	525/572 (92%)	462 (88%)	63 (12%)	5	14
1	B	516/572 (90%)	448 (87%)	68 (13%)	4	12
1	C	512/572 (90%)	433 (85%)	79 (15%)	2	8
1	D	524/572 (92%)	471 (90%)	53 (10%)	7	20
All	All	2077/2288 (91%)	1814 (87%)	263 (13%)	4	13

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	78	SER
1	A	90	ARG
1	A	111	ILE
1	A	116	SER
1	A	130	LEU
1	A	133	LEU
1	A	139	MET
1	A	147	MET
1	A	158	THR
1	A	199	ASN
1	A	201	SER
1	A	203	LEU
1	A	212	LYS
1	A	228	THR
1	A	236	ASP
1	A	248	ARG
1	A	250	LYS
1	A	256	VAL
1	A	268	ILE
1	A	269	GLU
1	A	286	MET
1	A	287	ASP
1	A	294	GLU
1	A	305	VAL
1	A	306	SER
1	A	307	ASP
1	A	309	LEU
1	A	311	LYS
1	A	336	SER
1	A	337	SER
1	A	339	MET
1	A	343	MET
1	A	359	THR
1	A	367	LEU
1	A	368	VAL
1	A	389	THR
1	A	402	LYS
1	A	425	LEU
1	A	435	SER
1	A	445	SER
1	A	452	MET
1	A	470	VAL

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Mol	Chain	Res	Type
1	A	478	ASP
1	A	481	THR
1	A	487	LEU
1	A	503	LYS
1	A	516	ILE
1	A	528	LEU
1	A	543	VAL
1	A	550	ILE
1	A	558	MET
1	A	563	THR
1	A	572	ILE
1	A	584	THR
1	A	601	SER
1	A	625	ASP
1	A	631	LEU
1	A	635	VAL
1	A	651	LYS
1	A	654	ASP
1	A	680	VAL
1	A	722	SER
1	B	74	VAL
1	B	78	SER
1	B	93	VAL
1	B	97	ASP
1	B	104	THR
1	B	134	THR
1	B	147	MET
1	B	152	SER
1	B	155	SER
1	B	163	THR
1	B	170	THR
1	B	171	VAL
1	B	178	SER
1	B	187	GLU
1	B	193	GLU
1	B	194	LEU
1	B	206	SER
1	B	225	LEU
1	B	226	ARG
1	B	253	ASN
1	B	255	ASP
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	274	LYS
1	B	287	ASP
1	B	296	LEU
1	B	303	SER
1	B	304	ASN
1	B	306	SER
1	B	308	VAL
1	B	313	GLU
1	B	325	MET
1	B	326	ASP
1	B	330	LEU
1	B	332	THR
1	B	387	MET
1	B	388	MET
1	B	389	THR
1	B	401	SER
1	B	415	LEU
1	B	416	THR
1	B	425	LEU
1	B	429	LEU
1	B	475	ASP
1	B	487	LEU
1	B	501	SER
1	B	514	ASP
1	B	523	GLN
1	B	528	LEU
1	B	540	SER
1	B	543	VAL
1	B	562	SER
1	B	580	SER
1	B	584	THR
1	B	604	ASP
1	B	623	GLU
1	B	630	SER
1	B	649	VAL
1	B	651	LYS
1	B	654	ASP
1	B	676	LEU
1	B	677	SER
1	B	680	VAL
1	B	683	LEU
1	B	693	ASN

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Mol	Chain	Res	Type
1	B	703	SER
1	B	714	THR
1	B	722	SER
1	B	723	PHE
1	C	74	VAL
1	C	78	SER
1	C	80	LEU
1	C	97	ASP
1	C	113	ASN
1	C	129	ARG
1	C	130	LEU
1	C	133	LEU
1	C	134	THR
1	C	140	LEU
1	C	151	THR
1	C	155	SER
1	C	201	SER
1	C	203	LEU
1	C	206	SER
1	C	233	GLN
1	C	235	ASP
1	C	244	THR
1	C	253	ASN
1	C	258	VAL
1	C	278	GLU
1	C	287	ASP
1	C	289	SER
1	C	293	ARG
1	C	302	LYS
1	C	303	SER
1	C	305	VAL
1	C	309	LEU
1	C	316	VAL
1	C	324	ILE
1	C	329	ARG
1	C	330	LEU
1	C	332	THR
1	C	334	ASP
1	C	341	MET
1	C	350	ARG
1	C	361	ARG
1	C	362	TRP

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Mol	Chain	Res	Type
1	C	363	ASP
1	C	364	ASP
1	C	366	LYS
1	C	368	VAL
1	C	369	THR
1	C	384	LYS
1	C	392	TYR
1	C	402	LYS
1	C	429	LEU
1	C	436	VAL
1	C	442	THR
1	C	467	SER
1	C	475	ASP
1	C	478	ASP
1	C	491	GLU
1	C	492	ARG
1	C	501	SER
1	C	516	ILE
1	C	524	LEU
1	C	529	GLN
1	C	553	SER
1	C	555	ARG
1	C	556	GLU
1	C	563	THR
1	C	584	THR
1	C	589	THR
1	C	593	LEU
1	C	619	LEU
1	C	627	SER
1	C	630	SER
1	C	648	VAL
1	C	649	VAL
1	C	653	PHE
1	C	654	ASP
1	C	663	SER
1	C	673	ASN
1	C	675	LYS
1	C	676	LEU
1	C	700	PHE
1	C	719	VAL
1	C	722	SER
1	D	78	SER

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Mol	Chain	Res	Type
1	D	112	ARG
1	D	116	SER
1	D	119	ASP
1	D	134	THR
1	D	140	LEU
1	D	146	ARG
1	D	152	SER
1	D	170	THR
1	D	185	GLU
1	D	197	ARG
1	D	226	ARG
1	D	230	ASN
1	D	261	THR
1	D	287	ASP
1	D	289	SER
1	D	303	SER
1	D	305	VAL
1	D	306	SER
1	D	308	VAL
1	D	332	THR
1	D	341	MET
1	D	388	MET
1	D	393	THR
1	D	426	ILE
1	D	433	ARG
1	D	442	THR
1	D	456	THR
1	D	470	VAL
1	D	491	GLU
1	D	510	VAL
1	D	516	ILE
1	D	523	GLN
1	D	528	LEU
1	D	543	VAL
1	D	545	VAL
1	D	556	GLU
1	D	561	SER
1	D	562	SER
1	D	563	THR
1	D	586	ASN
1	D	593	LEU
1	D	610	ILE

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Mol	Chain	Res	Type
1	D	613	LEU
1	D	619	LEU
1	D	630	SER
1	D	670	VAL
1	D	673	ASN
1	D	677	SER
1	D	687	ASP
1	D	693	ASN
1	D	705	ASN
1	D	714	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	131	ASN
1	A	230	ASN
1	A	523	GLN
1	A	529	GLN
1	B	76	GLN
1	B	145	ASN
1	B	507	ASN
1	B	523	GLN
1	B	638	GLN
1	B	645	GLN
1	B	665	ASN
1	C	135	ASN
1	C	199	ASN
1	C	230	ASN
1	C	233	GLN
1	C	253	ASN
1	C	346	GLN
1	C	523	GLN
1	C	529	GLN
1	C	547	GLN
1	C	665	ASN
1	D	76	GLN
1	D	131	ASN
1	D	253	ASN
1	D	397	GLN
1	D	536	GLN
1	D	691	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	657/723 (90%)	-1.01	0 100 100	42, 61, 91, 122	0
1	B	645/723 (89%)	-1.04	1 (0%) 91 90	40, 59, 85, 121	0
1	C	640/723 (88%)	-0.94	3 (0%) 87 83	44, 67, 102, 132	0
1	D	656/723 (90%)	-0.93	1 (0%) 91 90	44, 68, 101, 131	1 (0%)
All	All	2598/2892 (89%)	-0.98	5 (0%) 91 90	40, 64, 96, 132	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	514	ASP	3.0
1	C	443	LEU	2.4
1	C	389	THR	2.4
1	B	69	SER	2.4
1	C	701	GLY	2.3

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	A	801	1/1	0.99	0.04	85,85,85,85	0
2	CU	B	801	1/1	0.99	0.03	99,99,99,99	0
2	CU	D	801	1/1	0.99	0.04	98,98,98,98	0
2	CU	C	801	1/1	1.00	0.03	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.