



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3T53
Title : Crystal structures of the extrusion state of the CusBA adaptor-transporter complex
Authors : Su, C.-C.; Long, F.; Yu, E.W.
Deposited on : 2011-07-26
Resolution : 3.37 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

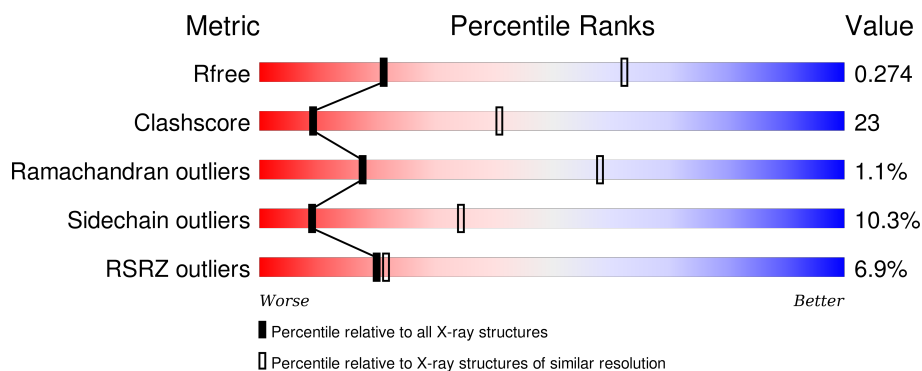
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.37 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

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>11%</div> <div>56% 36% . .</div> </div>
1	C	336	<div> <div>57% 35% . .</div> </div>
2	A	1054	<div> <div>11%</div> <div>51% 41% 5% .</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12876 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	324	Total	C	N	O	S	0	0	0
			2473	1563	430	474	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	1	Total Cu 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0
4	A	7	Total O 7 7	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.79 Å 159.79 Å 683.04 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.12 – 3.37 49.12 – 3.37	Depositor EDS
% Data completeness (in resolution range)	87.7 (49.12-3.37) 99.4 (49.12-3.37)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.248 , 0.286 0.241 , 0.274	Depositor DCC
R_{free} test set	2414 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 47756 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

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	B	0.22	0/2498	0.42	0/3401
1	C	0.22	0/2513	0.42	0/3421
2	A	0.21	0/8089	0.40	0/11015
All	All	0.21	0/13100	0.41	0/17837

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

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	118	0
1	C	2473	0	2533	103	0
2	A	7923	0	8166	408	0
3	A	1	0	0	0	0
4	A	7	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	0	0
All	All	12876	0	13221	600	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 23.

All (600) 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:C:256:TRP:CZ3	1:C:257:LEU:HD12	1.45	1.48
2:A:661:LEU:HD23	2:A:662:TRP:N	1.45	1.29
1:C:256:TRP:CZ3	1:C:257:LEU:CD1	2.34	1.11
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.17	1.05
1:C:256:TRP:CH2	1:C:257:LEU:CD1	2.44	1.01
2:A:550:VAL:HG13	2:A:913:TRP:CD1	1.96	1.01
2:A:550:VAL:HG13	2:A:913:TRP:HD1	1.24	1.00
2:A:661:LEU:HD23	2:A:661:LEU:C	1.81	0.99
1:C:256:TRP:CH2	1:C:257:LEU:HD12	1.97	0.98
2:A:660:ASN:ND2	2:A:660:ASN:H	1.65	0.94
2:A:48:ILE:HD11	2:A:131:PRO:HD2	1.47	0.94
2:A:661:LEU:C	2:A:661:LEU:CD2	2.35	0.94
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.48	0.93
2:A:550:VAL:HA	2:A:913:TRP:HE1	1.30	0.93
2:A:944:MET:HG2	2:A:980:ARG:HD3	1.52	0.92
2:A:660:ASN:N	2:A:660:ASN:HD22	1.64	0.91
2:A:298:ARG:HE	2:A:328:SER:HB2	1.36	0.90
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.53	0.90
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.55	0.89
2:A:950:HIS:HA	2:A:953:GLU:HG2	1.54	0.88
1:B:174:THR:H	1:B:177:GLN:HE21	1.18	0.87
1:C:181:ILE:HG22	1:C:182:LEU:HD12	1.57	0.86
2:A:660:ASN:H	2:A:660:ASN:HD22	0.89	0.86
2:A:904:VAL:HG23	2:A:905:PRO:HD3	1.59	0.85
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.61	0.83
2:A:961:PRO:HA	2:A:1043:HIS:HE1	1.44	0.83
2:A:661:LEU:CD2	2:A:662:TRP:N	2.37	0.83
2:A:240:LEU:HD21	2:A:267:ILE:HD11	1.58	0.83
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.44	0.82
2:A:661:LEU:HD21	2:A:663:VAL:HG13	1.61	0.81
2:A:365:VAL:HG11	2:A:501:MET:HB3	1.63	0.80
2:A:973:LEU:HD21	2:A:1036:LYS:HB3	1.64	0.79
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.66	0.78
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.65	0.77
2:A:48:ILE:HD13	2:A:48:ILE:H	1.47	0.77
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.65	0.77
1:C:302:ASN:HD21	1:C:307:LEU:H	1.31	0.77
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.67	0.76
1:B:120:GLN:NE2	1:B:243:PRO:HD2	1.98	0.76
2:A:969:LEU:HD21	2:A:1036:LYS:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:891:PHE:HE2	2:A:942:VAL:HG13	1.52	0.75
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.69	0.74
1:B:204:ILE:HD12	1:B:204:ILE:H	1.51	0.74
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.21	0.74
2:A:712:SER:HB3	2:A:827:ASP:HB3	1.69	0.74
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.69	0.74
2:A:980:ARG:NH1	2:A:1028:LEU:HA	2.02	0.74
2:A:940:PHE:HE1	2:A:984:LYS:HG2	1.51	0.74
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.67	0.74
1:B:117:ASN:HD22	1:B:119:TYR:H	1.32	0.73
2:A:51:THR:HG23	2:A:127:ALA:HA	1.70	0.73
1:B:223:LEU:HD12	1:B:235:VAL:HG12	1.71	0.73
2:A:270:GLU:HG2	2:A:271:MET:H	1.54	0.72
2:A:365:VAL:HB	2:A:411:ILE:HD11	1.72	0.72
2:A:532:VAL:HG21	2:A:1029:PHE:HB3	1.72	0.71
1:C:132:ILE:HD11	1:C:229:ILE:HB	1.72	0.71
2:A:400:VAL:HA	2:A:403:MET:HG3	1.74	0.70
2:A:26:TRP:HD1	2:A:379:ILE:HD13	1.57	0.70
2:A:42:LEU:H	2:A:42:LEU:HD12	1.57	0.70
2:A:141:GLU:HG2	2:A:288:VAL:HG12	1.75	0.69
2:A:456:ILE:HG12	2:A:886:LEU:HD13	1.73	0.69
2:A:955:VAL:HG13	2:A:956:PRO:HD3	1.75	0.69
1:B:104:LEU:HD22	1:B:361:SER:HB3	1.75	0.69
2:A:418:LEU:HG	2:A:438:VAL:HG21	1.75	0.69
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.74	0.68
2:A:701:GLU:HG2	2:A:705:ARG:HH22	1.56	0.68
2:A:153:LEU:H	2:A:153:LEU:HD12	1.57	0.68
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.24	0.68
2:A:237:LEU:HG	2:A:243:PHE:CE1	2.29	0.68
2:A:61:VAL:O	2:A:65:VAL:HG12	1.93	0.68
1:B:280:LYS:HA	1:B:280:LYS:HE3	1.76	0.67
2:A:550:VAL:HG12	2:A:909:VAL:HG22	1.76	0.67
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.77	0.67
1:B:93:GLY:HA3	2:A:146:ASP:O	1.94	0.67
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.29	0.66
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.76	0.66
2:A:364:LEU:O	2:A:368:ILE:HG12	1.94	0.66
1:B:117:ASN:ND2	1:B:119:TYR:H	1.93	0.66
2:A:893:ARG:HB3	2:A:896:GLU:HB2	1.78	0.66
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.78	0.65
2:A:466:THR:O	2:A:871:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:O	1:C:256:TRP:N	2.30	0.65
2:A:413:ASN:O	2:A:417:ARG:HB2	1.97	0.65
2:A:1024:PRO:O	2:A:1028:LEU:HG	1.97	0.65
2:A:715:ALA:HB2	2:A:824:ILE:HG12	1.80	0.64
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.78	0.64
2:A:550:VAL:HG11	2:A:909:VAL:HG13	1.78	0.64
1:C:256:TRP:CE3	1:C:257:LEU:HD12	2.25	0.64
1:B:84:ILE:HG12	1:B:85:ASP:N	2.13	0.63
2:A:330:LEU:HD22	2:A:567:GLU:HB3	1.79	0.63
2:A:475:PHE:HZ	2:A:562:LEU:HD21	1.63	0.63
2:A:315:LEU:HD11	2:A:321:ILE:HD11	1.80	0.63
2:A:572:TYR:HE2	2:A:592:THR:HG21	1.64	0.63
1:C:126:ALA:HB2	1:C:229:ILE:HD11	1.80	0.63
2:A:452:ILE:O	2:A:456:ILE:HG13	1.98	0.63
2:A:529:LEU:O	2:A:532:VAL:HG12	1.99	0.62
2:A:38:ALA:HB2	2:A:331:ILE:HD13	1.81	0.62
2:A:685:VAL:HG11	2:A:696:MET:HB3	1.81	0.62
2:A:729:ASN:ND2	2:A:732:LYS:H	1.96	0.62
1:B:114:VAL:HG12	1:B:309:PRO:HA	1.80	0.62
2:A:359:HIS:CD2	2:A:361:ARG:H	2.17	0.62
2:A:961:PRO:HA	2:A:1043:HIS:CE1	2.31	0.62
1:B:335:THR:HG22	1:B:391:ILE:HD12	1.80	0.62
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.82	0.62
2:A:377:ALA:O	2:A:381:MET:HG3	1.99	0.62
1:C:165:TYR:CE2	1:C:182:LEU:HD11	2.35	0.62
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.81	0.62
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.30	0.61
2:A:140:TYR:HE1	2:A:323:THR:HG1	1.46	0.61
2:A:456:ILE:HA	2:A:886:LEU:HD13	1.82	0.61
2:A:525:TYR:HE2	2:A:1029:PHE:HE2	1.48	0.61
1:C:287:VAL:HB	1:C:294:LEU:HD23	1.82	0.61
1:C:126:ALA:HB2	1:C:229:ILE:CD1	2.30	0.61
2:A:877:PRO:O	2:A:881:MET:HG2	2.00	0.61
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.82	0.61
2:A:297:ALA:O	2:A:301:ILE:HG13	2.01	0.61
2:A:243:PHE:HB3	2:A:265:VAL:HG21	1.81	0.61
1:C:388:GLU:HB2	2:A:657:GLY:H	1.66	0.61
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.01	0.60
2:A:999:LEU:HD23	2:A:1017:ILE:HD12	1.82	0.60
1:B:385:ILE:HG22	1:B:389:ALA:HB2	1.83	0.60
2:A:572:TYR:CE2	2:A:592:THR:HG21	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:409:VAL:HG11	2:A:450:LEU:HD21	1.83	0.60
2:A:488:GLY:O	2:A:492:LEU:HB2	2.01	0.60
1:C:80:SER:HA	1:C:397:ARG:HD2	1.83	0.60
2:A:6:ILE:HG21	2:A:444:VAL:HG22	1.82	0.60
2:A:20:ALA:HA	2:A:23:LEU:HB3	1.84	0.60
2:A:122:PRO:O	2:A:125:VAL:HG22	2.02	0.60
2:A:876:VAL:O	2:A:879:THR:HG22	2.02	0.60
2:A:536:PRO:HB2	2:A:1037:LEU:HD12	1.84	0.60
1:B:89:THR:H	2:A:590:GLN:HE22	1.49	0.59
2:A:880:LEU:O	2:A:883:ILE:HG22	2.03	0.59
2:A:861:GLN:HA	2:A:864:LEU:HD12	1.84	0.59
2:A:642:MET:HE3	2:A:642:MET:HA	1.85	0.59
1:B:307:LEU:HD12	1:B:307:LEU:H	1.67	0.59
2:A:270:GLU:HG2	2:A:271:MET:N	2.17	0.59
2:A:141:GLU:HB2	2:A:325:TYR:HB3	1.84	0.59
1:C:359:GLN:HG3	1:C:360:ALA:N	2.18	0.59
2:A:786:LEU:HB3	2:A:798:LEU:HB2	1.84	0.58
1:B:123:ILE:HB	1:C:227:MET:CG	2.33	0.58
2:A:729:ASN:HB3	2:A:732:LYS:HB2	1.85	0.58
1:C:151:LEU:HD11	1:C:210:LEU:HD12	1.85	0.58
1:B:94:VAL:HG12	1:B:96:THR:HG23	1.86	0.58
2:A:980:ARG:HH12	2:A:1028:LEU:HA	1.67	0.58
2:A:883:ILE:O	2:A:887:LEU:HG	2.02	0.58
2:A:440:THR:O	2:A:444:VAL:HG23	2.03	0.58
2:A:458:THR:HB	2:A:483:THR:HG23	1.84	0.58
2:A:661:LEU:HD23	2:A:662:TRP:CA	2.31	0.58
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.86	0.58
2:A:535:TRP:NE1	2:A:537:LYS:HB3	2.18	0.58
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.04	0.57
1:C:317:LEU:C	1:C:317:LEU:HD12	2.24	0.57
1:B:385:ILE:HG13	2:A:272:ARG:HB2	1.86	0.57
1:B:378:VAL:HG21	1:B:383:PHE:CE2	2.38	0.57
2:A:411:ILE:HG23	2:A:415:HIS:CE1	2.40	0.57
2:A:701:GLU:HG2	2:A:705:ARG:NH2	2.19	0.57
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.85	0.57
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.86	0.57
1:C:384:LEU:HD11	2:A:588:MET:HE2	1.85	0.57
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.86	0.57
2:A:402:ALA:HA	2:A:405:ASP:HB3	1.87	0.57
2:A:786:LEU:HD22	2:A:787:PRO:HD2	1.85	0.57
1:B:358:PHE:HE2	1:C:273:ASP:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:475:PHE:CZ	2:A:562:LEU:HD21	2.39	0.56
2:A:365:VAL:HG21	2:A:501:MET:HA	1.87	0.56
1:B:174:THR:H	1:B:177:GLN:NE2	1.95	0.56
2:A:872:LEU:O	2:A:876:VAL:HG23	2.05	0.56
1:B:123:ILE:HB	1:C:227:MET:HG2	1.87	0.56
2:A:399:ALA:HB2	2:A:482:LYS:HG2	1.88	0.56
2:A:384:GLN:HG3	2:A:386:LEU:HD13	1.87	0.56
2:A:550:VAL:HA	2:A:913:TRP:NE1	2.10	0.56
1:B:332:LEU:HA	1:B:341:VAL:HG12	1.86	0.56
1:C:174:THR:HG22	1:C:176:THR:H	1.70	0.56
2:A:574:PRO:HA	2:A:660:ASN:HA	1.88	0.56
2:A:660:ASN:ND2	2:A:660:ASN:N	2.30	0.56
2:A:522:ILE:O	2:A:526:HIS:HD2	1.87	0.56
1:B:386:ASP:HB2	2:A:269:PRO:O	2.05	0.56
2:A:40:PRO:O	2:A:42:LEU:HG	2.06	0.55
2:A:661:LEU:HD12	2:A:679:SER:HB3	1.88	0.55
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.88	0.55
1:C:330:GLN:O	1:C:382:LEU:HD12	2.07	0.55
2:A:340:GLY:O	2:A:344:GLU:HG2	2.06	0.55
2:A:413:ASN:HD22	2:A:442:ALA:HB1	1.70	0.55
2:A:732:LYS:HB3	2:A:801:VAL:HA	1.89	0.55
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.89	0.55
2:A:690:LEU:HD11	2:A:813:LEU:HD11	1.89	0.55
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.05	0.55
1:C:268:VAL:HG12	1:C:276:LEU:HD11	1.89	0.55
2:A:572:TYR:HE1	2:A:660:ASN:HB2	1.71	0.55
1:C:359:GLN:HG3	1:C:360:ALA:H	1.72	0.54
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.37	0.54
2:A:361:ARG:O	2:A:365:VAL:HG23	2.07	0.54
1:C:332:LEU:HD11	1:C:357:VAL:HG22	1.88	0.54
1:C:345:ASP:HB2	1:C:349:ARG:O	2.07	0.54
1:C:352:PRO:HG3	1:C:395:LEU:HD12	1.88	0.54
2:A:960:ASN:N	2:A:961:PRO:HD2	2.22	0.54
2:A:422:GLN:HG2	2:A:427:ASP:OD1	2.07	0.54
1:B:336:GLY:HA3	2:A:775:SER:OG	2.08	0.54
2:A:904:VAL:HG12	2:A:937:ALA:HB3	1.90	0.54
2:A:595:LEU:O	2:A:598:SER:HB3	2.07	0.54
1:C:120:GLN:OE1	1:C:243:PRO:HD2	2.08	0.54
2:A:349:VAL:HG11	2:A:404:VAL:HG11	1.89	0.54
1:C:158:TRP:O	1:C:162:GLN:HG3	2.08	0.54
2:A:243:PHE:O	2:A:246:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:715:ALA:CB	2:A:824:ILE:HG12	2.37	0.54
2:A:291:LEU:HD22	2:A:297:ALA:HA	1.89	0.53
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.08	0.53
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.88	0.53
1:B:245:TRP:CE3	1:B:297:ARG:HD3	2.43	0.53
2:A:223:GLU:O	2:A:224:LEU:HD23	2.08	0.53
1:B:124:VAL:O	1:B:235:VAL:HG22	2.08	0.53
2:A:453:SER:HA	2:A:456:ILE:HD12	1.90	0.53
1:C:138:LEU:HD21	1:C:144:VAL:HG11	1.90	0.53
2:A:871:LYS:O	2:A:875:MET:HB2	2.09	0.53
2:A:404:VAL:HG22	2:A:408:ILE:HG23	1.91	0.53
2:A:217:ALA:HB3	2:A:233:ALA:HB3	1.89	0.53
2:A:474:LEU:O	2:A:477:PRO:HD2	2.08	0.53
1:B:164:GLU:O	1:B:168:LEU:HD13	2.08	0.53
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.39	0.53
1:C:342:ILE:HB	1:C:378:VAL:HG12	1.90	0.53
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.90	0.53
1:B:252:GLU:CG	1:C:270:ALA:HB2	2.39	0.53
1:B:274:LYS:O	1:B:276:LEU:HD23	2.09	0.53
1:B:250:ILE:HG21	1:B:258:VAL:HG11	1.91	0.53
2:A:140:TYR:HD2	2:A:304:VAL:HG11	1.73	0.53
2:A:13:ARG:HA	2:A:499:ILE:HD13	1.90	0.53
2:A:432:ASN:HA	2:A:435:ARG:HG2	1.90	0.53
2:A:940:PHE:CE1	2:A:984:LYS:HG2	2.39	0.52
2:A:991:ILE:HG21	2:A:1020:MET:SD	2.49	0.52
1:B:174:THR:HG22	1:B:176:THR:H	1.75	0.52
1:C:124:VAL:HB	1:C:235:VAL:HG13	1.92	0.52
2:A:118:GLN:HE22	2:A:126:SER:HA	1.75	0.52
1:B:255:ALA:HB3	1:C:270:ALA:HB1	1.91	0.52
2:A:69:LEU:HD11	2:A:121:LEU:HD11	1.91	0.52
2:A:184:VAL:HG23	2:A:270:GLU:HB3	1.91	0.52
1:B:271:ARG:CD	1:B:306:ALA:HB1	2.39	0.52
2:A:882:ILE:O	2:A:886:LEU:HG	2.10	0.52
2:A:97:PHE:CZ	2:A:106:ALA:HB1	2.44	0.52
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.75	0.52
2:A:534:HIS:C	2:A:534:HIS:CD2	2.83	0.52
2:A:519:ARG:O	2:A:523:ARG:HG3	2.10	0.52
2:A:620:PRO:HB2	2:A:622:GLU:HG3	1.92	0.52
2:A:661:LEU:HD22	2:A:661:LEU:C	2.29	0.51
2:A:275:ILE:CD1	2:A:586:ALA:HB2	2.36	0.51
1:C:166:LEU:O	1:C:170:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:TRP:C	2:A:436:TRP:CD1	2.83	0.51
2:A:49:ILE:HB	2:A:93:VAL:HB	1.92	0.51
1:B:307:LEU:N	1:B:307:LEU:HD12	2.25	0.51
1:C:106:PHE:O	1:C:318:ASN:HA	2.10	0.51
1:B:158:TRP:O	1:B:162:GLN:HG3	2.10	0.51
1:B:132:ILE:HD11	1:B:229:ILE:HB	1.92	0.51
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.93	0.51
2:A:1028:LEU:O	2:A:1032:PRO:HG2	2.10	0.51
2:A:421:TRP:O	2:A:425:HIS:HB2	2.10	0.51
2:A:446:VAL:HG12	2:A:946:MET:HE3	1.93	0.51
2:A:554:LEU:HD21	2:A:912:ILE:HG12	1.93	0.51
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.46	0.51
1:C:298:LEU:HD11	1:C:315:LEU:HD13	1.92	0.51
1:C:256:TRP:CH2	1:C:257:LEU:HD13	2.38	0.51
2:A:327:ARG:NH1	2:A:666:ILE:HG12	2.26	0.51
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.92	0.51
1:C:327:ILE:HD13	1:C:367:LEU:HD21	1.93	0.51
2:A:420:GLU:HG3	2:A:421:TRP:N	2.25	0.51
1:C:388:GLU:HB2	2:A:657:GLY:N	2.26	0.51
2:A:906:PHE:O	2:A:909:VAL:HG12	2.11	0.50
1:C:302:ASN:ND2	1:C:307:LEU:H	2.03	0.50
2:A:74:LEU:HD11	2:A:817:ASN:HA	1.93	0.50
1:B:104:LEU:HD11	1:B:359:GLN:O	2.12	0.50
1:C:223:LEU:C	1:C:224:ARG:HD2	2.32	0.50
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.92	0.50
2:A:342:LEU:HD21	2:A:397:ALA:HA	1.92	0.50
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.92	0.50
2:A:49:ILE:HD11	2:A:73:MET:HE3	1.94	0.50
1:C:384:LEU:HD21	2:A:588:MET:HE2	1.93	0.50
2:A:925:ALA:O	2:A:1012:ILE:HG13	2.11	0.50
2:A:764:ALA:O	2:A:765:ARG:HG3	2.11	0.50
2:A:992:ILE:O	2:A:996:LEU:HB2	2.11	0.50
1:B:391:ILE:HG13	2:A:774:GLN:OE1	2.12	0.50
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.47	0.50
2:A:837:VAL:O	2:A:841:GLN:HG3	2.11	0.50
1:B:174:THR:HB	1:B:177:GLN:HG3	1.93	0.50
1:B:162:GLN:OE1	1:B:198:LEU:HD13	2.10	0.50
1:B:356:ALA:HB1	1:B:368:ARG:NH1	2.27	0.50
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.94	0.50
2:A:546:SER:O	2:A:550:VAL:HG23	2.11	0.50
2:A:690:LEU:HD22	2:A:718:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:56:GLN:HB3	2:A:60:ILE:HG23	1.93	0.50
2:A:950:HIS:HA	2:A:953:GLU:CG	2.34	0.50
2:A:984:LYS:HG3	2:A:1028:LEU:HD21	1.94	0.49
2:A:667:ARG:HH11	2:A:861:GLN:HE22	1.60	0.49
1:C:124:VAL:O	1:C:235:VAL:HG12	2.11	0.49
2:A:408:ILE:HD12	2:A:986:MET:HB3	1.93	0.49
1:B:94:VAL:HG21	1:B:350:PHE:HZ	1.76	0.49
2:A:122:PRO:HB2	2:A:125:VAL:HG13	1.93	0.49
2:A:291:LEU:HD13	2:A:300:VAL:HG11	1.94	0.49
2:A:744:GLN:O	2:A:748:THR:HG23	2.12	0.49
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.48	0.49
1:C:254:ILE:O	1:C:255:ALA:C	2.51	0.49
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.11	0.49
1:B:339:GLN:HG3	1:B:357:VAL:HG22	1.94	0.49
2:A:956:PRO:HA	2:A:959:ASN:ND2	2.27	0.49
2:A:153:LEU:CD1	2:A:153:LEU:H	2.24	0.49
2:A:276:ALA:HB3	2:A:284:VAL:O	2.12	0.49
2:A:46:GLN:HG2	2:A:134:THR:HG22	1.94	0.49
2:A:143:ALA:HB2	2:A:606:PHE:HE1	1.77	0.49
2:A:550:VAL:O	2:A:550:VAL:HG12	2.11	0.49
2:A:411:ILE:HG12	2:A:501:MET:HE3	1.93	0.49
1:B:340:ARG:HD3	1:B:395:LEU:HD12	1.94	0.49
2:A:402:ALA:HB3	2:A:486:MET:CE	2.42	0.49
2:A:83:ARG:HG2	2:A:816:GLU:HG3	1.94	0.49
1:C:110:PHE:CE1	1:C:250:ILE:HG13	2.47	0.49
1:B:223:LEU:C	1:B:224:ARG:HD2	2.33	0.49
1:B:280:LYS:HE3	1:B:281:TRP:H	1.77	0.49
2:A:455:LEU:HD13	2:A:455:LEU:O	2.12	0.49
1:B:125:GLN:NE2	1:C:228:ASN:H	2.10	0.49
1:B:144:VAL:HG21	1:B:238:ILE:HD13	1.95	0.49
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.95	0.49
2:A:868:ALA:O	2:A:872:LEU:HG	2.13	0.49
1:B:195:ILE:O	1:B:198:LEU:HB3	2.13	0.48
2:A:143:ALA:HB2	2:A:606:PHE:CE1	2.48	0.48
1:B:153:LEU:HD23	1:B:153:LEU:N	2.28	0.48
2:A:969:LEU:O	2:A:973:LEU:HD13	2.13	0.48
2:A:403:MET:SD	2:A:485:ALA:HB1	2.53	0.48
2:A:910:GLY:HA3	2:A:1022:THR:OG1	2.12	0.48
2:A:601:GLU:OE2	2:A:637:ARG:HD3	2.13	0.48
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.43	0.48
2:A:522:ILE:HG23	2:A:526:HIS:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:395:GLY:HA2	2:A:398:ILE:HG22	1.95	0.48
2:A:56:GLN:HB3	2:A:60:ILE:CG2	2.43	0.48
1:B:344:VAL:HG13	1:B:348:GLY:HA2	1.94	0.48
1:B:271:ARG:NE	1:B:306:ALA:HB1	2.28	0.48
2:A:898:LEU:C	2:A:898:LEU:HD23	2.34	0.48
2:A:419:GLU:O	2:A:423:HIS:HD2	1.96	0.48
1:B:222:ASP:HB2	1:B:234:VAL:O	2.13	0.48
1:B:117:ASN:HD22	1:B:117:ASN:C	2.16	0.48
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.44	0.48
2:A:461:PHE:CZ	2:A:464:ILE:HD12	2.49	0.48
2:A:608:LYS:HE2	2:A:625:GLU:HG2	1.95	0.48
2:A:550:VAL:CG1	2:A:909:VAL:HG22	2.43	0.48
2:A:114:LEU:HD11	2:A:127:ALA:HB1	1.94	0.48
2:A:368:ILE:HG22	2:A:368:ILE:O	2.14	0.48
2:A:376:ILE:HD13	2:A:488:GLY:HA2	1.96	0.48
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.44	0.48
2:A:842:LYS:O	2:A:846:GLU:HG2	2.14	0.48
2:A:525:TYR:CE1	2:A:977:ALA:HB1	2.49	0.48
2:A:644:LYS:HB3	2:A:644:LYS:NZ	2.29	0.48
2:A:48:ILE:HG22	2:A:94:TYR:CD2	2.49	0.47
2:A:37:ASP:OD2	2:A:297:ALA:HB3	2.14	0.47
1:B:360:ALA:HA	1:B:365:THR:HA	1.95	0.47
2:A:952:ILE:HA	2:A:957:SER:CB	2.44	0.47
2:A:700:ILE:HA	2:A:703:VAL:HG22	1.95	0.47
2:A:525:TYR:CE2	2:A:1029:PHE:HE2	2.31	0.47
2:A:185:LYS:HG2	2:A:766:TYR:CD2	2.49	0.47
2:A:57:ALA:O	2:A:61:VAL:HG23	2.14	0.47
2:A:630:LEU:HD13	2:A:642:MET:HE1	1.96	0.47
1:B:386:ASP:O	1:B:387:SER:C	2.53	0.47
1:B:252:GLU:HG2	1:C:270:ALA:HB2	1.97	0.47
1:B:322:GLU:O	1:B:324:MET:HG3	2.14	0.47
2:A:324:THR:HG21	2:A:606:PHE:CD1	2.48	0.47
2:A:965:SER:HB2	2:A:968:LYS:HB2	1.96	0.47
2:A:376:ILE:HD13	2:A:488:GLY:CA	2.45	0.47
2:A:482:LYS:O	2:A:486:MET:HG2	2.14	0.47
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.79	0.47
2:A:48:ILE:HG12	2:A:130:GLY:HA3	1.95	0.47
2:A:666:ILE:O	2:A:670:ILE:HG13	2.14	0.47
2:A:456:ILE:HG12	2:A:886:LEU:CD1	2.44	0.47
2:A:995:LEU:C	2:A:1017:ILE:HD11	2.35	0.47
2:A:76:VAL:HG13	2:A:77:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:139:ILE:O	2:A:325:TYR:HD1	1.97	0.47
2:A:45:VAL:HG11	2:A:103:PRO:HA	1.97	0.47
2:A:988:VAL:O	2:A:988:VAL:HG12	2.15	0.47
2:A:240:LEU:HD22	2:A:265:VAL:HG12	1.97	0.47
2:A:291:LEU:HD21	2:A:295:LYS:O	2.15	0.47
2:A:431:ASP:CG	2:A:432:ASN:H	2.18	0.47
1:C:389:ALA:O	1:C:394:ALA:HB3	2.15	0.47
1:B:358:PHE:CD2	1:C:272:PRO:HB2	2.50	0.47
2:A:392:SER:O	2:A:396:ILE:HG13	2.15	0.47
2:A:42:LEU:HD12	2:A:42:LEU:N	2.25	0.47
1:B:291:THR:O	1:B:293:THR:N	2.48	0.47
1:B:143:LYS:HD2	1:B:216:GLY:O	2.15	0.47
2:A:1037:LEU:HD23	2:A:1037:LEU:O	2.16	0.46
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.97	0.46
2:A:571:LEU:HD23	2:A:627:THR:HA	1.97	0.46
2:A:459:LEU:HB3	2:A:882:ILE:HD13	1.98	0.46
2:A:729:ASN:HD22	2:A:729:ASN:C	2.19	0.46
1:C:223:LEU:HD21	1:C:233:ASN:HD22	1.80	0.46
2:A:573:MET:HA	2:A:624:VAL:O	2.15	0.46
2:A:771:ARG:HD2	2:A:777:ARG:NE	2.31	0.46
2:A:296:ASN:HB3	2:A:299:GLU:HB3	1.97	0.46
2:A:985:ALA:O	2:A:989:ALA:HB2	2.15	0.46
2:A:637:ARG:HH11	2:A:637:ARG:HB2	1.79	0.46
2:A:497:ILE:HB	2:A:498:PRO:HD3	1.96	0.46
2:A:620:PRO:HB2	2:A:622:GLU:CG	2.45	0.46
2:A:771:ARG:HG3	2:A:772:TYR:N	2.29	0.46
2:A:551:LEU:HD23	2:A:551:LEU:C	2.35	0.46
2:A:952:ILE:HG12	2:A:1039:TRP:HE1	1.80	0.46
1:C:266:LEU:HG	1:C:278:ILE:HD11	1.98	0.46
2:A:65:VAL:HA	2:A:121:LEU:HD22	1.98	0.46
2:A:813:LEU:HA	2:A:813:LEU:HD13	1.81	0.46
2:A:137:GLY:O	2:A:290:ILE:HA	2.15	0.46
1:B:372:ALA:HB3	1:B:375:GLU:HG3	1.98	0.46
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.97	0.46
2:A:298:ARG:O	2:A:298:ARG:HD3	2.15	0.46
2:A:297:ALA:O	2:A:300:VAL:HG12	2.16	0.46
1:C:223:LEU:HD12	1:C:235:VAL:HB	1.98	0.46
1:C:91:ASN:O	2:A:591:LYS:HD3	2.16	0.46
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.16	0.46
2:A:580:ILE:HG22	2:A:622:GLU:HB3	1.97	0.46
1:B:271:ARG:HD2	1:B:306:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:446:VAL:HG12	2:A:946:MET:CE	2.46	0.45
2:A:625:GLU:HG3	2:A:625:GLU:O	2.16	0.45
2:A:454:LEU:HA	2:A:457:ILE:HG22	1.97	0.45
2:A:467:LEU:O	2:A:472:GLY:HA3	2.16	0.45
2:A:884:PHE:CD1	2:A:884:PHE:C	2.90	0.45
1:C:332:LEU:HA	1:C:341:VAL:HG12	1.98	0.45
2:A:279:ASN:ND2	2:A:605:VAL:H	2.14	0.45
1:B:390:ASN:HA	2:A:774:GLN:HE22	1.81	0.45
2:A:408:ILE:HG13	2:A:409:VAL:N	2.32	0.45
2:A:740:VAL:O	2:A:744:GLN:HG3	2.16	0.45
2:A:984:LYS:HD2	2:A:984:LYS:C	2.37	0.45
2:A:153:LEU:N	2:A:153:LEU:HD12	2.26	0.45
1:B:84:ILE:CD1	2:A:594:LYS:HB2	2.47	0.45
1:B:196:ARG:O	1:B:199:ILE:HG12	2.16	0.45
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.41	0.45
2:A:991:ILE:O	2:A:995:LEU:HD13	2.17	0.45
2:A:53:TYR:CE1	2:A:56:GLN:HG3	2.51	0.45
2:A:31:ILE:HG13	2:A:378:PHE:CZ	2.51	0.45
2:A:575:SER:O	2:A:658:LEU:HD12	2.16	0.45
2:A:661:LEU:HD23	2:A:662:TRP:H	1.63	0.45
1:B:123:ILE:HD12	1:B:237:LYS:HG3	1.99	0.45
1:B:220:ALA:HB3	1:B:237:LYS:HB3	1.99	0.45
2:A:67:TYR:N	2:A:68:PRO:HD2	2.31	0.45
2:A:404:VAL:O	2:A:408:ILE:HG12	2.17	0.45
1:B:302:ASN:HD21	1:B:306:ALA:N	2.15	0.45
2:A:462:ILE:N	2:A:463:PRO:CD	2.80	0.45
2:A:988:VAL:HG11	2:A:1024:PRO:HG2	1.99	0.45
2:A:816:GLU:O	2:A:817:ASN:HB2	2.17	0.45
1:C:114:VAL:HG12	1:C:309:PRO:HA	1.99	0.45
2:A:637:ARG:HB2	2:A:640:MET:HG3	1.99	0.45
2:A:988:VAL:CG1	2:A:1024:PRO:HG2	2.46	0.45
2:A:38:ALA:O	2:A:390:ILE:HG22	2.17	0.45
2:A:42:LEU:HB3	2:A:470:GLN:HG3	1.99	0.45
2:A:117:VAL:HG12	2:A:117:VAL:O	2.16	0.45
2:A:944:MET:HG2	2:A:980:ARG:CD	2.37	0.44
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.41	0.44
2:A:561:PHE:CE1	2:A:864:LEU:HB3	2.51	0.44
2:A:222:ILE:HG23	2:A:229:TYR:HB2	1.98	0.44
1:C:358:PHE:HD2	1:C:368:ARG:NH2	2.14	0.44
2:A:494:ILE:O	2:A:494:ILE:HG12	2.17	0.44
2:A:723:TYR:O	2:A:806:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:980:ARG:C	2:A:983:PRO:HD2	2.36	0.44
2:A:359:HIS:HD2	2:A:360:VAL:N	2.14	0.44
2:A:6:ILE:O	2:A:6:ILE:HD13	2.17	0.44
1:C:384:LEU:HD21	2:A:588:MET:CE	2.48	0.44
2:A:453:SER:O	2:A:456:ILE:HB	2.18	0.44
2:A:876:VAL:HB	2:A:877:PRO:HD3	2.00	0.44
2:A:571:LEU:HB3	2:A:573:MET:HE2	2.00	0.44
1:C:134:LYS:HB3	1:C:152:ASP:HB2	1.98	0.44
1:C:156:PRO:O	1:C:159:VAL:HG22	2.17	0.44
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.82	0.44
2:A:526:HIS:N	2:A:527:PRO:CD	2.81	0.44
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.99	0.44
1:B:383:PHE:C	1:B:384:LEU:HD12	2.38	0.44
2:A:837:VAL:HG21	2:A:862:PHE:CD2	2.52	0.44
2:A:921:HIS:O	2:A:926:THR:HG21	2.18	0.44
2:A:525:TYR:HE1	2:A:977:ALA:HB1	1.83	0.44
1:B:252:GLU:HG3	1:C:270:ALA:HB2	2.00	0.44
2:A:599:VAL:O	2:A:602:VAL:HG13	2.18	0.44
2:A:729:ASN:HD22	2:A:732:LYS:H	1.65	0.44
1:B:385:ILE:CG2	1:B:389:ALA:HB2	2.46	0.44
2:A:193:PRO:HB3	2:A:787:PRO:HB2	2.00	0.44
1:B:123:ILE:HG12	1:C:224:ARG:HB2	1.99	0.44
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.48	0.44
2:A:27:GLY:HA3	2:A:375:CYS:HB3	2.00	0.44
2:A:28:THR:O	2:A:32:ILE:HG13	2.18	0.44
1:C:171:THR:O	1:C:172:GLY:C	2.55	0.44
2:A:619:ALA:HB1	2:A:623:MET:HG2	2.00	0.44
2:A:1020:MET:HA	2:A:1020:MET:CE	2.48	0.43
2:A:534:HIS:CD2	2:A:534:HIS:O	2.71	0.43
1:C:284:LEU:HB3	1:C:285:PRO:HD2	2.00	0.43
2:A:904:VAL:N	2:A:905:PRO:CD	2.81	0.43
2:A:1032:PRO:C	2:A:1034:ALA:H	2.22	0.43
1:B:85:ASP:HA	1:B:86:PRO:HD3	1.87	0.43
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.48	0.43
2:A:212:ALA:C	2:A:215:GLN:HE22	2.21	0.43
1:B:327:ILE:CD1	1:B:341:VAL:HG11	2.48	0.43
2:A:999:LEU:HD21	2:A:1014:ALA:HA	2.00	0.43
1:C:174:THR:H	1:C:177:GLN:NE2	2.17	0.43
2:A:557:VAL:HG12	2:A:921:HIS:HA	1.99	0.43
1:B:340:ARG:HH21	1:B:354:ARG:CG	2.32	0.43
1:C:127:ARG:O	1:C:231:LYS:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:636:TRP:CD1	2:A:636:TRP:N	2.86	0.43
2:A:1001:GLY:O	2:A:1002:THR:C	2.56	0.43
2:A:746:PHE:O	2:A:750:ALA:HB3	2.18	0.43
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.99	0.43
2:A:952:ILE:HA	2:A:957:SER:OG	2.17	0.43
2:A:272:ARG:NH2	2:A:283:GLU:OE1	2.51	0.43
2:A:965:SER:HB3	2:A:968:LYS:HD3	2.01	0.43
2:A:575:SER:N	2:A:659:ALA:O	2.51	0.43
2:A:414:ALA:HB3	2:A:501:MET:HE1	2.01	0.43
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.83	0.43
1:C:331:ALA:O	1:C:341:VAL:HG12	2.19	0.43
1:C:224:ARG:N	1:C:224:ARG:HD2	2.33	0.43
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.53	0.43
2:A:70:THR:O	2:A:74:LEU:HG	2.19	0.42
2:A:851:LYS:HB3	2:A:852:PRO:HD2	2.01	0.42
1:B:114:VAL:HG22	1:B:246:VAL:HG22	2.01	0.42
2:A:203:LEU:HD12	2:A:746:PHE:CD2	2.54	0.42
1:B:399:ARG:O	1:B:400:SER:HB2	2.19	0.42
1:C:189:GLY:O	1:C:190:MET:C	2.58	0.42
2:A:969:LEU:CD2	2:A:1036:LYS:HE3	2.48	0.42
2:A:277:GLU:OE2	2:A:590:GLN:HG3	2.19	0.42
1:B:302:ASN:HD21	1:B:307:LEU:H	1.66	0.42
2:A:195:ARG:HD3	2:A:261:ASP:O	2.19	0.42
2:A:756:VAL:HG12	2:A:756:VAL:O	2.18	0.42
2:A:590:GLN:O	2:A:594:LYS:HG3	2.19	0.42
1:B:384:LEU:HD21	1:B:395:LEU:HD23	2.01	0.42
1:C:268:VAL:HA	1:C:269:PRO:HD3	1.93	0.42
1:C:153:LEU:HD23	1:C:153:LEU:H	1.83	0.42
2:A:783:LEU:O	2:A:798:LEU:HB3	2.19	0.42
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.54	0.42
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.88	0.42
1:C:86:PRO:O	1:C:90:GLN:HG3	2.19	0.42
1:C:264:PHE:HB3	1:C:315:LEU:HD11	2.02	0.42
2:A:897:ALA:O	2:A:901:ILE:HG13	2.20	0.42
2:A:370:LEU:HB2	2:A:371:PRO:HD3	2.02	0.42
2:A:927:GLY:O	2:A:931:ILE:HG12	2.20	0.42
1:B:384:LEU:N	1:B:384:LEU:HD12	2.35	0.42
1:B:343:THR:HA	1:B:377:VAL:HA	2.02	0.42
2:A:552:TRP:N	2:A:553:PRO:CD	2.83	0.42
2:A:191:ILE:HD11	2:A:206:VAL:HG11	2.01	0.42
2:A:497:ILE:O	2:A:501:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.85	0.42
2:A:955:VAL:N	2:A:956:PRO:CD	2.83	0.42
1:B:307:LEU:H	1:B:307:LEU:CD1	2.33	0.42
2:A:884:PHE:HB2	2:A:901:ILE:HD11	2.01	0.42
2:A:327:ARG:O	2:A:331:ILE:HG12	2.20	0.41
2:A:57:ALA:HB1	2:A:58:PRO:HD2	2.01	0.41
2:A:381:MET:HE2	2:A:381:MET:HB2	1.83	0.41
1:C:167:LEU:HD12	1:C:167:LEU:C	2.41	0.41
2:A:611:LYS:HA	2:A:617:ASP:OD2	2.20	0.41
2:A:140:TYR:HE1	2:A:323:THR:OG1	2.02	0.41
2:A:992:ILE:HD11	2:A:1020:MET:O	2.20	0.41
2:A:994:GLY:O	2:A:997:PRO:HD2	2.20	0.41
1:B:271:ARG:HB3	1:B:274:LYS:HB2	2.02	0.41
1:C:343:THR:OG1	1:C:353:LYS:HD3	2.20	0.41
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.41
2:A:65:VAL:HA	2:A:121:LEU:CD2	2.50	0.41
2:A:121:LEU:HB3	2:A:125:VAL:HG21	2.01	0.41
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.56	0.41
2:A:534:HIS:O	2:A:534:HIS:HD2	2.04	0.41
2:A:342:LEU:HD23	2:A:342:LEU:HA	1.83	0.41
2:A:85:PHE:CD1	2:A:812:MET:HE3	2.55	0.41
1:B:335:THR:HG23	1:B:338:GLU:O	2.21	0.41
1:B:302:ASN:HD21	1:B:306:ALA:H	1.68	0.41
1:B:132:ILE:CD1	1:B:229:ILE:HB	2.50	0.41
1:C:281:TRP:HB2	1:C:298:LEU:HD23	2.02	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	0.41
1:C:329:SER:HA	1:C:365:THR:HG22	2.01	0.41
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.82	0.41
2:A:178:ALA:HB2	2:A:614:THR:HB	2.03	0.41
2:A:189:VAL:HG22	2:A:265:VAL:HG22	2.01	0.41
1:C:220:ALA:HB3	1:C:237:LYS:HB3	2.02	0.41
1:B:291:THR:O	1:B:293:THR:HG23	2.21	0.41
1:B:259:LYS:HG3	1:B:260:ASP:N	2.36	0.41
2:A:661:LEU:CD1	2:A:679:SER:HB3	2.51	0.41
1:B:330:GLN:NE2	2:A:267:ILE:HB	2.36	0.41
2:A:184:VAL:HG21	2:A:270:GLU:OE1	2.21	0.41
1:B:264:PHE:HE1	1:B:281:TRP:CE2	2.39	0.41
1:B:308:LYS:HA	1:B:309:PRO:HD3	1.97	0.41
2:A:595:LEU:HB3	2:A:653:VAL:HG22	2.03	0.41
1:B:125:GLN:HE21	1:C:227:MET:HB3	1.85	0.41
2:A:834:VAL:HA	2:A:837:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:392:SER:O	2:A:481:THR:HG21	2.21	0.41
2:A:462:ILE:N	2:A:463:PRO:HD2	2.36	0.41
2:A:1016:MET:HB2	2:A:1016:MET:HE2	1.91	0.41
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.55	0.41
2:A:641:THR:H	2:A:644:LYS:HB2	1.86	0.41
2:A:356:PHE:HE2	2:A:985:ALA:O	2.04	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.82	0.41
2:A:201:ILE:HD13	2:A:248:LEU:HB3	2.02	0.41
2:A:904:VAL:O	2:A:908:LEU:HG	2.20	0.40
1:C:357:VAL:HA	1:C:367:LEU:HD12	2.03	0.40
2:A:533:LEU:HD22	2:A:1036:LYS:HD2	2.03	0.40
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.36	0.40
2:A:876:VAL:O	2:A:880:LEU:HG	2.21	0.40
2:A:999:LEU:CD2	2:A:1017:ILE:HD12	2.49	0.40
1:B:242:ASP:CB	1:B:243:PRO:CD	2.98	0.40
2:A:590:GLN:HG2	2:A:594:LYS:HE3	2.02	0.40
1:C:322:GLU:O	1:C:324:MET:HG2	2.21	0.40
1:C:108:GLN:OE1	1:C:108:GLN:HA	2.22	0.40
2:A:899:LEU:HD22	2:A:899:LEU:HA	1.90	0.40
2:A:359:HIS:CD2	2:A:360:VAL:N	2.90	0.40
2:A:960:ASN:HA	2:A:963:THR:O	2.22	0.40
1:B:335:THR:HG22	1:B:391:ILE:CD1	2.48	0.40
1:C:94:VAL:CG2	1:C:385:ILE:HD11	2.51	0.40
1:C:353:LYS:HE2	1:C:375:GLU:OE2	2.21	0.40
2:A:421:TRP:O	2:A:421:TRP:HD1	2.04	0.40
1:B:360:ALA:CB	1:B:365:THR:HG22	2.49	0.40
2:A:834:VAL:HG22	2:A:838:HIS:HD2	1.85	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	B	320/336 (95%)	284 (89%)	31 (10%)	5 (2%)	12	49
1	C	322/336 (96%)	300 (93%)	19 (6%)	3 (1%)	21	63
2	A	1024/1054 (97%)	923 (90%)	91 (9%)	10 (1%)	19	60
All	All	1666/1726 (96%)	1507 (90%)	141 (8%)	18 (1%)	17	58

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	ALA
2	A	638	PRO
2	A	852	PRO
1	B	292	ARG
1	C	172	GLY
1	B	390	ASN
2	A	574	PRO
2	A	813	LEU
1	B	388	GLU
2	A	56	GLN
2	A	812	MET
2	A	998	ILE
2	A	1024	PRO
2	A	665	PRO
1	B	137	PRO
1	C	137	PRO
1	B	156	PRO
2	A	426	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	B	263/275 (96%)	235 (89%)	28 (11%)	8	32
1	C	265/275 (96%)	236 (89%)	29 (11%)	8	31
2	A	847/871 (97%)	762 (90%)	85 (10%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1375/1421 (97%)	1233 (90%)	142 (10%)	9 34

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	105	THR
1	B	117	ASN
1	B	121	TYR
1	B	151	LEU
1	B	206	THR
1	B	239	GLN
1	B	247	THR
1	B	266	LEU
1	B	267	THR
1	B	268	VAL
1	B	275	THR
1	B	276	LEU
1	B	280	LYS
1	B	282	THR
1	B	298	LEU
1	B	322	GLU
1	B	332	LEU
1	B	335	THR
1	B	340	ARG
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	364	VAL
1	B	378	VAL
1	B	390	ASN
1	B	395	LEU
1	B	396	GLU
1	C	87	THR
1	C	96	THR
1	C	104	LEU
1	C	120	GLN
1	C	121	TYR
1	C	150	LEU
1	C	151	LEU
1	C	185	LEU
1	C	207	ARG

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Mol	Chain	Res	Type
1	C	247	THR
1	C	253	SER
1	C	257	LEU
1	C	260	ASP
1	C	268	VAL
1	C	283	LEU
1	C	287	VAL
1	C	292	ARG
1	C	304	ASP
1	C	316	GLN
1	C	317	LEU
1	C	324	MET
1	C	325	LEU
1	C	330	GLN
1	C	339	GLN
1	C	354	ARG
1	C	364	VAL
1	C	365	THR
1	C	367	LEU
1	C	382	LEU
2	A	6	ILE
2	A	8	ARG
2	A	34	THR
2	A	42	LEU
2	A	48	ILE
2	A	51	THR
2	A	53	TYR
2	A	65	VAL
2	A	88	PHE
2	A	105	TRP
2	A	114	LEU
2	A	140	TYR
2	A	145	VAL
2	A	157	ARG
2	A	184	VAL
2	A	203	LEU
2	A	211	ASP
2	A	215	GLN
2	A	236	TYR
2	A	259	LEU
2	A	260	ARG
2	A	298	ARG

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Mol	Chain	Res	Type
2	A	338	LEU
2	A	343	LEU
2	A	374	LEU
2	A	403	MET
2	A	412	GLU
2	A	418	LEU
2	A	434	THR
2	A	436	TRP
2	A	464	ILE
2	A	492	LEU
2	A	521	LEU
2	A	524	VAL
2	A	531	LYS
2	A	532	VAL
2	A	534	HIS
2	A	541	LEU
2	A	545	LEU
2	A	547	VAL
2	A	567	GLU
2	A	569	ASP
2	A	573	MET
2	A	602	VAL
2	A	623	MET
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	642	MET
2	A	643	ASP
2	A	660	ASN
2	A	661	LEU
2	A	663	VAL
2	A	688	THR
2	A	693	ILE
2	A	722	ARG
2	A	725	ASN
2	A	729	ASN
2	A	748	THR
2	A	769	ASN
2	A	771	ARG
2	A	778	ASP
2	A	781	GLN
2	A	786	LEU

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Mol	Chain	Res	Type
2	A	789	LEU
2	A	804	ILE
2	A	812	MET
2	A	813	LEU
2	A	884	PHE
2	A	885	VAL
2	A	888	TYR
2	A	899	LEU
2	A	904	VAL
2	A	909	VAL
2	A	945	LEU
2	A	946	MET
2	A	955	VAL
2	A	958	LEU
2	A	969	LEU
2	A	970	ASP
2	A	984	LYS
2	A	999	LEU
2	A	1020	MET
2	A	1035	TYR
2	A	1039	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	120	GLN
1	B	125	GLN
1	B	177	GLN
1	B	295	GLN
1	B	302	ASN
1	B	330	GLN
1	B	390	ASN
1	C	125	GLN
1	C	177	GLN
1	C	295	GLN
1	C	302	ASN
2	A	87	GLN
2	A	118	GLN
2	A	151	HIS
2	A	215	GLN
2	A	238	GLN

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Mol	Chain	Res	Type
2	A	279	ASN
2	A	329	GLN
2	A	359	HIS
2	A	413	ASN
2	A	423	HIS
2	A	470	GLN
2	A	534	HIS
2	A	564	GLN
2	A	590	GLN
2	A	629	GLN
2	A	633	GLN
2	A	635	GLN
2	A	660	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	921	HIS
2	A	1043	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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%)	-0.04	3 (0%) 85 88	24, 58, 112, 176	0
1	C	324/336 (96%)	0.01	2 (0%) 90 91	25, 58, 110, 174	0
2	A	1028/1054 (97%)	0.43	111 (10%) 8 8	28, 106, 212, 312	0
All	All	1674/1726 (96%)	0.26	116 (6%) 20 21	24, 79, 194, 312	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	15	LEU	11.0
2	A	890	ALA	8.5
2	A	887	LEU	7.9
2	A	365	VAL	7.9
2	A	495	VAL	5.9
2	A	889	LEU	5.5
2	A	886	LEU	5.3
2	A	891	PHE	5.0
2	A	494	ILE	5.0
2	A	496	VAL	5.0
2	A	418	LEU	4.9
2	A	1036	LYS	4.9
2	A	368	ILE	4.8
2	A	888	TYR	4.8
2	A	429	THR	4.7
2	A	18	MET	4.7
2	A	17	LEU	4.6
2	A	436	TRP	4.6
2	A	873	LYS	4.5
1	C	402	SER	4.5
2	A	73	MET	4.4
2	A	872	LEU	4.3
2	A	499	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	A	14	PHE	4.2
2	A	853	GLY	4.2
2	A	7	ARG	4.2
2	A	355	LEU	4.2
2	A	538	THR	4.1
2	A	848	VAL	4.0
2	A	1001	GLY	3.9
2	A	449	ALA	3.9
2	A	29	TRP	3.8
2	A	1043	HIS	3.8
2	A	428	ALA	3.8
2	A	504	TRP	3.7
2	A	35	PRO	3.7
2	A	1039	TRP	3.6
2	A	437	GLN	3.6
2	A	1035	TYR	3.6
2	A	704	ALA	3.6
2	A	445	GLU	3.5
2	A	528	LEU	3.5
2	A	502	GLY	3.5
2	A	874	LEU	3.5
2	A	847	LYS	3.4
2	A	392	SER	3.4
2	A	703	VAL	3.3
2	A	500	LEU	3.3
2	A	423	HIS	3.3
2	A	427	ASP	3.2
2	A	450	LEU	3.2
2	A	71	THR	3.1
2	A	451	PHE	3.1
2	A	396	ILE	3.1
2	A	434	THR	3.0
2	A	554	LEU	3.0
2	A	430	LEU	3.0
2	A	539	THR	2.9
2	A	426	PRO	2.9
2	A	498	PRO	2.9
2	A	530	LEU	2.8
2	A	417	ARG	2.8
2	A	16	VAL	2.8
2	A	366	ALA	2.7
2	A	895	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	A	896	GLU	2.6
2	A	946	MET	2.6
2	A	956	PRO	2.6
2	A	871	LYS	2.6
2	A	36	VAL	2.6
2	A	26	TRP	2.6
2	A	421	TRP	2.6
2	A	439	ILE	2.6
1	B	79	ALA	2.5
2	A	1037	LEU	2.5
2	A	497	ILE	2.5
1	B	387	SER	2.5
2	A	875	MET	2.5
2	A	669	ARG	2.4
2	A	438	VAL	2.4
2	A	448	PRO	2.4
2	A	846	GLU	2.4
2	A	1041	HIS	2.4
2	A	480	PHE	2.4
2	A	970	ASP	2.4
1	B	386	ASP	2.4
2	A	503	TYR	2.4
2	A	700	ILE	2.3
2	A	388	ALA	2.3
2	A	948	LEU	2.3
2	A	520	PHE	2.3
2	A	462	ILE	2.3
2	A	623	MET	2.3
2	A	32	ILE	2.3
2	A	120	LYS	2.3
2	A	849	GLN	2.3
2	A	960	ASN	2.3
2	A	954	ALA	2.3
2	A	973	LEU	2.3
2	A	78	GLY	2.2
2	A	850	LEU	2.2
2	A	441	ASP	2.2
2	A	549	THR	2.2
2	A	11	ALA	2.2
2	A	33	ASN	2.2
2	A	517	LEU	2.2
1	C	242	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	854	THR	2.1
2	A	969	LEU	2.1
2	A	433	LYS	2.1
2	A	406	ALA	2.1
2	A	10	VAL	2.1
2	A	947	TYR	2.0
2	A	519	ARG	2.0
2	A	844	ILE	2.0
2	A	97	PHE	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(\AA^2)	Q<0.9
3	CU	A	1048	1/1	0.92	0.19	-2.85	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.