



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3T51
Title : Crystal structures of the pre-extrusion and extrusion states of the CusBA adaptor-transporter complex
Authors : Su, C.-C.; Long, F.; Yu, E.W.
Deposited on : 2011-07-26
Resolution : 3.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

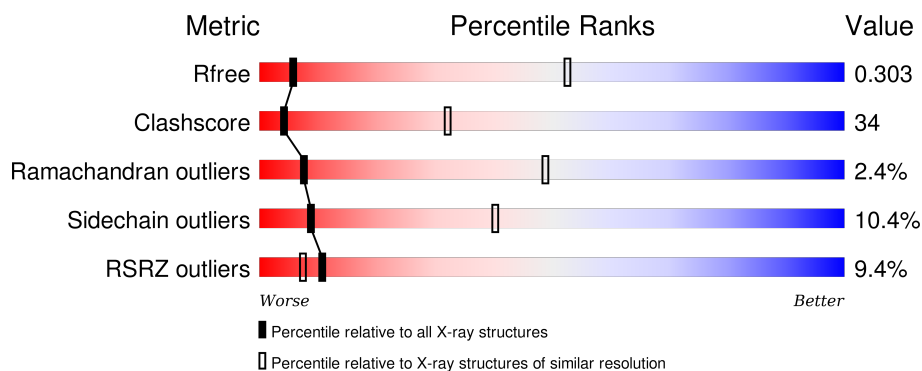
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	336	<div> <div>14%</div> <div>54%</div> <div>37%</div> <div>5%</div> <div>.</div> </div>
1	C	336	<div> <div>49%</div> <div>41%</div> <div>6%</div> <div>.</div> </div>
2	A	1054	<div> <div>14%</div> <div>42%</div> <div>48%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12841 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 Cation efflux system protein CusB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			
1	C	322	Total	C	N	O	S	0	0	0
			2458	1555	428	469	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	HIS	-	EXPRESSION TAG	UNP P77239
B	409	HIS	-	EXPRESSION TAG	UNP P77239
B	410	HIS	-	EXPRESSION TAG	UNP P77239
B	411	HIS	-	EXPRESSION TAG	UNP P77239
B	412	HIS	-	EXPRESSION TAG	UNP P77239
B	413	HIS	-	EXPRESSION TAG	UNP P77239
C	408	HIS	-	EXPRESSION TAG	UNP P77239
C	409	HIS	-	EXPRESSION TAG	UNP P77239
C	410	HIS	-	EXPRESSION TAG	UNP P77239
C	411	HIS	-	EXPRESSION TAG	UNP P77239
C	412	HIS	-	EXPRESSION TAG	UNP P77239
C	413	HIS	-	EXPRESSION TAG	UNP P77239

- Molecule 2 is a protein called Cation efflux system protein CusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1028	Total	C	N	O	S	0	0	0
			7923	5124	1330	1433	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P38054
A	-5	HIS	-	EXPRESSION TAG	UNP P38054

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	EXPRESSION TAG	UNP P38054
A	-3	HIS	-	EXPRESSION TAG	UNP P38054
A	-2	HIS	-	EXPRESSION TAG	UNP P38054
A	-1	HIS	-	EXPRESSION TAG	UNP P38054
A	0	HIS	-	EXPRESSION TAG	UNP P38054

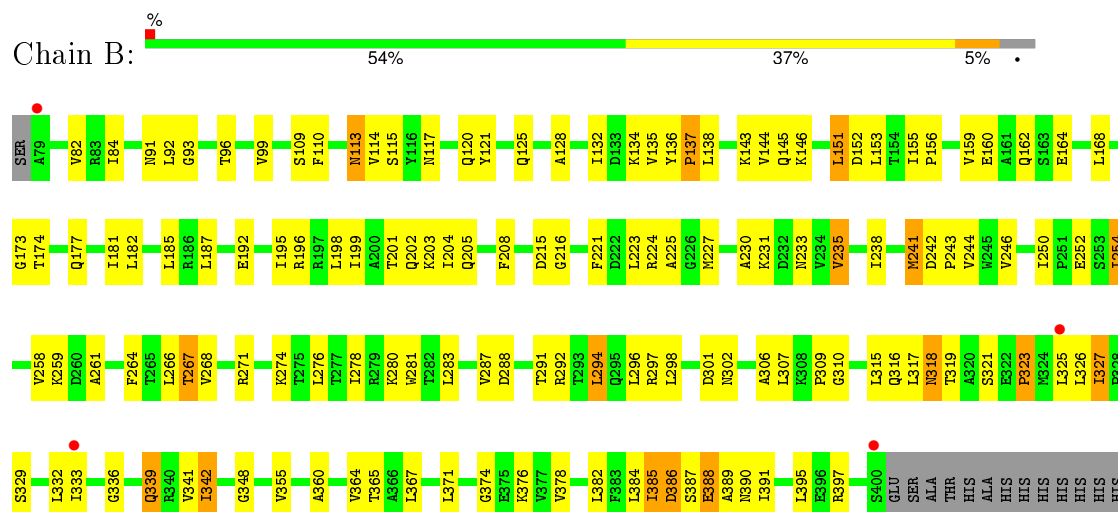
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cu	0	0
			2	2		

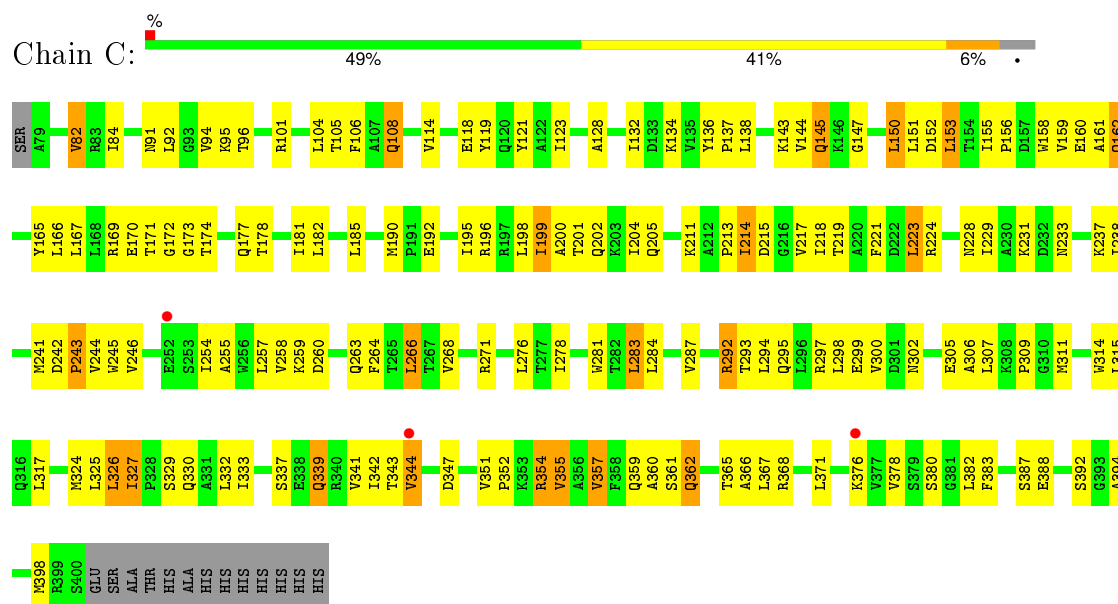
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Cation efflux system protein CusB

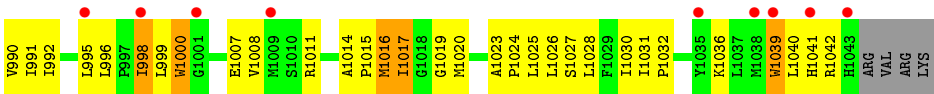


• Molecule 1: Cation efflux system protein CusB



• Molecule 2: Cation efflux system protein CusA





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.64Å 159.64Å 679.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.90 128.06 – 3.90	Depositor EDS
% Data completeness (in resolution range)	82.5 (50.00-3.90) 89.3 (128.06-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.259 , 0.325 0.242 , 0.303	Depositor DCC
R_{free} test set	1410 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	104.0	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 115.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 27748 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12841	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.21	0/2498	0.42	0/3401
1	C	0.22	0/2498	0.41	0/3401
2	A	0.22	0/8089	0.41	0/11015
All	All	0.22	0/13085	0.41	0/17817

There are no bond length outliers.

There are no bond angle outliers.

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	B	2458	0	2522	133	0
1	C	2458	0	2522	146	0
2	A	7923	0	8166	631	0
3	A	2	0	0	0	0
All	All	12841	0	13210	873	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 34.

All (873) 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)
2:A:48:ILE:CD1	2:A:130:GLY:HA3	1.48	1.40
2:A:933:LEU:HD11	2:A:1019:GLY:CA	1.55	1.35
2:A:48:ILE:CG1	2:A:130:GLY:HA3	1.63	1.29
2:A:879:THR:CG2	2:A:880:LEU:HD23	1.63	1.27
2:A:933:LEU:HD11	2:A:1019:GLY:C	1.55	1.25
2:A:933:LEU:CD1	2:A:1019:GLY:HA3	1.66	1.25
2:A:879:THR:HG23	2:A:880:LEU:CD2	1.67	1.23
2:A:876:VAL:O	2:A:879:THR:HG22	1.35	1.22
2:A:48:ILE:HD11	2:A:130:GLY:CA	1.71	1.19
2:A:927:GLY:O	2:A:931:ILE:HD13	1.42	1.19
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	1.82	1.15
2:A:107:ARG:HH11	2:A:129:LEU:HD12	1.14	1.10
2:A:107:ARG:NH1	2:A:129:LEU:HD12	1.68	1.06
2:A:933:LEU:HD11	2:A:1019:GLY:HA3	1.17	1.06
2:A:879:THR:CG2	2:A:880:LEU:CD2	2.30	1.06
2:A:48:ILE:HD11	2:A:130:GLY:HA3	1.06	1.04
2:A:459:LEU:HA	2:A:462:ILE:HG13	1.32	1.04
2:A:881:MET:N	2:A:881:MET:SD	2.30	1.03
2:A:107:ARG:HH11	2:A:129:LEU:CD1	1.73	1.00
2:A:879:THR:HG23	2:A:880:LEU:HD23	1.00	1.00
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.42	0.97
1:B:278:ILE:HG12	1:B:298:LEU:HD23	1.47	0.96
2:A:39:LEU:HG	2:A:40:PRO:HD2	1.48	0.94
2:A:54:PRO:HD3	2:A:122:PRO:HG3	1.50	0.94
2:A:880:LEU:HD23	2:A:880:LEU:N	1.83	0.93
2:A:932:ALA:HB1	2:A:1016:MET:CE	1.99	0.92
2:A:40:PRO:HG3	2:A:474:LEU:HD13	1.48	0.92
2:A:995:LEU:HA	2:A:998:ILE:HD11	1.52	0.92
2:A:933:LEU:HD21	2:A:1020:MET:HB2	1.50	0.90
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.50	0.90
1:B:121:TYR:HD1	1:C:224:ARG:HG2	1.37	0.89
2:A:48:ILE:HG12	2:A:130:GLY:HA3	1.54	0.89
2:A:48:ILE:CD1	2:A:130:GLY:CA	2.39	0.89
2:A:930:PHE:HE2	2:A:1015:PRO:HB3	1.37	0.89
2:A:48:ILE:CG1	2:A:130:GLY:CA	2.50	0.89
2:A:135:GLY:HA3	2:A:673:LEU:HD21	1.53	0.89
2:A:404:VAL:HG11	2:A:990:VAL:HG11	1.55	0.88
2:A:460:SER:HB3	2:A:882:ILE:HD11	1.51	0.88
1:B:204:ILE:H	1:B:204:ILE:HD12	1.36	0.88
2:A:145:VAL:HG12	2:A:284:VAL:HG11	1.55	0.88
2:A:668:ASN:O	2:A:678:LYS:HG2	1.74	0.88
2:A:876:VAL:O	2:A:879:THR:CG2	2.22	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:668:ASN:HA	2:A:678:LYS:CG	2.05	0.86
2:A:933:LEU:HD12	2:A:1019:GLY:HA3	1.55	0.86
2:A:48:ILE:HD11	2:A:130:GLY:C	1.96	0.85
2:A:933:LEU:CD1	2:A:1019:GLY:CA	2.36	0.84
2:A:876:VAL:HG23	2:A:877:PRO:HD3	1.60	0.84
2:A:932:ALA:HB1	2:A:1016:MET:HE3	1.60	0.83
2:A:550:VAL:HG11	2:A:909:VAL:HG13	1.59	0.83
1:B:121:TYR:CD1	1:C:224:ARG:HG2	2.14	0.82
2:A:933:LEU:CD1	2:A:1019:GLY:C	2.43	0.82
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.61	0.82
2:A:404:VAL:HG12	2:A:408:ILE:CG2	2.09	0.82
1:C:95:LYS:H	1:C:380:SER:HB3	1.45	0.81
2:A:410:MET:HB2	2:A:446:VAL:HG11	1.62	0.81
2:A:525:TYR:HE1	2:A:977:ALA:HB1	1.45	0.81
2:A:456:ILE:HG12	2:A:886:LEU:HD13	1.63	0.80
2:A:460:SER:HA	2:A:882:ILE:HD12	1.63	0.80
2:A:459:LEU:HA	2:A:462:ILE:CG1	2.11	0.80
2:A:930:PHE:CD2	2:A:1015:PRO:HB3	2.17	0.80
1:B:259:LYS:HD2	1:C:271:ARG:HH12	1.48	0.79
1:B:132:ILE:HD11	1:B:223:LEU:HD13	1.65	0.79
2:A:133:ALA:HB2	2:A:292:ARG:HA	1.65	0.79
2:A:459:LEU:CA	2:A:462:ILE:HG13	2.12	0.79
2:A:679:SER:OG	2:A:825:TYR:HB3	1.83	0.78
1:C:355:VAL:HG21	1:C:367:LEU:HD13	1.65	0.78
2:A:82:VAL:HG23	2:A:817:ASN:HA	1.66	0.78
2:A:877:PRO:O	2:A:881:MET:SD	2.41	0.78
2:A:462:ILE:O	2:A:465:PHE:HD2	1.66	0.77
2:A:1000:TRP:CE3	2:A:1000:TRP:HA	2.20	0.77
1:C:387:SER:HA	2:A:577:LEU:HD12	1.67	0.77
2:A:407:ALA:O	2:A:497:ILE:CD1	2.33	0.77
2:A:879:THR:HG22	2:A:880:LEU:HD23	1.67	0.76
2:A:932:ALA:HB1	2:A:1016:MET:HE2	1.67	0.76
2:A:477:PRO:HA	2:A:480:PHE:CE2	2.20	0.76
2:A:131:PRO:HG3	2:A:616:THR:CG2	2.15	0.76
1:C:333:ILE:HD11	1:C:382:LEU:HD22	1.67	0.76
2:A:944:MET:SD	2:A:980:ARG:HD3	2.25	0.75
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.68	0.75
1:B:182:LEU:HD21	1:B:199:ILE:HD11	1.69	0.75
2:A:927:GLY:O	2:A:931:ILE:CD1	2.30	0.74
2:A:131:PRO:HG3	2:A:616:THR:HG23	1.70	0.73
1:C:341:VAL:HG21	1:C:371:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:139:ILE:HD13	2:A:327:ARG:HD2	1.68	0.73
1:B:114:VAL:HG23	1:B:310:GLY:H	1.51	0.73
1:B:274:LYS:HE2	1:B:276:LEU:HD11	1.70	0.73
2:A:365:VAL:HG21	2:A:411:ILE:HD12	1.69	0.73
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.71	0.73
2:A:546:SER:O	2:A:550:VAL:HG13	1.89	0.72
1:C:344:VAL:HG12	1:C:376:LYS:HB3	1.71	0.72
2:A:408:ILE:HA	2:A:411:ILE:HG22	1.70	0.72
1:C:327:ILE:HD12	1:C:367:LEU:HD11	1.70	0.72
2:A:933:LEU:HD21	2:A:1020:MET:CB	2.20	0.72
1:C:132:ILE:HD11	1:C:229:ILE:HB	1.69	0.72
2:A:548:LEU:HD22	2:A:548:LEU:H	1.53	0.72
1:B:113:ASN:N	1:B:113:ASN:HD22	1.88	0.72
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.72	0.72
2:A:1000:TRP:HE3	2:A:1000:TRP:HA	1.54	0.71
2:A:763:ILE:HD12	2:A:763:ILE:H	1.56	0.71
2:A:968:LYS:HD2	2:A:968:LYS:H	1.56	0.71
2:A:460:SER:HB3	2:A:882:ILE:CD1	2.21	0.71
1:B:292:ARG:HG3	2:A:199:TYR:CE2	2.26	0.70
1:C:161:ALA:HB1	1:C:185:LEU:HD11	1.73	0.70
1:B:355:VAL:HG21	1:B:367:LEU:HD23	1.73	0.70
2:A:253:ASN:HB3	2:A:255:VAL:HG22	1.72	0.70
2:A:411:ILE:HB	2:A:497:ILE:HD13	1.73	0.70
2:A:893:ARG:HG3	2:A:896:GLU:H	1.56	0.70
2:A:880:LEU:H	2:A:880:LEU:HD23	1.57	0.70
2:A:26:TRP:HE1	2:A:379:ILE:HA	1.55	0.70
2:A:668:ASN:HA	2:A:678:LYS:HG2	1.73	0.70
2:A:980:ARG:HD2	2:A:1028:LEU:HD23	1.74	0.70
1:C:217:VAL:HG21	1:C:241:MET:HE3	1.74	0.70
2:A:48:ILE:H	2:A:48:ILE:HD13	1.57	0.69
2:A:880:LEU:CD2	2:A:880:LEU:N	2.56	0.69
2:A:475:PHE:HZ	2:A:562:LEU:HD21	1.55	0.69
2:A:138:TRP:CZ3	2:A:665:PRO:HB2	2.28	0.69
2:A:379:ILE:HG23	2:A:380:VAL:HG23	1.74	0.69
1:C:284:LEU:HD21	1:C:297:ARG:NH2	2.08	0.69
2:A:880:LEU:O	2:A:884:PHE:N	2.24	0.69
1:B:134:LYS:HG2	1:B:152:ASP:HB2	1.75	0.69
1:B:388:GLU:HG2	2:A:777:ARG:NH2	2.08	0.69
1:B:388:GLU:HG2	2:A:777:ARG:HH21	1.57	0.68
2:A:48:ILE:HG12	2:A:130:GLY:CA	2.17	0.68
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:925:ALA:O	2:A:928:THR:HG23	1.91	0.68
2:A:404:VAL:HG12	2:A:408:ILE:HG21	1.73	0.68
2:A:399:ALA:HB2	2:A:482:LYS:HA	1.76	0.68
1:C:137:PRO:O	1:C:138:LEU:HD12	1.94	0.68
2:A:222:ILE:HG22	2:A:229:TYR:HB2	1.76	0.68
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.76	0.67
2:A:831:ARG:HG2	2:A:832:ASP:H	1.59	0.67
2:A:955:VAL:H	2:A:956:PRO:HD2	1.58	0.67
2:A:219:GLY:HA3	2:A:231:VAL:HG13	1.77	0.67
1:B:317:LEU:HD23	1:B:318:ASN:N	2.10	0.67
2:A:54:PRO:CD	2:A:122:PRO:HG3	2.23	0.67
2:A:1024:PRO:O	2:A:1028:LEU:HG	1.94	0.67
2:A:36:VAL:HG22	2:A:331:ILE:HD11	1.76	0.67
2:A:987:THR:O	2:A:991:ILE:HG12	1.94	0.67
2:A:571:LEU:HD23	2:A:572:TYR:N	2.10	0.66
2:A:980:ARG:NH1	2:A:1028:LEU:HA	2.09	0.66
1:B:259:LYS:HD2	1:C:271:ARG:NH1	2.09	0.66
2:A:279:ASN:HA	2:A:605:VAL:HG23	1.75	0.66
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.78	0.66
2:A:61:VAL:O	2:A:65:VAL:HG12	1.95	0.66
1:C:101:ARG:HH21	1:C:325:LEU:HD11	1.59	0.66
2:A:353:CYS:O	2:A:357:LEU:HB3	1.96	0.65
2:A:399:ALA:HB1	2:A:485:ALA:HB3	1.78	0.65
2:A:275:ILE:HG13	2:A:586:ALA:HB2	1.79	0.65
2:A:243:PHE:O	2:A:246:ILE:HG12	1.95	0.65
1:B:287:VAL:HG12	1:B:294:LEU:HB3	1.79	0.65
2:A:114:LEU:HD11	2:A:127:ALA:HB3	1.77	0.65
2:A:328:SER:HA	2:A:331:ILE:HG22	1.79	0.65
2:A:404:VAL:O	2:A:408:ILE:HG23	1.96	0.65
2:A:1026:LEU:O	2:A:1030:ILE:HB	1.97	0.64
2:A:357:LEU:HD21	2:A:362:SER:HB2	1.78	0.64
2:A:430:LEU:HD23	2:A:430:LEU:H	1.62	0.64
2:A:386:LEU:O	2:A:387:ASN:HB2	1.97	0.64
2:A:315:LEU:HB3	2:A:319:VAL:HG11	1.79	0.64
1:B:252:GLU:HG3	1:C:311:MET:HG2	1.80	0.64
2:A:933:LEU:CD2	2:A:1020:MET:HB2	2.24	0.64
1:C:82:VAL:HG21	1:C:392:SER:HB3	1.78	0.64
2:A:462:ILE:O	2:A:465:PHE:CD2	2.50	0.64
2:A:812:MET:O	2:A:812:MET:HG2	1.97	0.64
2:A:39:LEU:HD12	2:A:390:ILE:HG21	1.80	0.64
2:A:542:VAL:O	2:A:545:LEU:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:SER:OG	1:B:365:THR:HG23	1.98	0.63
1:B:109:SER:HA	1:B:316:GLN:HA	1.79	0.63
2:A:759:THR:HG23	2:A:768:ILE:HD11	1.79	0.63
2:A:462:ILE:N	2:A:463:PRO:CD	2.62	0.63
2:A:357:LEU:HD11	2:A:362:SER:HB3	1.79	0.63
2:A:780:PRO:O	2:A:784:ARG:HG2	1.98	0.63
1:C:276:LEU:HD21	1:C:307:LEU:HD11	1.81	0.63
1:B:297:ARG:C	1:B:298:LEU:HD12	2.19	0.63
2:A:977:ALA:HA	2:A:980:ARG:HH21	1.64	0.63
1:C:114:VAL:HG23	1:C:311:MET:O	1.98	0.63
2:A:404:VAL:HG12	2:A:408:ILE:HG23	1.80	0.63
2:A:392:SER:HA	2:A:481:THR:HG21	1.79	0.62
2:A:529:LEU:HA	2:A:532:VAL:HG13	1.79	0.62
1:C:138:LEU:HD23	1:C:218:ILE:HD11	1.81	0.62
2:A:661:LEU:HD12	2:A:827:ASP:HB2	1.81	0.62
2:A:829:ARG:HD3	2:A:829:ARG:H	1.64	0.62
1:C:166:LEU:HD22	1:C:202:GLN:HB3	1.82	0.62
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.81	0.62
1:B:326:LEU:HD13	1:B:364:VAL:HG21	1.82	0.62
2:A:879:THR:CG2	2:A:880:LEU:HD21	2.27	0.62
1:C:114:VAL:O	1:C:309:PRO:HA	1.99	0.62
2:A:199:TYR:HE1	2:A:261:ASP:HB2	1.65	0.62
1:B:386:ASP:HB3	2:A:271:MET:HA	1.80	0.61
2:A:280:GLY:O	2:A:594:LYS:HG2	1.99	0.61
1:B:241:MET:O	1:B:244:VAL:HG23	2.01	0.61
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.83	0.61
2:A:368:ILE:HG13	2:A:500:LEU:HD21	1.82	0.61
2:A:83:ARG:HB2	2:A:94:TYR:HB2	1.82	0.61
1:B:385:ILE:HG23	1:B:389:ALA:HB2	1.83	0.61
2:A:365:VAL:CG2	2:A:411:ILE:HD12	2.31	0.61
2:A:547:VAL:O	2:A:550:VAL:HG22	1.99	0.61
1:B:342:ILE:O	1:B:378:VAL:HG12	2.01	0.60
2:A:48:ILE:HG22	2:A:94:TYR:CD2	2.36	0.60
1:C:169:ARG:HE	1:C:202:GLN:HE22	1.50	0.60
1:B:241:MET:HB2	1:B:244:VAL:HG22	1.83	0.60
2:A:474:LEU:HD21	2:A:562:LEU:HD11	1.83	0.60
2:A:191:ILE:HA	2:A:263:ALA:HB2	1.84	0.60
2:A:546:SER:O	2:A:549:THR:HG22	2.01	0.60
1:B:332:LEU:HA	1:B:341:VAL:HG12	1.84	0.60
2:A:960:ASN:N	2:A:961:PRO:HD2	2.16	0.59
2:A:19:GLY:O	2:A:23:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG23	1:B:374:GLY:H	1.66	0.59
2:A:931:ILE:CD1	2:A:931:ILE:N	2.66	0.59
1:B:274:LYS:HG3	1:B:276:LEU:HD21	1.84	0.59
1:B:384:LEU:HD22	1:B:391:ILE:HD13	1.84	0.59
2:A:554:LEU:O	2:A:557:VAL:HG22	2.02	0.59
2:A:669:ARG:O	2:A:673:LEU:HD22	2.01	0.59
2:A:984:LYS:HG3	2:A:1028:LEU:HD21	1.83	0.59
2:A:577:LEU:HB3	2:A:578:PRO:HD2	1.84	0.59
1:C:266:LEU:HD12	1:C:266:LEU:H	1.67	0.59
1:B:144:VAL:HG21	1:B:238:ILE:HD13	1.83	0.59
2:A:589:LEU:HD12	2:A:609:THR:HB	1.84	0.59
2:A:291:LEU:HD22	2:A:297:ALA:HA	1.85	0.59
2:A:876:VAL:O	2:A:880:LEU:CD2	2.51	0.59
1:B:271:ARG:NE	1:B:306:ALA:HB1	2.18	0.59
2:A:933:LEU:HD21	2:A:1020:MET:CA	2.33	0.59
2:A:931:ILE:HD12	2:A:931:ILE:N	2.18	0.59
2:A:986:MET:O	2:A:990:VAL:HG22	2.03	0.59
2:A:771:ARG:HD2	2:A:777:ARG:NH1	2.17	0.59
2:A:463:PRO:HB2	2:A:875:MET:SD	2.42	0.59
2:A:728:ILE:HA	2:A:802:ALA:HB2	1.84	0.58
2:A:572:TYR:HB3	2:A:626:THR:OG1	2.03	0.58
1:C:281:TRP:HB3	1:C:298:LEU:HD21	1.84	0.58
2:A:83:ARG:HG3	2:A:94:TYR:HB2	1.83	0.58
1:C:104:LEU:HD12	1:C:366:ALA:HB2	1.85	0.58
2:A:608:LYS:O	2:A:624:VAL:HG23	2.03	0.58
2:A:454:LEU:HD12	2:A:490:ALA:HB2	1.85	0.58
2:A:152:ASP:O	2:A:156:LEU:HG	2.03	0.58
2:A:85:PHE:CD2	2:A:94:TYR:HE1	2.22	0.58
2:A:460:SER:CA	2:A:882:ILE:HD12	2.33	0.58
2:A:346:PHE:CE2	2:A:367:ILE:HG23	2.38	0.58
2:A:199:TYR:CE1	2:A:261:ASP:HB2	2.39	0.58
2:A:70:THR:HG23	2:A:82:VAL:HB	1.86	0.57
2:A:952:ILE:O	2:A:957:SER:HB3	2.04	0.57
2:A:561:PHE:CE1	2:A:864:LEU:HB3	2.39	0.57
2:A:114:LEU:O	2:A:117:VAL:HG23	2.04	0.57
2:A:664:PRO:HG2	2:A:667:ARG:HB3	1.85	0.57
2:A:572:TYR:HE1	2:A:653:VAL:HG11	1.69	0.57
2:A:550:VAL:C	2:A:553:PRO:HD2	2.24	0.57
2:A:168:LEU:HA	2:A:171:ILE:HD13	1.87	0.57
2:A:596:ILE:O	2:A:599:VAL:HG22	2.05	0.57
2:A:410:MET:HG3	2:A:411:ILE:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.39	0.57
2:A:641:THR:H	2:A:644:LYS:HB3	1.69	0.57
2:A:995:LEU:CA	2:A:998:ILE:HD11	2.29	0.57
2:A:880:LEU:HB2	2:A:881:MET:SD	2.45	0.57
2:A:54:PRO:HD3	2:A:122:PRO:CG	2.30	0.57
2:A:896:GLU:HG3	2:A:945:LEU:HG	1.87	0.57
2:A:380:VAL:HB	2:A:484:TYR:CZ	2.38	0.57
2:A:595:LEU:HD13	2:A:653:VAL:HA	1.85	0.56
2:A:372:LEU:O	2:A:376:ILE:HG13	2.05	0.56
2:A:143:ALA:HB2	2:A:606:PHE:CE1	2.40	0.56
1:C:241:MET:O	1:C:244:VAL:HB	2.05	0.56
2:A:196:LEU:HD22	2:A:201:ILE:O	2.04	0.56
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.39	0.56
2:A:879:THR:HG22	2:A:880:LEU:CD2	2.28	0.56
2:A:554:LEU:HD23	2:A:912:ILE:HG21	1.87	0.56
2:A:497:ILE:HB	2:A:498:PRO:HD3	1.86	0.56
2:A:452:ILE:O	2:A:456:ILE:HG13	2.06	0.56
2:A:918:MET:HE1	2:A:1000:TRP:CZ3	2.41	0.56
2:A:649:LEU:HB3	2:A:662:TRP:CH2	2.40	0.56
2:A:668:ASN:HA	2:A:678:LYS:HG3	1.85	0.56
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.35	0.56
2:A:96:ILE:O	2:A:96:ILE:HG23	2.03	0.56
2:A:876:VAL:C	2:A:879:THR:HG22	2.20	0.56
2:A:573:MET:CE	2:A:668:ASN:HD21	2.18	0.56
2:A:408:ILE:O	2:A:411:ILE:HG22	2.05	0.56
2:A:387:ASN:O	2:A:388:ALA:HB3	2.05	0.56
1:B:164:GLU:O	1:B:168:LEU:HG	2.04	0.56
2:A:153:LEU:H	2:A:153:LEU:HD12	1.71	0.56
2:A:572:TYR:HE2	2:A:574:PRO:HB3	1.70	0.56
1:B:266:LEU:HD12	1:B:267:THR:H	1.69	0.56
1:C:343:THR:HB	1:C:351:VAL:HG13	1.88	0.56
2:A:773:PRO:HG2	2:A:776:TRP:CD1	2.40	0.56
2:A:572:TYR:C	2:A:572:TYR:HD2	2.09	0.56
2:A:138:TRP:CE2	2:A:141:GLU:OE1	2.59	0.56
2:A:188:GLN:HA	2:A:769:ASN:ND2	2.20	0.56
1:C:174:THR:HB	1:C:177:GLN:HG2	1.88	0.56
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.88	0.56
1:C:162:GLN:HE22	1:C:205:GLN:HB2	1.70	0.56
2:A:637:ARG:HB2	2:A:640:MET:CG	2.36	0.56
1:C:192:GLU:O	1:C:195:ILE:HG22	2.06	0.56
2:A:701:GLU:HB2	2:A:715:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HB	1:B:376:LYS:HD3	1.88	0.55
2:A:930:PHE:CE2	2:A:1015:PRO:CB	2.75	0.55
2:A:550:VAL:O	2:A:554:LEU:HG	2.06	0.55
2:A:926:THR:HG22	2:A:1011:ARG:O	2.06	0.55
2:A:370:LEU:HD22	2:A:400:VAL:HG23	1.88	0.55
2:A:948:LEU:HD21	2:A:1032:PRO:HA	1.88	0.55
1:C:136:TYR:HB3	1:C:137:PRO:HD2	1.89	0.55
1:B:387:SER:OG	2:A:271:MET:HB2	2.05	0.55
2:A:241:ASP:HA	2:A:244:ASN:HB2	1.89	0.55
1:B:195:ILE:O	1:B:198:LEU:HB3	2.06	0.55
2:A:746:PHE:CE2	2:A:788:ILE:HG13	2.42	0.55
2:A:699:GLN:NE2	2:A:848:VAL:HG13	2.22	0.55
2:A:522:ILE:HG22	2:A:981:VAL:HG11	1.89	0.55
2:A:918:MET:HE1	2:A:1000:TRP:HZ3	1.70	0.55
2:A:311:LEU:C	2:A:313:SER:H	2.10	0.55
1:B:385:ILE:O	1:B:389:ALA:HB3	2.07	0.55
2:A:571:LEU:HD22	2:A:668:ASN:ND2	2.21	0.55
1:C:362:GLN:HE21	1:C:362:GLN:HA	1.72	0.55
2:A:45:VAL:HG11	2:A:103:PRO:HA	1.89	0.55
2:A:887:LEU:HD13	2:A:897:ALA:HA	1.89	0.55
2:A:143:ALA:HB2	2:A:606:PHE:HE1	1.72	0.55
1:C:366:ALA:O	1:C:367:LEU:HD23	2.07	0.55
2:A:315:LEU:HB3	2:A:319:VAL:CG1	2.37	0.55
2:A:609:THR:HB	2:A:624:VAL:HB	1.89	0.55
2:A:1023:ALA:N	2:A:1024:PRO:HD2	2.22	0.55
2:A:26:TRP:NE1	2:A:30:THR:HG21	2.22	0.55
2:A:685:VAL:HG21	2:A:697:ALA:HB2	1.87	0.55
2:A:995:LEU:O	2:A:998:ILE:CD1	2.55	0.55
2:A:681:ILE:HB	2:A:826:ILE:HB	1.87	0.55
1:B:291:THR:HG21	2:A:255:VAL:HG23	1.89	0.55
1:B:382:LEU:HD13	2:A:154:ALA:HB2	1.89	0.55
1:C:388:GLU:HB2	2:A:657:GLY:N	2.22	0.55
2:A:572:TYR:C	2:A:572:TYR:CD2	2.80	0.54
2:A:316:PRO:O	2:A:319:VAL:HG12	2.08	0.54
2:A:930:PHE:HE2	2:A:1015:PRO:CB	2.17	0.54
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.25	0.54
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.43	0.54
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.41	0.54
2:A:432:ASN:HA	2:A:435:ARG:HG2	1.89	0.54
2:A:26:TRP:HE1	2:A:379:ILE:CA	2.18	0.54
2:A:709:GLY:HA3	2:A:831:ARG:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.90	0.54
1:B:291:THR:HG21	2:A:255:VAL:CG2	2.38	0.54
2:A:278:LEU:HD23	2:A:279:ASN:N	2.23	0.54
1:C:214:ILE:HG12	1:C:215:ASP:N	2.22	0.54
2:A:876:VAL:CG2	2:A:877:PRO:HD3	2.33	0.54
2:A:551:LEU:HD23	2:A:554:LEU:HD12	1.89	0.54
1:B:250:ILE:HB	1:B:294:LEU:HD12	1.89	0.54
1:C:242:ASP:O	1:C:243:PRO:C	2.45	0.54
1:B:261:ALA:HB3	1:B:281:TRP:HZ2	1.72	0.54
2:A:181:GLY:HA3	2:A:276:ALA:HB3	1.89	0.54
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.27	0.54
2:A:571:LEU:HD22	2:A:668:ASN:HD22	1.72	0.54
1:C:327:ILE:HD13	1:C:327:ILE:H	1.72	0.54
2:A:537:LYS:HE3	2:A:541:LEU:HD21	1.88	0.54
2:A:555:ASN:HD22	2:A:556:LYS:HG3	1.71	0.54
2:A:395:GLY:HA3	2:A:481:THR:OG1	2.07	0.54
2:A:188:GLN:HG2	2:A:769:ASN:HD21	1.72	0.54
1:B:114:VAL:HG12	1:B:246:VAL:HB	1.90	0.54
2:A:131:PRO:HD3	2:A:615:ALA:HB3	1.89	0.54
2:A:876:VAL:O	2:A:880:LEU:HD21	2.08	0.53
2:A:525:TYR:CE1	2:A:977:ALA:HB1	2.34	0.53
1:B:333:ILE:HD11	1:B:342:ILE:HD11	1.90	0.53
2:A:20:ALA:HA	2:A:23:LEU:HD12	1.90	0.53
1:B:99:VAL:HG12	1:B:327:ILE:HG22	1.89	0.53
2:A:932:ALA:CB	2:A:1016:MET:HE2	2.36	0.53
1:C:284:LEU:HB2	1:C:295:GLN:HB2	1.90	0.53
2:A:960:ASN:H	2:A:961:PRO:HD2	1.73	0.53
1:C:199:ILE:HG13	1:C:200:ALA:N	2.21	0.53
1:C:302:ASN:ND2	1:C:307:LEU:HB2	2.23	0.53
2:A:297:ALA:O	2:A:301:ILE:HG13	2.08	0.53
2:A:80:LYS:HB2	2:A:98:GLU:HB3	1.90	0.53
1:B:382:LEU:HD22	2:A:183:VAL:HG11	1.89	0.53
2:A:407:ALA:O	2:A:497:ILE:HD11	2.09	0.53
2:A:146:ASP:OD1	2:A:148:SER:HB3	2.08	0.53
2:A:69:LEU:HD21	2:A:117:VAL:HG11	1.91	0.53
2:A:388:ALA:O	2:A:389:ASN:HB3	2.08	0.53
1:B:223:LEU:HD12	1:B:235:VAL:HG22	1.90	0.53
1:C:159:VAL:HG23	1:C:160:GLU:H	1.74	0.53
2:A:729:ASN:ND2	2:A:732:LYS:H	2.06	0.53
2:A:202:SER:OG	2:A:205:GLU:HB2	2.09	0.53
2:A:460:SER:CB	2:A:882:ILE:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:881:MET:O	2:A:885:VAL:HG23	2.09	0.53
1:B:204:ILE:H	1:B:204:ILE:CD1	2.12	0.53
1:C:314:TRP:CH2	2:A:195:ARG:HG2	2.43	0.53
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.09	0.53
2:A:915:LEU:HD21	2:A:1015:PRO:HG3	1.91	0.53
2:A:369:SER:O	2:A:403:MET:HE2	2.09	0.53
2:A:677:ILE:HG21	2:A:682:GLY:HA3	1.91	0.52
2:A:668:ASN:CA	2:A:678:LYS:HG2	2.37	0.52
1:C:161:ALA:HB1	1:C:185:LEU:CD1	2.38	0.52
2:A:906:PHE:HB3	2:A:1026:LEU:HD13	1.92	0.52
2:A:608:LYS:C	2:A:624:VAL:HG23	2.29	0.52
1:C:302:ASN:HD21	1:C:307:LEU:H	1.57	0.52
2:A:707:VAL:HG12	2:A:709:GLY:H	1.74	0.52
1:C:325:LEU:HD12	1:C:325:LEU:N	2.25	0.52
2:A:277:GLU:HG2	2:A:282:GLY:O	2.09	0.52
1:B:317:LEU:HD21	1:B:319:THR:HG22	1.90	0.52
1:C:158:TRP:CH2	1:C:190:MET:HA	2.44	0.52
2:A:460:SER:CB	2:A:882:ILE:HD11	2.34	0.52
2:A:932:ALA:CB	2:A:1016:MET:CE	2.80	0.52
1:C:339:GLN:HG2	1:C:355:VAL:O	2.09	0.52
1:B:113:ASN:ND2	1:B:113:ASN:N	2.57	0.52
1:B:385:ILE:HD13	1:B:386:ASP:O	2.10	0.52
2:A:175:ALA:HB3	2:A:290:ILE:O	2.10	0.52
2:A:637:ARG:HB2	2:A:640:MET:HG2	1.91	0.52
1:C:354:ARG:NH1	1:C:354:ARG:HB3	2.24	0.52
2:A:50:LYS:CG	2:A:92:TYR:HE2	2.22	0.52
2:A:138:TRP:HZ3	2:A:665:PRO:HB2	1.74	0.52
1:C:132:ILE:N	1:C:132:ILE:HD12	2.25	0.52
1:C:147:GLY:HA2	1:C:211:LYS:HB3	1.92	0.52
1:B:125:GLN:NE2	1:C:228:ASN:H	2.06	0.52
2:A:667:ARG:HD3	2:A:861:GLN:NE2	2.25	0.52
2:A:178:ALA:HB2	2:A:614:THR:HB	1.91	0.52
2:A:360:VAL:O	2:A:364:LEU:HD13	2.10	0.52
2:A:74:LEU:HG	2:A:82:VAL:HG11	1.92	0.52
2:A:307:LYS:O	2:A:311:LEU:HG	2.09	0.52
2:A:667:ARG:O	2:A:670:ILE:HD13	2.10	0.52
1:C:242:ASP:CB	1:C:243:PRO:HD2	2.40	0.52
1:B:261:ALA:HB3	1:B:281:TRP:CZ2	2.45	0.52
2:A:68:PRO:O	2:A:72:THR:HG23	2.10	0.52
2:A:248:LEU:HD12	2:A:262:VAL:HG21	1.91	0.52
1:B:246:VAL:CG1	1:B:298:LEU:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:781:GLN:H	2:A:781:GLN:CD	2.13	0.52
1:C:360:ALA:O	1:C:361:SER:HB2	2.09	0.52
2:A:829:ARG:HD3	2:A:829:ARG:N	2.24	0.52
1:B:187:LEU:HD13	1:C:159:VAL:HG11	1.92	0.52
2:A:729:ASN:C	2:A:729:ASN:HD22	2.14	0.52
1:B:201:THR:HG23	1:B:203:LYS:H	1.73	0.52
2:A:882:ILE:HD13	2:A:883:ILE:N	2.24	0.51
2:A:679:SER:O	2:A:680:PRO:C	2.49	0.51
1:C:217:VAL:CG2	1:C:241:MET:HE3	2.40	0.51
1:C:259:LYS:HD3	1:C:260:ASP:H	1.75	0.51
1:C:162:GLN:NE2	1:C:205:GLN:H	2.09	0.51
1:B:117:ASN:ND2	1:B:120:GLN:HG3	2.26	0.51
2:A:668:ASN:C	2:A:678:LYS:HG2	2.30	0.51
2:A:679:SER:O	2:A:681:ILE:N	2.44	0.51
2:A:560:GLU:O	2:A:923:SER:HA	2.11	0.51
2:A:311:LEU:O	2:A:315:LEU:HG	2.11	0.51
2:A:1025:LEU:HA	2:A:1028:LEU:HD12	1.93	0.51
1:B:385:ILE:HG23	1:B:389:ALA:CB	2.40	0.51
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.10	0.51
2:A:48:ILE:HG22	2:A:94:TYR:HD2	1.74	0.51
2:A:977:ALA:O	2:A:981:VAL:HG23	2.10	0.51
2:A:699:GLN:HE21	2:A:848:VAL:HG13	1.75	0.51
2:A:276:ALA:O	2:A:283:GLU:HG3	2.11	0.51
2:A:59:GLN:NE2	2:A:63:ASN:HD21	2.08	0.51
2:A:676:GLY:C	2:A:677:ILE:HG12	2.30	0.51
1:B:264:PHE:CE2	1:B:317:LEU:HD12	2.45	0.51
2:A:178:ALA:HB3	2:A:288:VAL:HG13	1.93	0.51
2:A:790:THR:HB	2:A:791:PRO:HD2	1.92	0.51
2:A:49:ILE:HG13	2:A:93:VAL:HB	1.93	0.51
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.92	0.51
2:A:467:LEU:HD13	2:A:871:LYS:HG2	1.93	0.51
1:B:223:LEU:O	1:B:224:ARG:HD2	2.11	0.51
2:A:187:TYR:HE2	2:A:759:THR:HG1	1.58	0.51
1:C:281:TRP:HB3	1:C:298:LEU:CD2	2.40	0.51
2:A:879:THR:HG23	2:A:880:LEU:N	2.26	0.50
2:A:300:VAL:O	2:A:304:VAL:HG23	2.11	0.50
2:A:44:ASP:HB2	2:A:96:ILE:HD11	1.93	0.50
2:A:96:ILE:CG2	2:A:96:ILE:O	2.59	0.50
1:C:276:LEU:HD13	1:C:307:LEU:HD21	1.93	0.50
1:B:336:GLY:HA3	2:A:775:SER:HB2	1.94	0.50
2:A:980:ARG:HD2	2:A:1028:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:TRP:NE1	1:C:299:GLU:HG2	2.26	0.50
2:A:832:ASP:O	2:A:836:VAL:HG23	2.11	0.50
2:A:957:SER:O	2:A:959:ASN:N	2.45	0.50
2:A:723:TYR:O	2:A:806:VAL:HG23	2.12	0.50
2:A:955:VAL:H	2:A:956:PRO:CD	2.24	0.50
1:C:231:LYS:HB3	1:C:231:LYS:HZ2	1.77	0.50
2:A:325:TYR:HB2	2:A:627:THR:HG21	1.94	0.50
2:A:42:LEU:HD22	2:A:470:GLN:HB3	1.93	0.50
1:C:383:PHE:CE1	2:A:580:ILE:HB	2.47	0.50
2:A:341:LYS:O	2:A:345:GLU:HG2	2.11	0.50
1:B:250:ILE:HB	1:B:294:LEU:CD1	2.41	0.50
2:A:139:ILE:HG22	2:A:140:TYR:N	2.26	0.50
2:A:38:ALA:HB2	2:A:331:ILE:HB	1.93	0.50
2:A:45:VAL:CG1	2:A:103:PRO:HA	2.42	0.50
2:A:4:TRP:CE3	2:A:5:ILE:HG13	2.47	0.50
2:A:83:ARG:CG	2:A:94:TYR:HB2	2.42	0.50
2:A:952:ILE:HG23	2:A:957:SER:HB3	1.94	0.50
1:C:145:GLN:HA	1:C:215:ASP:OD2	2.12	0.50
2:A:933:LEU:HD21	2:A:1020:MET:N	2.27	0.49
2:A:998:ILE:H	2:A:998:ILE:HD13	1.77	0.49
2:A:410:MET:HG2	2:A:497:ILE:HD12	1.94	0.49
2:A:454:LEU:HA	2:A:457:ILE:HG22	1.95	0.49
2:A:395:GLY:HA2	2:A:478:LEU:HG	1.94	0.49
1:B:391:ILE:HG12	2:A:774:GLN:NE2	2.26	0.49
1:B:159:VAL:HG23	1:B:160:GLU:H	1.76	0.49
2:A:687:GLY:O	2:A:820:PRO:HB2	2.12	0.49
1:C:287:VAL:HG23	1:C:293:THR:O	2.13	0.49
2:A:668:ASN:HA	2:A:678:LYS:HE2	1.95	0.49
2:A:173:ASP:O	2:A:291:LEU:HD12	2.13	0.49
2:A:408:ILE:HA	2:A:411:ILE:CG2	2.42	0.49
2:A:56:GLN:NE2	2:A:61:VAL:HG23	2.27	0.49
1:C:324:MET:CE	1:C:368:ARG:HA	2.43	0.49
2:A:135:GLY:O	2:A:138:TRP:HB2	2.11	0.49
1:C:217:VAL:O	1:C:238:ILE:HA	2.12	0.49
2:A:454:LEU:O	2:A:457:ILE:HG22	2.12	0.49
2:A:67:TYR:HD2	2:A:67:TYR:C	2.15	0.49
2:A:140:TYR:O	2:A:289:VAL:HG22	2.13	0.49
1:C:245:TRP:CD1	1:C:299:GLU:HG2	2.47	0.49
2:A:47:VAL:HG12	2:A:95:VAL:O	2.12	0.49
1:C:315:LEU:HD23	1:C:315:LEU:C	2.33	0.49
2:A:39:LEU:CG	2:A:40:PRO:HD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:C	1:B:224:ARG:HD2	2.33	0.49
1:C:245:TRP:CD2	1:C:297:ARG:HD3	2.47	0.49
2:A:666:ILE:HG22	2:A:667:ARG:N	2.26	0.49
1:C:254:ILE:HG23	1:C:257:LEU:HD12	1.94	0.49
2:A:142:TYR:CE1	2:A:164:LEU:HD13	2.48	0.49
2:A:577:LEU:CB	2:A:578:PRO:HD2	2.42	0.49
1:C:324:MET:HE2	1:C:368:ARG:HA	1.95	0.49
2:A:67:TYR:CD2	2:A:67:TYR:C	2.86	0.49
2:A:789:LEU:HD21	2:A:793:LYS:HA	1.95	0.49
2:A:984:LYS:C	2:A:984:LYS:HD2	2.33	0.49
1:C:242:ASP:HB3	1:C:243:PRO:HD2	1.93	0.49
2:A:18:MET:O	2:A:21:LEU:HG	2.13	0.49
2:A:914:LEU:CD2	2:A:1017:ILE:HB	2.42	0.49
1:B:151:LEU:HD21	1:B:235:VAL:HG22	1.94	0.49
2:A:403:MET:CE	2:A:489:ALA:HB2	2.42	0.49
2:A:1027:SER:OG	2:A:1031:ILE:HD12	2.12	0.48
2:A:132:ASP:OD2	2:A:292:ARG:HD3	2.13	0.48
2:A:730:ARG:NH2	2:A:740:VAL:HG21	2.28	0.48
1:C:284:LEU:HD12	1:C:295:GLN:HB3	1.95	0.48
2:A:784:ARG:HD3	2:A:804:ILE:HG13	1.94	0.48
2:A:273:ARG:O	2:A:621:LEU:HD21	2.12	0.48
1:B:223:LEU:HD12	1:B:235:VAL:CG2	2.44	0.48
2:A:185:LYS:O	2:A:766:TYR:HB3	2.13	0.48
2:A:467:LEU:HD12	2:A:471:GLU:HG3	1.94	0.48
2:A:678:LYS:HD2	2:A:678:LYS:HA	1.49	0.48
2:A:923:SER:HB3	2:A:926:THR:HG23	1.96	0.48
1:C:118:GLU:HB2	1:C:245:TRP:CZ3	2.48	0.48
2:A:291:LEU:HD11	2:A:295:LYS:HB2	1.95	0.48
1:B:128:ALA:HA	1:B:231:LYS:HE2	1.95	0.48
2:A:50:LYS:HG3	2:A:92:TYR:HE2	1.78	0.48
2:A:888:TYR:OH	2:A:894:VAL:HG23	2.13	0.48
2:A:788:ILE:CG2	2:A:796:ILE:HG13	2.43	0.48
2:A:671:ASP:HB2	2:A:678:LYS:HD3	1.95	0.48
2:A:831:ARG:HD3	2:A:836:VAL:HG22	1.96	0.48
2:A:478:LEU:O	2:A:478:LEU:HD23	2.13	0.48
1:B:281:TRP:HZ3	1:B:283:LEU:HB2	1.78	0.48
2:A:633:GLN:HG2	2:A:636:TRP:CZ2	2.49	0.48
1:B:325:LEU:HD12	1:B:325:LEU:O	2.13	0.48
2:A:348:VAL:HA	2:A:351:VAL:HG22	1.95	0.48
2:A:475:PHE:CZ	2:A:562:LEU:HD21	2.44	0.48
1:B:156:PRO:O	1:B:159:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:PRO:HB2	1:C:398:MET:SD	2.53	0.48
2:A:883:ILE:O	2:A:887:LEU:HG	2.14	0.48
1:B:367:LEU:HD12	1:B:367:LEU:N	2.28	0.48
2:A:272:ARG:HD2	2:A:275:ILE:HD13	1.95	0.48
1:B:84:ILE:HG22	1:C:91:ASN:CG	2.33	0.48
2:A:957:SER:O	2:A:960:ASN:N	2.32	0.48
2:A:462:ILE:N	2:A:463:PRO:HD3	2.29	0.48
2:A:191:ILE:O	2:A:193:PRO:HD3	2.14	0.48
2:A:168:LEU:HB3	2:A:177:VAL:HG21	1.94	0.47
2:A:526:HIS:HB2	2:A:527:PRO:HD3	1.96	0.47
2:A:940:PHE:CE1	2:A:1027:SER:HB3	2.48	0.47
1:C:153:LEU:HD12	1:C:229:ILE:HG21	1.96	0.47
2:A:26:TRP:HE1	2:A:379:ILE:CB	2.27	0.47
2:A:696:MET:CE	2:A:851:LYS:HG2	2.44	0.47
2:A:879:THR:O	2:A:882:ILE:HG23	2.12	0.47
1:C:181:ILE:O	1:C:185:LEU:HD13	2.14	0.47
1:C:119:TYR:CD1	1:C:245:TRP:HZ2	2.32	0.47
1:B:159:VAL:HG23	1:B:160:GLU:N	2.29	0.47
2:A:904:VAL:N	2:A:905:PRO:CD	2.78	0.47
2:A:952:ILE:HG23	2:A:957:SER:CB	2.44	0.47
2:A:85:PHE:HB2	2:A:92:TYR:O	2.15	0.47
1:C:382:LEU:HD23	1:C:382:LEU:O	2.15	0.47
1:C:138:LEU:HD22	1:C:150:LEU:HD12	1.95	0.47
2:A:357:LEU:HD11	2:A:362:SER:CB	2.44	0.47
1:B:271:ARG:HE	1:B:306:ALA:HB1	1.79	0.47
1:C:192:GLU:O	1:C:196:ARG:HG3	2.14	0.47
2:A:759:THR:O	2:A:761:GLU:HG3	2.14	0.47
1:B:397:ARG:HH12	2:A:583:ALA:C	2.18	0.47
2:A:572:TYR:HE2	2:A:574:PRO:CB	2.28	0.47
1:C:245:TRP:CE2	1:C:297:ARG:HD3	2.49	0.47
2:A:328:SER:HA	2:A:331:ILE:CG2	2.44	0.47
1:B:280:LYS:HD2	1:B:280:LYS:HA	1.62	0.47
2:A:929:GLY:O	2:A:932:ALA:HB3	2.14	0.47
2:A:868:ALA:O	2:A:872:LEU:HG	2.14	0.47
2:A:545:LEU:O	2:A:548:LEU:HD22	2.15	0.47
2:A:482:LYS:O	2:A:486:MET:HB3	2.15	0.47
2:A:834:VAL:HG13	2:A:838:HIS:CD2	2.50	0.47
1:C:278:ILE:HA	1:C:300:VAL:HG12	1.97	0.47
1:C:214:ILE:H	1:C:214:ILE:HD13	1.80	0.47
2:A:837:VAL:HG21	2:A:862:PHE:CD2	2.50	0.47
2:A:642:MET:O	2:A:646:ILE:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:HE21	2:A:785:GLN:HG2	1.79	0.47
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.97	0.46
1:B:287:VAL:O	1:B:287:VAL:HG23	2.14	0.46
1:C:314:TRP:CZ3	2:A:194:GLN:HB3	2.50	0.46
2:A:718:LEU:HD13	2:A:814:LYS:HG2	1.96	0.46
1:B:110:PHE:CZ	1:B:250:ILE:HG23	2.50	0.46
1:B:162:GLN:HG2	1:B:185:LEU:HD21	1.97	0.46
2:A:361:ARG:HG3	2:A:362:SER:N	2.30	0.46
2:A:812:MET:CG	2:A:812:MET:O	2.63	0.46
2:A:773:PRO:HG2	2:A:776:TRP:NE1	2.31	0.46
2:A:305:LYS:O	2:A:309:GLU:HG2	2.15	0.46
1:B:201:THR:HG23	1:B:203:LYS:N	2.29	0.46
2:A:157:ARG:HH12	2:A:613:GLU:CG	2.29	0.46
2:A:199:TYR:HD2	2:A:199:TYR:N	2.14	0.46
2:A:399:ALA:O	2:A:403:MET:HG2	2.16	0.46
2:A:356:PHE:HD1	2:A:986:MET:HG2	1.79	0.46
1:B:99:VAL:HG12	1:B:327:ILE:CG2	2.45	0.46
2:A:988:VAL:O	2:A:988:VAL:HG12	2.16	0.46
2:A:991:ILE:O	2:A:995:LEU:HD13	2.15	0.46
2:A:460:SER:CA	2:A:882:ILE:CD1	2.94	0.46
2:A:931:ILE:CD1	2:A:931:ILE:H	2.28	0.46
2:A:143:ALA:HB1	2:A:284:VAL:HG21	1.97	0.46
2:A:940:PHE:HE1	2:A:1027:SER:HB3	1.80	0.46
2:A:199:TYR:CD2	2:A:199:TYR:N	2.83	0.46
2:A:386:LEU:O	2:A:387:ASN:CB	2.62	0.46
2:A:21:LEU:O	2:A:25:ILE:HG12	2.16	0.46
2:A:599:VAL:O	2:A:602:VAL:HG12	2.15	0.46
2:A:944:MET:O	2:A:948:LEU:HD13	2.16	0.46
1:C:371:LEU:N	1:C:371:LEU:HD12	2.30	0.46
2:A:379:ILE:HG23	2:A:380:VAL:N	2.31	0.46
2:A:771:ARG:HH21	2:A:777:ARG:CZ	2.28	0.46
1:C:360:ALA:HB3	2:A:781:GLN:NE2	2.31	0.46
1:C:258:VAL:HG11	1:C:283:LEU:HD23	1.97	0.46
2:A:83:ARG:CB	2:A:94:TYR:HB2	2.46	0.46
2:A:324:THR:HG21	2:A:606:PHE:CD1	2.51	0.46
1:C:332:LEU:HD11	1:C:357:VAL:HG22	1.98	0.46
2:A:396:ILE:HA	2:A:399:ALA:HB3	1.98	0.46
2:A:193:PRO:HG3	2:A:772:TYR:CE2	2.50	0.45
2:A:223:GLU:O	2:A:224:LEU:HD23	2.17	0.45
2:A:144:LEU:N	2:A:144:LEU:HD12	2.31	0.45
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:571:LEU:C	2:A:571:LEU:HD23	2.37	0.45
2:A:944:MET:HE2	2:A:1032:PRO:HG3	1.97	0.45
1:B:367:LEU:HD22	1:B:371:LEU:HD13	1.98	0.45
1:C:174:THR:HB	1:C:177:GLN:CG	2.47	0.45
1:B:201:THR:C	1:B:203:LYS:H	2.19	0.45
1:C:182:LEU:HD12	1:C:182:LEU:HA	1.83	0.45
2:A:492:LEU:O	2:A:495:VAL:HG22	2.17	0.45
1:C:284:LEU:HD11	1:C:297:ARG:NH1	2.31	0.45
2:A:331:ILE:HG23	2:A:332:ASP:N	2.31	0.45
2:A:753:GLY:O	2:A:769:ASN:HB2	2.16	0.45
1:B:371:LEU:HD12	1:B:371:LEU:N	2.32	0.45
2:A:450:LEU:O	2:A:453:SER:HB3	2.15	0.45
2:A:683:ILE:O	2:A:823:TRP:HA	2.17	0.45
1:B:339:GLN:HB3	1:B:339:GLN:HE21	1.58	0.45
2:A:8:ARG:N	2:A:8:ARG:HD3	2.32	0.45
2:A:64:GLN:OE1	2:A:64:GLN:HA	2.16	0.45
2:A:930:PHE:CD2	2:A:1015:PRO:CB	2.95	0.45
2:A:968:LYS:N	2:A:968:LYS:HD2	2.26	0.45
1:B:384:LEU:HD12	1:B:384:LEU:N	2.31	0.45
1:C:254:ILE:CG2	1:C:257:LEU:HD12	2.46	0.45
1:B:268:VAL:HG21	1:B:307:LEU:HD13	1.97	0.45
2:A:563:PRO:HG2	2:A:1008:VAL:HA	1.98	0.45
2:A:450:LEU:HD23	2:A:453:SER:HB3	1.97	0.45
2:A:533:LEU:HD22	2:A:973:LEU:HD23	1.98	0.45
2:A:893:ARG:HD3	2:A:894:VAL:H	1.82	0.45
2:A:580:ILE:HD11	2:A:584:GLU:HG3	1.98	0.45
2:A:526:HIS:NE2	2:A:978:VAL:HG22	2.31	0.45
1:C:165:TYR:CE2	1:C:182:LEU:HD13	2.52	0.45
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.98	0.45
1:B:230:ALA:H	1:B:233:ASN:ND2	2.14	0.45
2:A:1030:ILE:HD12	2:A:1030:ILE:N	2.32	0.45
2:A:550:VAL:CG1	2:A:909:VAL:HG13	2.40	0.45
2:A:589:LEU:HG	2:A:624:VAL:HG21	1.97	0.45
2:A:380:VAL:HB	2:A:484:TYR:CE1	2.52	0.45
2:A:355:LEU:HD12	2:A:356:PHE:CE2	2.52	0.45
2:A:1042:ARG:HD2	2:A:1042:ARG:N	2.32	0.45
2:A:834:VAL:HG13	2:A:838:HIS:HD2	1.82	0.45
2:A:693:ILE:HG23	2:A:694:ASP:H	1.81	0.45
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.98	0.45
2:A:85:PHE:HD2	2:A:94:TYR:HE1	1.64	0.45
2:A:191:ILE:N	2:A:191:ILE:HD12	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:58:PRO:O	2:A:61:VAL:HB	2.17	0.45
1:B:177:GLN:O	1:B:181:ILE:HG22	2.17	0.45
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.98	0.45
2:A:236:TYR:CZ	2:A:760:VAL:HG11	2.52	0.45
2:A:48:ILE:N	2:A:48:ILE:HD13	2.28	0.44
2:A:557:VAL:HG23	2:A:922:LEU:HG	1.98	0.44
2:A:471:GLU:HA	2:A:474:LEU:HB3	1.99	0.44
2:A:325:TYR:HA	2:A:629:GLN:NE2	2.32	0.44
1:B:135:VAL:HG12	1:B:225:ALA:HB2	1.99	0.44
2:A:135:GLY:CA	2:A:673:LEU:HD21	2.35	0.44
2:A:816:GLU:O	2:A:817:ASN:HB2	2.18	0.44
2:A:279:ASN:HA	2:A:605:VAL:CG2	2.44	0.44
2:A:561:PHE:HB2	2:A:865:LEU:HG	1.99	0.44
1:C:128:ALA:HB3	1:C:155:ILE:HG21	2.00	0.44
2:A:391:MET:HA	2:A:391:MET:CE	2.47	0.44
1:B:91:ASN:O	2:A:147:ARG:HG2	2.17	0.44
1:B:246:VAL:HG13	1:B:298:LEU:HB2	1.99	0.44
2:A:365:VAL:HA	2:A:500:LEU:HD22	1.98	0.44
2:A:193:PRO:HG3	2:A:772:TYR:CD2	2.52	0.44
1:C:276:LEU:CD1	1:C:307:LEU:HD21	2.47	0.44
2:A:92:TYR:HD1	2:A:618:SER:HG	1.65	0.44
2:A:879:THR:CG2	2:A:880:LEU:N	2.80	0.44
2:A:296:ASN:HD22	2:A:299:GLU:HB2	1.82	0.44
2:A:495:VAL:O	2:A:499:ILE:HD13	2.18	0.44
2:A:346:PHE:CZ	2:A:367:ILE:HG23	2.52	0.44
2:A:933:LEU:HD23	2:A:933:LEU:HA	1.77	0.44
2:A:499:ILE:HG22	2:A:500:LEU:HD12	1.98	0.44
1:B:250:ILE:HD13	1:B:258:VAL:HG11	2.00	0.44
2:A:893:ARG:NH2	2:A:1042:ARG:HE	2.15	0.44
2:A:728:ILE:HA	2:A:802:ALA:CB	2.46	0.44
1:B:382:LEU:HD23	2:A:269:PRO:HD3	2.00	0.44
1:C:156:PRO:O	1:C:159:VAL:HG22	2.17	0.44
2:A:340:GLY:O	2:A:344:GLU:HG3	2.17	0.44
2:A:883:ILE:HG22	2:A:884:PHE:N	2.33	0.44
2:A:376:ILE:HD11	2:A:492:LEU:HG	2.00	0.44
2:A:157:ARG:HG2	2:A:182:GLY:HA3	1.99	0.44
1:B:114:VAL:HG23	1:B:309:PRO:HA	2.00	0.44
2:A:572:TYR:HD2	2:A:573:MET:N	2.16	0.44
2:A:381:MET:HG2	2:A:484:TYR:HE2	1.83	0.44
2:A:771:ARG:HG3	2:A:772:TYR:O	2.17	0.44
1:B:266:LEU:HD12	1:B:267:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:LEU:HB3	2:A:470:GLN:CG	2.48	0.44
2:A:4:TRP:HB3	2:A:5:ILE:H	1.61	0.44
1:B:82:VAL:HG13	1:B:82:VAL:O	2.17	0.44
1:B:192:GLU:O	1:B:196:ARG:HG3	2.18	0.44
2:A:109:ARG:HD3	2:A:109:ARG:HA	1.85	0.44
2:A:237:LEU:HD22	2:A:242:ASP:HB3	2.00	0.44
2:A:610:GLY:HA2	2:A:619:ALA:O	2.18	0.44
1:B:143:LYS:HG3	1:B:216:GLY:O	2.18	0.44
2:A:995:LEU:O	2:A:998:ILE:HD11	2.18	0.43
1:B:384:LEU:HD23	1:B:391:ILE:HA	1.99	0.43
2:A:156:LEU:HA	2:A:159:LEU:HB3	2.00	0.43
1:B:136:TYR:HA	1:B:137:PRO:HD3	1.85	0.43
2:A:924:VAL:O	2:A:928:THR:HG22	2.18	0.43
2:A:400:VAL:O	2:A:403:MET:HB2	2.18	0.43
2:A:80:LYS:HB3	2:A:96:ILE:HG23	2.00	0.43
2:A:1039:TRP:O	2:A:1039:TRP:HE3	2.01	0.43
1:C:359:GLN:HG3	1:C:360:ALA:N	2.33	0.43
1:B:384:LEU:CD2	1:B:391:ILE:HD13	2.48	0.43
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.18	0.43
2:A:1026:LEU:HG	2:A:1030:ILE:HD13	2.00	0.43
2:A:172:PRO:O	2:A:173:ASP:HB2	2.19	0.43
1:C:326:LEU:N	1:C:326:LEU:HD23	2.34	0.43
1:B:316:GLN:HG2	1:B:317:LEU:N	2.34	0.43
2:A:455:LEU:O	2:A:455:LEU:HD13	2.18	0.43
2:A:464:ILE:O	2:A:467:LEU:HD23	2.19	0.43
2:A:53:TYR:CG	2:A:54:PRO:HD2	2.54	0.43
2:A:137:GLY:O	2:A:139:ILE:HG12	2.19	0.43
1:C:317:LEU:C	1:C:317:LEU:HD12	2.39	0.43
2:A:624:VAL:HG22	2:A:626:THR:HG23	2.01	0.43
1:C:219:THR:HB	1:C:237:LYS:HE2	2.00	0.43
2:A:771:ARG:HD2	2:A:777:ARG:CZ	2.48	0.43
1:C:325:LEU:HD12	1:C:325:LEU:H	1.83	0.43
1:C:223:LEU:HD23	1:C:233:ASN:HB3	2.00	0.43
2:A:497:ILE:O	2:A:501:MET:HG2	2.19	0.43
2:A:760:VAL:O	2:A:760:VAL:HG13	2.18	0.43
1:C:84:ILE:HD13	2:A:656:PRO:HB3	2.00	0.43
2:A:474:LEU:C	2:A:477:PRO:HD2	2.39	0.43
2:A:408:ILE:CA	2:A:411:ILE:HG22	2.44	0.43
2:A:521:LEU:HG	2:A:522:ILE:N	2.33	0.43
2:A:567:GLU:C	2:A:569:ASP:H	2.22	0.43
2:A:240:LEU:HA	2:A:240:LEU:HD23	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:995:LEU:HD22	2:A:1020:MET:CE	2.49	0.43
2:A:552:TRP:HB3	2:A:553:PRO:HD3	2.00	0.43
2:A:938:ALA:O	2:A:942:VAL:HG23	2.18	0.43
2:A:728:ILE:HD13	2:A:743:VAL:HG13	2.01	0.43
1:C:211:LYS:O	1:C:213:PRO:HD3	2.19	0.43
2:A:671:ASP:OD2	2:A:678:LYS:HD3	2.19	0.42
1:B:287:VAL:HG12	1:B:294:LEU:CB	2.47	0.42
2:A:891:PHE:O	2:A:892:ARG:HB2	2.18	0.42
1:B:84:ILE:HD11	2:A:594:LYS:HB3	2.01	0.42
2:A:454:LEU:HD23	2:A:939:GLU:OE2	2.18	0.42
2:A:59:GLN:HE21	2:A:63:ASN:HD21	1.66	0.42
1:C:329:SER:HA	1:C:365:THR:HG22	2.00	0.42
1:B:254:ILE:O	1:B:254:ILE:HG23	2.19	0.42
1:C:167:LEU:HD23	1:C:167:LEU:O	2.19	0.42
1:C:143:LYS:HE3	1:C:305:GLU:OE1	2.19	0.42
2:A:704:ALA:O	2:A:710:VAL:HG11	2.19	0.42
2:A:879:THR:O	2:A:883:ILE:HB	2.19	0.42
1:C:271:ARG:NE	1:C:306:ALA:HB1	2.34	0.42
1:C:104:LEU:HD23	1:C:105:THR:N	2.34	0.42
1:B:276:LEU:HD22	1:B:276:LEU:H	1.85	0.42
2:A:942:VAL:O	2:A:946:MET:HG2	2.19	0.42
2:A:272:ARG:HD2	2:A:275:ILE:CD1	2.49	0.42
2:A:694:ASP:CG	2:A:718:LEU:H	2.23	0.42
1:C:92:LEU:HA	2:A:591:LYS:HE2	2.01	0.42
1:B:145:GLN:HA	1:B:215:ASP:HB3	2.01	0.42
1:C:96:THR:OG1	1:C:376:LYS:HG2	2.18	0.42
2:A:545:LEU:O	2:A:548:LEU:CD2	2.67	0.42
1:C:169:ARG:HE	1:C:202:GLN:NE2	2.15	0.42
2:A:746:PHE:HA	2:A:750:ALA:HB3	2.00	0.42
2:A:337:ASN:O	2:A:341:LYS:HG2	2.19	0.42
2:A:906:PHE:O	2:A:909:VAL:HB	2.20	0.42
1:B:110:PHE:CD2	1:B:250:ILE:HG12	2.54	0.42
2:A:74:LEU:HD11	2:A:82:VAL:HG21	2.00	0.42
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.54	0.42
2:A:998:ILE:HG12	2:A:999:LEU:N	2.34	0.42
2:A:571:LEU:HD13	2:A:668:ASN:ND2	2.34	0.42
2:A:891:PHE:CZ	2:A:945:LEU:HB3	2.54	0.42
1:C:144:VAL:HG21	1:C:238:ILE:HD13	2.01	0.42
1:B:386:ASP:O	1:B:387:SER:C	2.57	0.42
2:A:346:PHE:HE2	2:A:367:ILE:HG23	1.81	0.42
2:A:790:THR:HG21	2:A:794:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:LEU:HB3	2:A:470:GLN:HG2	2.01	0.42
2:A:134:THR:HG23	2:A:136:VAL:H	1.85	0.42
2:A:912:ILE:CD1	2:A:930:PHE:CE1	3.02	0.42
2:A:301:ILE:O	2:A:304:VAL:HB	2.19	0.42
2:A:684:LYS:O	2:A:685:VAL:HG13	2.19	0.42
1:C:92:LEU:O	2:A:591:LYS:HE2	2.19	0.42
2:A:467:LEU:HD12	2:A:471:GLU:CG	2.49	0.42
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.78	0.42
2:A:27:GLY:HA3	2:A:375:CYS:SG	2.59	0.42
1:C:264:PHE:HE1	1:C:281:TRP:CE2	2.38	0.42
1:B:187:LEU:CD1	1:C:159:VAL:HG11	2.49	0.42
2:A:86:SER:HB2	2:A:813:LEU:HB2	2.01	0.42
2:A:517:LEU:N	2:A:517:LEU:HD12	2.35	0.42
1:B:321:SER:O	1:B:323:PRO:HD3	2.20	0.42
2:A:376:ILE:HG22	2:A:376:ILE:O	2.19	0.42
2:A:403:MET:SD	2:A:485:ALA:HB1	2.60	0.42
2:A:490:ALA:HA	2:A:494:ILE:HD13	2.01	0.42
1:C:292:ARG:HD3	1:C:292:ARG:HA	1.91	0.42
2:A:980:ARG:HH12	2:A:1032:PRO:CG	2.33	0.42
1:B:391:ILE:O	1:B:395:LEU:HG	2.19	0.42
1:C:264:PHE:CD2	1:C:317:LEU:HB3	2.54	0.42
1:B:201:THR:O	1:B:202:GLN:HB2	2.19	0.42
1:C:201:THR:HG23	1:C:201:THR:O	2.19	0.42
2:A:143:ALA:HB1	2:A:284:VAL:CG2	2.50	0.41
2:A:57:ALA:O	2:A:61:VAL:HG23	2.20	0.41
1:C:195:ILE:O	1:C:198:LEU:HB3	2.20	0.41
2:A:528:LEU:O	2:A:528:LEU:HD23	2.19	0.41
2:A:578:PRO:HB2	2:A:579:GLY:H	1.63	0.41
1:C:162:GLN:NE2	1:C:205:GLN:HB2	2.35	0.41
2:A:47:VAL:CG1	2:A:95:VAL:HB	2.49	0.41
2:A:83:ARG:HH22	2:A:676:GLY:CA	2.33	0.41
2:A:1041:HIS:HB3	2:A:1042:ARG:HH11	1.84	0.41
1:B:264:PHE:CD1	1:B:315:LEU:HD21	2.55	0.41
2:A:237:LEU:C	2:A:238:GLN:HG2	2.40	0.41
2:A:947:TYR:CD2	2:A:979:LEU:HD23	2.55	0.41
2:A:668:ASN:CA	2:A:678:LYS:CG	2.88	0.41
2:A:376:ILE:CD1	2:A:492:LEU:HG	2.51	0.41
1:C:153:LEU:CD2	1:C:153:LEU:H	2.34	0.41
2:A:379:ILE:C	2:A:379:ILE:HD13	2.41	0.41
1:C:392:SER:C	1:C:394:ALA:H	2.24	0.41
2:A:779:SER:OG	2:A:781:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:637:ARG:HB2	2:A:640:MET:HG3	2.02	0.41
2:A:992:ILE:HG12	2:A:1020:MET:SD	2.61	0.41
2:A:596:ILE:HG12	2:A:653:VAL:HG21	2.03	0.41
2:A:175:ALA:HB2	2:A:292:ARG:HB2	2.01	0.41
2:A:114:LEU:HD11	2:A:127:ALA:CB	2.48	0.41
1:B:198:LEU:HD13	1:B:205:GLN:HG2	2.01	0.41
2:A:746:PHE:CD2	2:A:788:ILE:HG13	2.56	0.41
2:A:686:SER:O	2:A:854:THR:HA	2.21	0.41
2:A:550:VAL:O	2:A:553:PRO:HD2	2.20	0.41
2:A:572:TYR:CE1	2:A:653:VAL:HG11	2.52	0.41
1:B:355:VAL:CG2	1:B:367:LEU:HD23	2.48	0.41
1:C:317:LEU:O	1:C:317:LEU:HD12	2.20	0.41
1:C:201:THR:CG2	1:C:201:THR:O	2.68	0.41
1:C:170:GLU:HG3	1:C:171:THR:HG23	2.03	0.41
2:A:784:ARG:HD3	2:A:804:ILE:CG1	2.50	0.41
1:B:391:ILE:HG12	2:A:774:GLN:HE22	1.85	0.41
2:A:142:TYR:HE1	2:A:144:LEU:HD11	1.85	0.41
2:A:559:GLY:HA2	2:A:922:LEU:N	2.36	0.41
2:A:461:PHE:CZ	2:A:464:ILE:HD12	2.56	0.41
1:C:378:VAL:HG13	1:C:382:LEU:HG	2.03	0.41
2:A:105:TRP:C	2:A:105:TRP:CD1	2.93	0.41
2:A:1039:TRP:C	2:A:1041:HIS:H	2.24	0.41
2:A:377:ALA:O	2:A:381:MET:HG3	2.20	0.41
1:C:138:LEU:HD23	1:C:218:ILE:CD1	2.49	0.41
1:B:264:PHE:HE1	1:B:296:LEU:CD1	2.33	0.41
2:A:386:LEU:HD12	2:A:388:ALA:H	1.84	0.41
2:A:244:ASN:HB3	2:A:260:ARG:HB3	2.03	0.41
2:A:25:ILE:O	2:A:29:TRP:HB2	2.21	0.41
2:A:834:VAL:HA	2:A:837:VAL:HG22	2.02	0.41
2:A:131:PRO:C	2:A:133:ALA:N	2.74	0.41
2:A:814:LYS:HB3	2:A:814:LYS:NZ	2.36	0.41
2:A:296:ASN:ND2	2:A:299:GLU:HB2	2.36	0.41
1:C:151:LEU:N	1:C:151:LEU:HD12	2.36	0.41
2:A:940:PHE:O	2:A:944:MET:HG2	2.21	0.40
2:A:80:LYS:HE3	2:A:98:GLU:HB3	2.02	0.40
1:B:168:LEU:HD12	1:B:181:ILE:HG21	2.02	0.40
2:A:878:MET:O	2:A:882:ILE:HG22	2.21	0.40
2:A:480:PHE:CD1	2:A:480:PHE:C	2.94	0.40
1:C:104:LEU:HD12	1:C:366:ALA:CB	2.51	0.40
1:C:361:SER:O	1:C:362:GLN:HB3	2.21	0.40
2:A:214:ASN:O	2:A:215:GLN:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LEU:N	1:B:276:LEU:HD22	2.36	0.40
2:A:27:GLY:HA2	2:A:30:THR:OG1	2.20	0.40
1:B:115:SER:HA	1:B:309:PRO:HB3	2.02	0.40
1:B:258:VAL:O	1:B:259:LYS:C	2.60	0.40
2:A:137:GLY:HA3	2:A:290:ILE:HG23	2.02	0.40
2:A:891:PHE:CZ	2:A:942:VAL:HG13	2.56	0.40
1:B:155:ILE:HB	1:B:208:PHE:CE2	2.57	0.40
2:A:53:TYR:CD1	2:A:54:PRO:HD2	2.57	0.40
1:C:95:LYS:N	1:C:380:SER:HB3	2.25	0.40
1:C:268:VAL:HG21	1:C:311:MET:CE	2.52	0.40
2:A:189:VAL:HG22	2:A:769:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/336 (95%)	263 (82%)	49 (15%)	8 (2%)	7	48
1	C	320/336 (95%)	274 (86%)	39 (12%)	7 (2%)	8	50
2	A	1024/1054 (97%)	883 (86%)	116 (11%)	25 (2%)	7	49
All	All	1664/1726 (96%)	1420 (85%)	204 (12%)	40 (2%)	7	49

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	ASP
1	C	243	PRO
2	A	54	PRO
2	A	138	TRP
2	A	387	ASN
2	A	389	ASN

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Mol	Chain	Res	Type
2	A	578	PRO
1	C	221	PHE
2	A	181	GLY
2	A	235	GLY
2	A	388	ALA
2	A	447	GLY
2	A	955	VAL
2	A	958	LEU
1	B	173	GLY
1	B	241	MET
1	B	288	ASP
1	B	348	GLY
2	A	312	LYS
2	A	636	TRP
2	A	75	SER
2	A	215	GLN
2	A	677	ILE
2	A	760	VAL
1	B	137	PRO
1	C	94	VAL
1	C	173	GLY
1	C	255	ALA
1	C	337	SER
2	A	470	GLN
2	A	484	TYR
2	A	574	PRO
2	A	680	PRO
2	A	558	GLY
1	B	323	PRO
2	A	5	ILE
2	A	1017	ILE
1	C	172	GLY
1	B	93	GLY
2	A	653	VAL

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	B	263/275 (96%)	241 (92%)	22 (8%)	14	51
1	C	263/275 (96%)	235 (89%)	28 (11%)	8	39
2	A	847/871 (97%)	754 (89%)	93 (11%)	8	38
All	All	1373/1421 (97%)	1230 (90%)	143 (10%)	9	40

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	LEU
1	B	113	ASN
1	B	138	LEU
1	B	146	LYS
1	B	151	LEU
1	B	153	LEU
1	B	174	THR
1	B	221	PHE
1	B	227	MET
1	B	235	VAL
1	B	254	ILE
1	B	267	THR
1	B	294	LEU
1	B	301	ASP
1	B	302	ASN
1	B	318	ASN
1	B	327	ILE
1	B	339	GLN
1	B	342	ILE
1	B	385	ILE
1	B	388	GLU
1	B	390	ASN
1	C	82	VAL
1	C	108	GLN
1	C	121	TYR
1	C	145	GLN
1	C	150	LEU
1	C	153	LEU
1	C	162	GLN
1	C	178	THR
1	C	199	ILE
1	C	204	ILE
1	C	214	ILE
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	246	VAL
1	C	263	GLN
1	C	266	LEU
1	C	283	LEU
1	C	292	ARG
1	C	294	LEU
1	C	326	LEU
1	C	327	ILE
1	C	330	GLN
1	C	339	GLN
1	C	344	VAL
1	C	347	ASP
1	C	354	ARG
1	C	355	VAL
1	C	357	VAL
1	C	362	GLN
2	A	4	TRP
2	A	6	ILE
2	A	8	ARG
2	A	21	LEU
2	A	22	PHE
2	A	48	ILE
2	A	49	ILE
2	A	51	THR
2	A	65	VAL
2	A	67	TYR
2	A	76	VAL
2	A	82	VAL
2	A	96	ILE
2	A	105	TRP
2	A	109	ARG
2	A	112	GLU
2	A	117	VAL
2	A	129	LEU
2	A	138	TRP
2	A	157	ARG
2	A	160	GLN
2	A	205	GLU
2	A	232	ARG
2	A	238	GLN
2	A	253	ASN
2	A	267	ILE

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Mol	Chain	Res	Type
2	A	271	MET
2	A	281	GLU
2	A	298	ARG
2	A	338	LEU
2	A	343	LEU
2	A	358	TRP
2	A	359	HIS
2	A	361	ARG
2	A	379	ILE
2	A	390	ILE
2	A	408	ILE
2	A	410	MET
2	A	412	GLU
2	A	450	LEU
2	A	457	ILE
2	A	521	LEU
2	A	532	VAL
2	A	545	LEU
2	A	546	SER
2	A	548	LEU
2	A	549	THR
2	A	569	ASP
2	A	572	TYR
2	A	605	VAL
2	A	608	LYS
2	A	624	VAL
2	A	630	LEU
2	A	660	ASN
2	A	663	VAL
2	A	666	ILE
2	A	670	ILE
2	A	673	LEU
2	A	675	THR
2	A	677	ILE
2	A	678	LYS
2	A	685	VAL
2	A	710	VAL
2	A	727	GLU
2	A	729	ASN
2	A	769	ASN
2	A	781	GLN
2	A	785	GLN

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Mol	Chain	Res	Type
2	A	795	GLN
2	A	814	LYS
2	A	823	TRP
2	A	829	ARG
2	A	849	GLN
2	A	873	LYS
2	A	874	LEU
2	A	880	LEU
2	A	881	MET
2	A	882	ILE
2	A	883	ILE
2	A	909	VAL
2	A	921	HIS
2	A	928	THR
2	A	931	ILE
2	A	933	LEU
2	A	945	LEU
2	A	955	VAL
2	A	975	HIS
2	A	984	LYS
2	A	996	LEU
2	A	998	ILE
2	A	1000	TRP
2	A	1016	MET
2	A	1039	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	120	GLN
1	B	125	GLN
1	B	205	GLN
1	B	233	ASN
1	B	239	GLN
1	B	330	GLN
1	B	339	GLN
1	C	145	GLN
1	C	162	GLN
1	C	202	GLN
1	C	228	ASN
1	C	233	ASN

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Mol	Chain	Res	Type
1	C	263	GLN
1	C	316	GLN
1	C	362	GLN
2	A	63	ASN
2	A	194	GLN
2	A	215	GLN
2	A	337	ASN
2	A	555	ASN
2	A	564	GLN
2	A	629	GLN
2	A	635	GLN
2	A	660	ASN
2	A	668	ASN
2	A	699	GLN
2	A	725	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	950	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	B	322/336 (95%)	0.33	4 (1%) 81 72	40, 90, 163, 246	0
1	C	322/336 (95%)	0.25	3 (0%) 85 79	37, 88, 148, 212	0
2	A	1028/1054 (97%)	0.86	151 (14%) 3 3	39, 154, 305, 551	0
All	All	1672/1726 (96%)	0.64	158 (9%) 11 7	37, 115, 275, 551	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	954	ALA	8.8
2	A	955	VAL	8.6
2	A	871	LYS	6.8
2	A	392	SER	6.6
2	A	872	LEU	6.5
2	A	815	THR	6.5
2	A	448	PRO	6.2
2	A	873	LYS	5.7
2	A	503	TYR	5.6
2	A	956	PRO	5.6
2	A	868	ALA	5.3
2	A	418	LEU	5.1
2	A	473	ARG	5.0
2	A	951	ALA	4.9
2	A	450	LEU	4.9
2	A	712	SER	4.8
2	A	63	ASN	4.7
2	A	891	PHE	4.7
2	A	713	ALA	4.7
2	A	519	ARG	4.7
2	A	918	MET	4.7
2	A	709	GLY	4.6
2	A	520	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	A	504	TRP	4.5
2	A	814	LYS	4.4
2	A	517	LEU	4.3
2	A	400	VAL	4.1
2	A	890	ALA	4.1
2	A	493	ALA	4.1
2	A	846	GLU	4.0
2	A	441	ASP	4.0
2	A	415	HIS	4.0
2	A	959	ASN	3.9
2	A	938	ALA	3.9
2	A	434	THR	3.9
2	A	711	ALA	3.8
2	A	427	ASP	3.8
2	A	497	ILE	3.8
2	A	867	ARG	3.8
2	A	704	ALA	3.7
2	A	947	TYR	3.7
2	A	639	GLY	3.6
2	A	979	LEU	3.6
1	B	400	SER	3.6
2	A	539	THR	3.5
2	A	45	VAL	3.5
2	A	437	GLN	3.5
2	A	688	THR	3.4
1	B	79	ALA	3.4
2	A	501	MET	3.4
1	B	325	LEU	3.4
2	A	396	ILE	3.3
2	A	678	LYS	3.3
2	A	464	ILE	3.3
2	A	613	GLU	3.3
2	A	953	GLU	3.2
2	A	869	ASN	3.2
2	A	38	ALA	3.2
2	A	420	GLU	3.2
2	A	1043	HIS	3.2
2	A	496	VAL	3.1
2	A	283	GLU	3.1
2	A	946	MET	3.1
2	A	449	ALA	3.1
2	A	279	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	677	ILE	3.1
2	A	828	ALA	3.1
2	A	909	VAL	3.0
2	A	399	ALA	3.0
2	A	387	ASN	3.0
2	A	1001	GLY	3.0
2	A	908	LEU	3.0
2	A	853	GLY	2.9
2	A	416	LYS	2.9
2	A	1009	MET	2.9
2	A	381	MET	2.9
2	A	378	PHE	2.9
2	A	393	LEU	2.9
2	A	447	GLY	2.8
2	A	388	ALA	2.8
2	A	438	VAL	2.8
2	A	461	PHE	2.8
2	A	715	ALA	2.8
2	A	404	VAL	2.8
2	A	705	ARG	2.7
2	A	958	LEU	2.7
2	A	124	GLY	2.7
2	A	1039	TRP	2.7
2	A	460	SER	2.7
2	A	895	GLY	2.7
2	A	1035	TYR	2.7
2	A	830	ASP	2.7
2	A	531	LYS	2.6
2	A	183	VAL	2.6
2	A	31	ILE	2.6
2	A	917	TRP	2.6
2	A	426	PRO	2.6
2	A	40	PRO	2.6
2	A	445	GLU	2.5
2	A	714	LEU	2.5
2	A	35	PRO	2.5
2	A	73	MET	2.5
2	A	436	TRP	2.5
2	A	46	GLN	2.5
2	A	36	VAL	2.4
2	A	285	ALA	2.4
2	A	848	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	906	PHE	2.4
2	A	561	PHE	2.4
2	A	97	PHE	2.4
2	A	439	ILE	2.4
2	A	833	MET	2.4
2	A	564	GLN	2.4
2	A	99	ASP	2.4
2	A	717	ARG	2.3
2	A	998	ILE	2.3
2	A	920	PHE	2.3
2	A	588	MET	2.3
2	A	969	LEU	2.3
2	A	485	ALA	2.3
2	A	939	GLU	2.3
1	B	333	ILE	2.3
2	A	524	VAL	2.3
2	A	406	ALA	2.3
2	A	699	GLN	2.2
2	A	785	GLN	2.2
1	C	252	GLU	2.2
2	A	273	ARG	2.2
2	A	849	GLN	2.2
2	A	578	PRO	2.2
2	A	1041	HIS	2.2
2	A	854	THR	2.2
2	A	1038	MET	2.2
2	A	405	ASP	2.2
2	A	502	GLY	2.2
2	A	950	HIS	2.2
2	A	521	LEU	2.1
2	A	698	GLU	2.1
1	C	344	VAL	2.1
2	A	81	THR	2.1
2	A	444	VAL	2.1
2	A	67	TYR	2.1
2	A	995	LEU	2.1
2	A	618	SER	2.1
2	A	703	VAL	2.1
2	A	87	GLN	2.1
2	A	433	LYS	2.1
2	A	875	MET	2.1
2	A	499	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	376	LYS	2.1
2	A	482	LYS	2.1
2	A	894	VAL	2.0
2	A	94	TYR	2.0
2	A	425	HIS	2.0
2	A	80	LYS	2.0
2	A	886	LEU	2.0
2	A	887	LEU	2.0
2	A	56	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CU	A	1049	1/1	0.91	0.13	-2.99	150,150,150,150	0
3	CU	A	1048	1/1	0.91	0.19	-	159,159,159,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.