



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 3T53 / pdb_00003t53
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

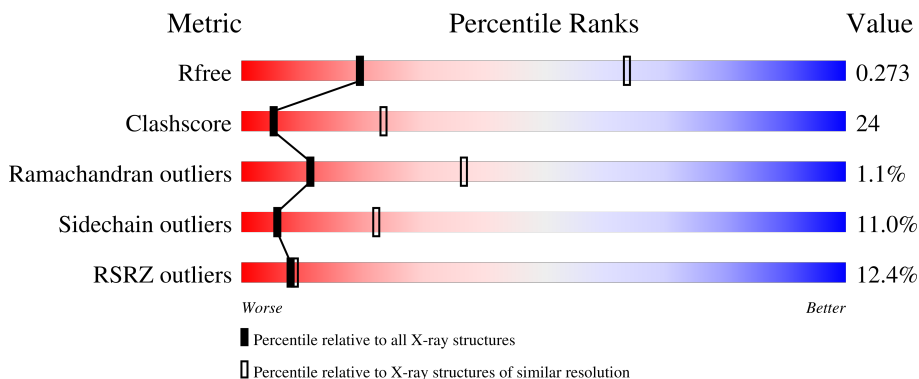
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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

Mol	Chain	Length	Quality of chain
1	B	336	
1	C	336	
2	A	1054	

2 Entry composition i

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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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 (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0

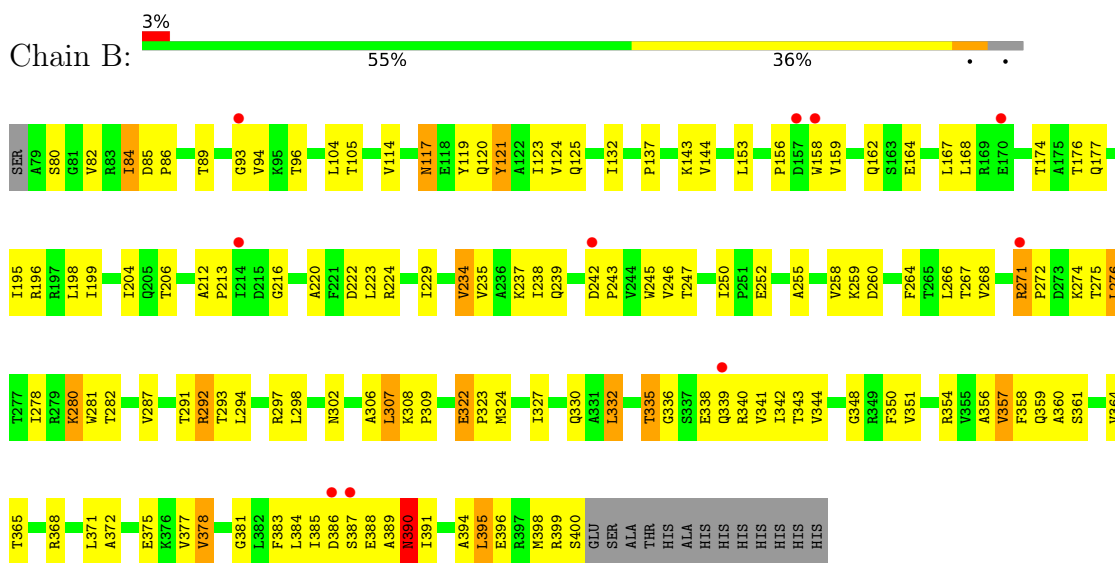
- Molecule 4 is water.

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

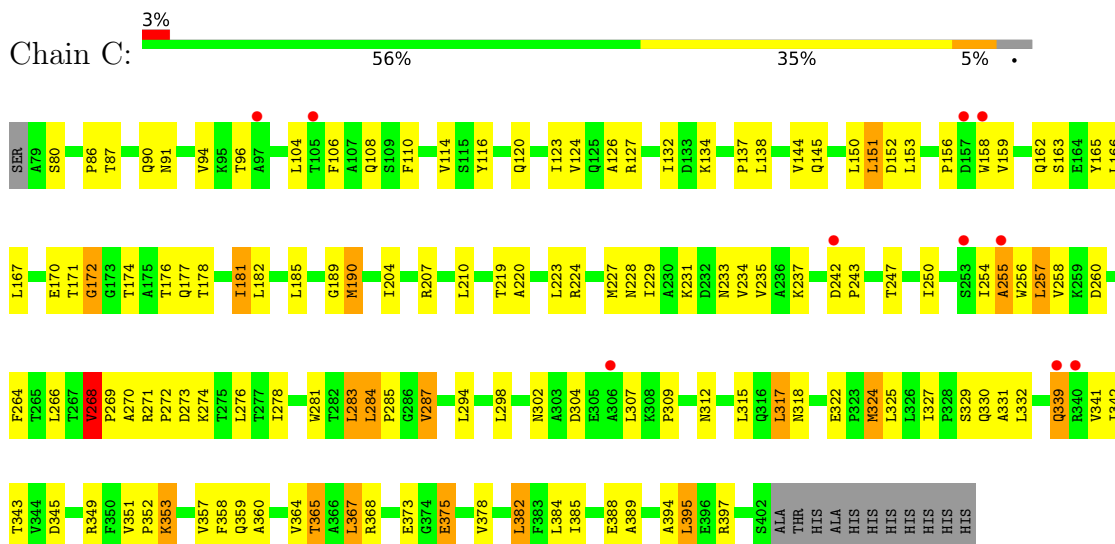
3 Residue-property plots [i](#)

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

- 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	159.79Å 159.79Å 683.04Å 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) 99.3 (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 3.40Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.248 , 0.286 0.243 , 0.273	Depositor DCC
R_{free} test set	2415 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.28	0/2498	0.75	3/3401 (0.1%)
1	C	0.28	0/2513	0.76	6/3421 (0.2%)
2	A	0.28	0/8089	0.75	2/11015 (0.0%)
All	All	0.28	0/13100	0.75	11/17837 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	521	LEU	N-CA-C	-5.86	107.94	114.62
1	B	381	GLY	N-CA-C	-5.55	106.06	115.34
1	C	284	LEU	CA-C-N	5.38	125.00	119.56
1	C	284	LEU	C-N-CA	5.38	125.00	119.56
2	A	455	LEU	N-CA-C	-5.16	106.49	112.89
1	C	268	VAL	CA-C-N	5.14	125.18	119.32
1	C	268	VAL	C-N-CA	5.14	125.18	119.32
1	B	271	ARG	CA-C-N	5.11	125.18	119.87
1	B	271	ARG	C-N-CA	5.11	125.18	119.87
1	C	190	MET	CA-C-N	5.03	124.94	119.76
1	C	190	MET	C-N-CA	5.03	124.94	119.76

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	123	0
1	C	2473	0	2533	106	0
2	A	7923	0	8166	431	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	631	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 24.

All (631) 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
2:A:661:LEU:HD23	2:A:661:LEU:C	1.81	1.04
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:C	2:A:661:LEU:CD2	2.35	0.99
1:C:256:TRP:CH2	1:C:257:LEU:HD12	1.97	0.98
2:A:660:ASN:H	2:A:660:ASN:ND2	1.65	0.94
2:A:48:ILE:HD11	2:A:131:PRO:HD2	1.47	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:HD22	2:A:660:ASN:N	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
2:A:446:VAL:HG12	2:A:946:MET:HE1	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:240:LEU:HD21	2:A:267:ILE:HD11	1.58	0.83
2:A:661:LEU:CD2	2:A:662:TRP:N	2.37	0.83
2:A:391:MET:HE3	2:A:474:LEU:HD11	1.59	0.82
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:85:PHE:HD1	2:A:812:MET:HE1	1.46	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
2:A:402:ALA:HB3	2:A:486:MET:HE1	1.67	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:120:GLN:NE2	1:B:243:PRO:HD2	1.98	0.76
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.67	0.76
2:A:85:PHE:CD1	2:A:812:MET:HE1	2.21	0.75
2:A:969:LEU:HD21	2:A:1036:LYS:HB2	1.68	0.75
2:A:891:PHE:HE2	2:A:942:VAL:HG13	1.52	0.75
1:B:204:ILE:HD12	1:B:204:ILE:H	1.51	0.74
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.69	0.74
2:A:712:SER:HB3	2:A:827:ASP:HB3	1.69	0.74
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.21	0.74
2:A:980:ARG:NH1	2:A:1028:LEU:HA	2.02	0.74
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.69	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:398:ILE:HG13	2:A:1016:MET:HE1	1.72	0.71
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:HD12	2:A:42:LEU:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:701:GLU:HG2	2:A:705:ARG:HH22	1.56	0.68
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.74	0.68
2:A:153:LEU:HD12	2:A:153:LEU:H	1.57	0.68
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.24	0.68
2:A:61:VAL:O	2:A:65:VAL:HG12	1.93	0.68
2:A:237:LEU:HG	2:A:243:PHE:CE1	2.29	0.68
1:B:280:LYS:HE3	1:B:280:LYS:HA	1.76	0.67
1:B:93:GLY:HA3	2:A:146:ASP:O	1.94	0.67
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.77	0.67
2:A:550:VAL:HG12	2:A:909:VAL:HG22	1.76	0.67
2:A:630:LEU:HD13	2:A:642:MET:HE1	1.76	0.66
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:466:THR:O	2:A:871:LYS:HE2	1.96	0.65
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.78	0.65
1:C:254:ILE:O	1:C:256:TRP:N	2.30	0.65
2:A:1020:MET:HE3	2:A:1020:MET:HA	1.77	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:425:HIS:HB3	2:A:426:PRO:HD2	1.78	0.64
2:A:715:ALA:HB2	2:A:824:ILE:HG12	1.80	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:315:LEU:HD11	2:A:321:ILE:HD11	1.80	0.63
2:A:475:PHE:HZ	2:A:562:LEU:HD21	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:729:ASN:ND2	2:A:732:LYS:H	1.96	0.62
1:C:317:LEU:C	1:C:317:LEU:HD12	2.24	0.62
1:B:114:VAL:HG12	1:B:309:PRO:HA	1.80	0.62
1:C:384:LEU:HD11	2:A:588:MET:HE2	1.81	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:B:360:ALA:HB2	1:B:365:THR:HG22	1.81	0.62
1:C:165:TYR:CE2	1:C:182:LEU:HD11	2.35	0.62
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.30	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:297:ALA:O	2:A:301:ILE:HG13	2.01	0.61
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.82	0.61
1:C:388:GLU:HB2	2:A:657:GLY:H	1.66	0.61
2:A:243:PHE:HB3	2:A:265:VAL:HG21	1.81	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:409:VAL:HG11	2:A:450:LEU:HD21	1.83	0.60
2:A:572:TYR:CE2	2:A:592:THR:HG21	2.36	0.60
1:C:80:SER:HA	1:C:397:ARG:HD2	1.83	0.60
2:A:488:GLY:O	2:A:492:LEU:HB2	2.01	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:378:PHE:HA	2:A:381:MET:HE2	1.84	0.59
2:A:861:GLN:HA	2:A:864:LEU:HD12	1.84	0.59
2:A:880:LEU:O	2:A:883:ILE:HG22	2.03	0.59
1:B:307:LEU:HD12	1:B:307:LEU:H	1.67	0.59
1:C:359:GLN:HG3	1:C:360:ALA:N	2.18	0.59
2:A:141:GLU:HB2	2:A:325:TYR:HB3	1.84	0.59
2:A:270:GLU:HG2	2:A:271:MET:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HB	1:C:227:MET:CG	2.33	0.58
2:A:786:LEU:HB3	2:A:798:LEU:HB2	1.84	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:883:ILE:O	2:A:887:LEU:HG	2.02	0.58
2:A:980:ARG:HH12	2:A:1028:LEU:HA	1.67	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:535:TRP:NE1	2:A:537:LYS:HB3	2.18	0.58
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.86	0.58
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.04	0.57
1:B:378:VAL:HG21	1:B:383:PHE:CE2	2.38	0.57
1:B:385:ILE:HG13	2:A:272:ARG:HB2	1.86	0.57
2:A:411:ILE:HG23	2:A:415:HIS:CE1	2.40	0.57
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.86	0.57
2:A:186:GLU:HG3	2:A:767:PRO:HG2	1.85	0.57
2:A:701:GLU:HG2	2:A:705:ARG:NH2	2.19	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
1:B:358:PHE:HE2	1:C:273:ASP:HB3	1.70	0.57
2:A:786:LEU:HD22	2:A:787:PRO:HD2	1.85	0.57
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:123:ILE:HB	1:C:227:MET:HG2	1.87	0.56
1:B:174:THR:H	1:B:177:GLN:NE2	1.95	0.56
2:A:384:GLN:HG3	2:A:386:LEU:HD13	1.87	0.56
2:A:399:ALA:HB2	2:A:482:LYS:HG2	1.88	0.56
2:A:534:HIS:C	2:A:534:HIS:CD2	2.83	0.56
2:A:872:LEU:O	2:A:876:VAL:HG23	2.05	0.56
1:B:332:LEU:HA	1:B:341:VAL:HG12	1.86	0.56
2:A:436:TRP:CD1	2:A:436:TRP:C	2.83	0.56
2:A:550:VAL:HA	2:A:913:TRP:NE1	2.10	0.56
2:A:661:LEU:C	2:A:661:LEU:HD22	2.29	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:522:ILE:O	2:A:526:HIS:HD2	1.87	0.56
2:A:660:ASN:ND2	2:A:660:ASN:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:661:LEU:HD12	2:A:679:SER:HB3	1.88	0.55
1:B:324:MET:HE1	1:B:358:PHE:CG	2.41	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
1:C:223:LEU:C	1:C:224:ARG:HD2	2.32	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
1:C:268:VAL:HG12	1:C:276:LEU:HD11	1.89	0.55
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.05	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
1:C:332:LEU:HD11	1:C:357:VAL:HG22	1.88	0.54
2:A:361:ARG:O	2:A:365:VAL:HG23	2.07	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
1:B:336:GLY:HA3	2:A:775:SER:OG	2.08	0.54
1:C:254:ILE:O	1:C:255:ALA:C	2.51	0.54
2:A:422:GLN:HG2	2:A:427:ASP:OD1	2.07	0.54
2:A:960:ASN:N	2:A:961:PRO:HD2	2.22	0.54
2:A:411:ILE:HA	2:A:501:MET:HE1	1.90	0.54
2:A:595:LEU:O	2:A:598:SER:HB3	2.07	0.54
2:A:904:VAL:HG12	2:A:937:ALA:HB3	1.90	0.54
1:C:120:GLN:OE1	1:C:243:PRO:HD2	2.08	0.54
1:C:158:TRP:O	1:C:162:GLN:HG3	2.08	0.54
2:A:349:VAL:HG11	2:A:404:VAL:HG11	1.89	0.54
2:A:243:PHE:O	2:A:246:ILE:HG13	2.07	0.54
1:B:223:LEU:C	1:B:224:ARG:HD2	2.33	0.54
2:A:715:ALA:CB	2:A:824:ILE:HG12	2.37	0.54
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.08	0.53
1:B:245:TRP:CE3	1:B:297:ARG:HD3	2.43	0.53
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.88	0.53
2:A:223:GLU:O	2:A:224:LEU:HD23	2.08	0.53
2:A:291:LEU:HD22	2:A:297:ALA:HA	1.89	0.53
1:B:124:VAL:O	1:B:235:VAL:HG22	2.08	0.53
1:C:138:LEU:HD21	1:C:144:VAL:HG11	1.90	0.53
2:A:453:SER:HA	2:A:456:ILE:HD12	1.90	0.53
2:A:871:LYS:O	2:A:875:MET:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:217:ALA:HB3	2:A:233:ALA:HB3	1.89	0.53
2:A:404:VAL:HG22	2:A:408:ILE:HG23	1.91	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:B:252:GLU:CG	1:C:270:ALA:HB2	2.39	0.53
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.90	0.53
1:C:342:ILE:HB	1:C:378:VAL:HG12	1.90	0.53
2:A:898:LEU:C	2:A:898:LEU:HD23	2.34	0.53
1:B:117:ASN:HD22	1:B:117:ASN:C	2.16	0.53
1:B:250:ILE:HG21	1:B:258:VAL:HG11	1.91	0.53
1:B:274:LYS:O	1:B:276:LEU:HD23	2.09	0.53
2:A:13:ARG:HA	2:A:499:ILE:HD13	1.90	0.53
2:A:140:TYR:HD2	2:A:304:VAL:HG11	1.73	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
1:B:386:ASP:O	1:B:387:SER:C	2.53	0.52
2:A:69:LEU:HD11	2:A:121:LEU:HD11	1.91	0.52
1:B:271:ARG:CD	1:B:306:ALA:HB1	2.39	0.52
2:A:184:VAL:HG23	2:A:270:GLU:HB3	1.91	0.52
2:A:97:PHE:CZ	2:A:106:ALA:HB1	2.44	0.52
2:A:882:ILE:O	2:A:886:LEU:HG	2.10	0.52
2:A:995:LEU:C	2:A:1017:ILE:HD11	2.35	0.52
1:B:292:ARG:HG3	1:C:312:ASN:HD21	1.75	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
1:C:166:LEU:O	1:C:170:GLU:HG2	2.10	0.51
2:A:49:ILE:HB	2:A:93:VAL:HB	1.92	0.51
2:A:275:ILE:CD1	2:A:586:ALA:HB2	2.36	0.51
2:A:431:ASP:CG	2:A:432:ASN:H	2.18	0.51
1:B:307:LEU:HD12	1:B:307:LEU:N	2.25	0.51
1:C:106:PHE:O	1:C:318:ASN:HA	2.10	0.51
2:A:944:MET:HE2	2:A:1031:ILE:HB	1.91	0.51
1:B:132:ILE:HD11	1:B:229:ILE:HB	1.92	0.51
1:B:158:TRP:O	1:B:162:GLN:HG3	2.10	0.51
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:TRP:O	2:A:425:HIS:HB2	2.10	0.51
2:A:554:LEU:HD21	2:A:912:ILE:HG12	1.93	0.51
2:A:1028:LEU:O	2:A:1032:PRO:HG2	2.10	0.51
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.46	0.51
2:A:729:ASN:C	2:A:729:ASN:HD22	2.19	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:87:GLN:HE21	2:A:812:MET:HE2	1.75	0.51
2:A:327:ARG:NH1	2:A:666:ILE:HG12	2.26	0.51
2:A:551:LEU:C	2:A:551:LEU:HD23	2.35	0.51
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.92	0.51
1:B:342:ILE:HD13	1:B:398:MET:HE1	1.93	0.51
1:C:327:ILE:HD13	1:C:367:LEU:HD21	1.93	0.51
1:C:388:GLU:HB2	2:A:657:GLY:N	2.26	0.51
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
2:A:906:PHE:O	2:A:909:VAL:HG12	2.11	0.50
1:B:104:LEU:HD11	1:B:359:GLN:O	2.12	0.50
2:A:342:LEU:HD21	2:A:397:ALA:HA	1.92	0.50
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.92	0.50
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.92	0.50
2:A:764:ALA:O	2:A:765:ARG:HG3	2.11	0.50
2:A:884:PHE:CD1	2:A:884:PHE:C	2.90	0.50
2:A:925:ALA:O	2:A:1012:ILE:HG13	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
2:A:984:LYS:HD2	2:A:984:LYS:C	2.37	0.50
1:B:162:GLN:OE1	1:B:198:LEU:HD13	2.10	0.50
1:B:174:THR:HB	1:B:177:GLN:HG3	1.93	0.50
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.94	0.50
1:B:356:ALA:HB1	1:B:368:ARG:NH1	2.27	0.50
2:A:56:GLN:HB3	2:A:60:ILE:HG23	1.93	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
2:A:950:HIS:HA	2:A:953:GLU:CG	2.34	0.50
2:A:980:ARG:C	2:A:983:PRO:HD2	2.36	0.50
1:C:124:VAL:O	1:C:235:VAL:HG12	2.11	0.49
2:A:399:ALA:HB1	2:A:486:MET:HE2	1.94	0.49
2:A:420:GLU:HG3	2:A:421:TRP:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:667:ARG:HH11	2:A:861:GLN:HE22	1.60	0.49
2:A:984:LYS:HG3	2:A:1028:LEU:HD21	1.94	0.49
1:B:94:VAL:HG21	1:B:350:PHE:HZ	1.76	0.49
2:A:408:ILE:HD12	2:A:986:MET:HB3	1.93	0.49
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.48	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:B:339:GLN:HG3	1:B:357:VAL:HG22	1.94	0.49
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.11	0.49
2:A:153:LEU:H	2:A:153:LEU:CD1	2.24	0.49
2:A:573:MET:HE1	2:A:668:ASN:ND2	2.27	0.49
2:A:956:PRO:HA	2:A:959:ASN:ND2	2.27	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:276:ALA:HB3	2:A:284:VAL:O	2.12	0.49
1:B:340:ARG:HD3	1:B:395:LEU:HD12	1.94	0.49
1:C:110:PHE:CE1	1:C:250:ILE:HG13	2.47	0.49
2:A:83:ARG:HG2	2:A:816:GLU:HG3	1.94	0.49
2:A:402:ALA:HB3	2:A:486:MET:CE	2.42	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
1:B:383:PHE:C	1:B:384:LEU:HD12	2.38	0.49
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.95	0.49
2:A:550:VAL:HG12	2:A:550:VAL:O	2.11	0.49
2:A:868:ALA:O	2:A:872:LEU:HG	2.13	0.49
1:B:153:LEU:N	1:B:153:LEU:HD23	2.28	0.48
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
2:A:403:MET:SD	2:A:485:ALA:HB1	2.53	0.48
2:A:601:GLU:OE2	2:A:637:ARG:HD3	2.13	0.48
2:A:910:GLY:HA3	2:A:1022:THR:OG1	2.12	0.48
2:A:969:LEU:O	2:A:973:LEU:HD13	2.13	0.48
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.43	0.48
2:A:410:MET:HE1	2:A:493:ALA:O	2.13	0.48
1:C:171:THR:O	1:C:172:GLY:C	2.55	0.48
2:A:395:GLY:HA2	2:A:398:ILE:HG22	1.95	0.48
2:A:522:ILE:HG23	2:A:526:HIS:HE2	1.79	0.48
1:B:344:VAL:HG13	1:B:348:GLY:HA2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:56:GLN:HB3	2:A:60:ILE:CG2	2.43	0.48
1:B:222:ASP:HB2	1:B:234:VAL:O	2.13	0.48
1:B:271:ARG:NE	1:B:306:ALA:HB1	2.28	0.48
2:A:212:ALA:C	2:A:215:GLN:HE22	2.21	0.48
2:A:419:GLU:O	2:A:423:HIS:HD2	1.96	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:114:LEU:HD11	2:A:127:ALA:HB1	1.94	0.48
2:A:550:VAL:CG1	2:A:909:VAL:HG22	2.43	0.48
2:A:1001:GLY:O	2:A:1002:THR:C	2.56	0.48
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.44	0.48
2:A:368:ILE:O	2:A:368:ILE:HG22	2.14	0.48
2:A:376:ILE:HD13	2:A:488:GLY:HA2	1.96	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:NZ	2:A:644:LYS:HB3	2.29	0.48
2:A:37:ASP:OD2	2:A:297:ALA:HB3	2.14	0.47
2:A:48:ILE:HG22	2:A:94:TYR:CD2	2.49	0.47
1:B:360:ALA:HA	1:B:365:THR:HA	1.95	0.47
2:A:700:ILE:HA	2:A:703:VAL:HG22	1.95	0.47
2:A:952:ILE:HA	2:A:957:SER:CB	2.44	0.47
1:B:350:PHE:HB3	1:B:398:MET:HE2	1.97	0.47
2:A:185:LYS:HG2	2:A:766:TYR:CD2	2.49	0.47
2:A:525:TYR:CE2	2:A:1029:PHE:HE2	2.31	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:57:ALA:O	2:A:61:VAL:HG23	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
1:C:189:GLY:O	1:C:190:MET:C	2.58	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:76:VAL:HG13	2:A:77:PRO:HD2	1.95	0.47
2:A:456:ILE:HG12	2:A:886:LEU:CD1	2.44	0.47
2:A:666:ILE:O	2:A:670:ILE:HG13	2.14	0.47
2:A:45:VAL:HG11	2:A:103:PRO:HA	1.97	0.47
2:A:139:ILE:O	2:A:325:TYR:HD1	1.97	0.47
2:A:1032:PRO:C	2:A:1034:ALA:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ALA:O	1:C:394:ALA:HB3	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:988:VAL:HG12	2:A:988:VAL:O	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
1:B:143:LYS:HD2	1:B:216:GLY:O	2.15	0.47
1:B:291:THR:O	1:B:293:THR:N	2.48	0.47
2:A:42:LEU:HD12	2:A:42:LEU:N	2.25	0.47
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:1037:LEU:HD23	2:A:1037:LEU:O	2.16	0.46
2:A:390:ILE:HG23	2:A:391:MET:HE2	1.98	0.46
2:A:459:LEU:HB3	2:A:882:ILE:HD13	1.98	0.46
1:C:167:LEU:C	1:C:167:LEU:HD12	2.41	0.46
1:C:223:LEU:HD21	1:C:233:ASN:HD22	1.80	0.46
2:A:296:ASN:HB3	2:A:299:GLU:HB3	1.97	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:985:ALA:O	2:A:989:ALA:HB2	2.15	0.46
2:A:637:ARG:HB2	2:A:637:ARG:HH11	1.79	0.46
1:C:384:LEU:HD21	2:A:588:MET:HE2	1.98	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
1:C:266:LEU:HG	1:C:278:ILE:HD11	1.98	0.46
2:A:73:MET:HE1	2:A:110:VAL:HG13	1.96	0.46
2:A:952:ILE:HG12	2:A:1039:TRP:HE1	1.80	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:65:VAL:HA	2:A:121:LEU:HD22	1.98	0.46
2:A:137:GLY:O	2:A:290:ILE:HA	2.15	0.46
2:A:813:LEU:HD13	2:A:813:LEU:HA	1.81	0.46
1:C:91:ASN:O	2:A:591:LYS:HD3	2.16	0.46
1:C:223:LEU:HD12	1:C:235:VAL:HB	1.98	0.46
2:A:297:ALA:O	2:A:300:VAL:HG12	2.16	0.46
2:A:298:ARG:O	2:A:298:ARG:HD3	2.15	0.46
2:A:87:GLN:NE2	2:A:812:MET:HE2	2.31	0.46
2:A:580:ILE:HG22	2:A:622:GLU:HB3	1.97	0.46
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.16	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: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:625:GLU:O	2:A:625:GLU:HG3	2.16	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
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
2:A:87:GLN:CG	2:A:812:MET:HE2	2.46	0.45
2:A:153:LEU:HD12	2:A:153:LEU:N	2.26	0.45
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.41	0.45
2:A:31:ILE:HG13	2:A:378:PHE:CZ	2.51	0.45
2:A:53:TYR:CE1	2:A:56:GLN:HG3	2.51	0.45
2:A:991:ILE:O	2:A:995:LEU:HD13	2.17	0.45
2:A:575:SER:O	2:A:658:LEU:HD12	2.16	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:661:LEU:HD23	2:A:662:TRP:H	1.63	0.45
1:B:302:ASN:HD21	1:B:306:ALA:N	2.15	0.45
2:A:404:VAL:O	2:A:408:ILE:HG12	2.17	0.45
2:A:462:ILE:N	2:A:463:PRO:CD	2.80	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:816:GLU:O	2:A:817:ASN:HB2	2.17	0.45
2:A:988:VAL:HG11	2:A:1024:PRO:HG2	1.99	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:988:VAL:CG1	2:A:1024:PRO:HG2	2.46	0.45
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.41	0.44
1:C:358:PHE:HD2	1:C:368:ARG:NH2	2.14	0.44
2:A:222:ILE:HG23	2:A:229:TYR:HB2	1.98	0.44
2:A:494:ILE:HG12	2:A:494:ILE:O	2.17	0.44
2:A:561:PHE:CE1	2:A:864:LEU:HB3	2.51	0.44
2:A:723:TYR:O	2:A:806:VAL:HA	2.17	0.44
2:A:944:MET:HG2	2:A:980:ARG:CD	2.37	0.44
1:C:384:LEU:HD21	2:A:588:MET:CE	2.48	0.44
2:A:6:ILE:HD13	2:A:6:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:359:HIS:HD2	2:A:360:VAL:N	2.14	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: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: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
2:A:55:GLY:O	2:A:56:GLN:C	2.60	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
1:B:252:GLU:HG3	1:C:270:ALA:HB2	2.00	0.44
2:A:525:TYR:HE1	2:A:977:ALA:HB1	1.83	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
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: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
2:A:619:ALA:HB1	2:A:623:MET:HG2	2.00	0.44
1:C:284:LEU:HB3	1:C:285:PRO:HD2	2.00	0.43
2:A:534:HIS:CD2	2:A:534:HIS:O	2.71	0.43
2:A:1020:MET:HA	2:A:1020:MET:CE	2.48	0.43
2:A:904:VAL:N	2:A:905:PRO:CD	2.81	0.43
1:B:85:ASP:HA	1:B:86:PRO:HD3	1.87	0.43
2:A:399:ALA:CB	2:A:486:MET:HE2	2.48	0.43
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.48	0.43
1:B:327:ILE:CD1	1:B:341:VAL:HG11	2.48	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
2:A:999:LEU:HD21	2:A:1014:ALA:HA	2.00	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
2:A:636:TRP:CD1	2:A:636:TRP:N	2.86	0.43
2:A:746:PHE:O	2:A:750:ALA:HB3	2.18	0.43
2:A:831:ARG:HH22	2:A:839:ASP:CG	2.27	0.43
2:A:952:ILE:HA	2:A:957:SER:OG	2.17	0.43
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.99	0.43
2:A:40:PRO:O	2:A:41:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:272:ARG:NH2	2:A:283:GLU:OE1	2.51	0.43
2:A:367:ILE:C	2:A:369:SER:H	2.27	0.43
2:A:575:SER:N	2:A:659:ALA:O	2.51	0.43
2:A:965:SER:HB3	2:A:968:LYS:HD3	2.01	0.43
1:B:389:ALA:O	1:B:390:ASN:C	2.61	0.43
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.83	0.43
1:C:224:ARG:HD2	1:C:224:ARG:N	2.33	0.43
1:C:331:ALA:O	1:C:341:VAL:HG12	2.19	0.43
2:A:214:ASN:C	2:A:215:GLN:HG3	2.43	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
2:A:661:LEU:HD23	2:A:662:TRP:C	2.44	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:277:GLU:OE2	2:A:590:GLN:HG3	2.19	0.42
2:A:756:VAL:O	2:A:756:VAL:HG12	2.18	0.42
2:A:969:LEU:CD2	2:A:1036:LYS:HE3	2.48	0.42
1:B:384:LEU:HD21	1:B:395:LEU:HD23	2.01	0.42
1:C:153:LEU:HD23	1:C:153:LEU:H	1.83	0.42
1:C:268:VAL:HA	1:C:269:PRO:HD3	1.93	0.42
2:A:590:GLN:O	2:A:594:LYS:HG3	2.19	0.42
2:A:1025:LEU:HD23	2:A:1025:LEU:C	2.45	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
2:A:633:GLN:HA	2:A:636:TRP:CE2	2.54	0.42
2:A:783:LEU:O	2:A:798:LEU:HB3	2.19	0.42
1:C:264:PHE:HB3	1:C:315:LEU:HD11	2.02	0.42
2:A:370:LEU:HB2	2:A:371:PRO:HD3	2.02	0.42
2:A:897:ALA:O	2:A:901:ILE:HG13	2.20	0.42
2:A:927:GLY:O	2:A:931:ILE:HG12	2.20	0.42
1:B:343:THR:HA	1:B:377:VAL:HA	2.02	0.42
1:B:384:LEU:HD12	1:B:384:LEU:N	2.35	0.42
2:A:191:ILE:HD11	2:A:206:VAL:HG11	2.01	0.42
2:A:552:TRP:N	2:A:553:PRO:CD	2.83	0.42
2:A:567:GLU:CD	2:A:665:PRO:HD2	2.45	0.42
1:B:271:ARG:HA	1:B:272:PRO:HD3	1.85	0.42
2:A:497:ILE:O	2:A:501:MET:HG2	2.19	0.42
1:B:307:LEU:H	1:B:307:LEU:CD1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:ILE:C	2:A:337:ASN:H	2.27	0.42
2:A:884:PHE:HB2	2:A:901:ILE:HD11	2.01	0.42
2:A:955:VAL:N	2:A:956:PRO:CD	2.83	0.42
2:A:57:ALA:HB1	2:A:58:PRO:HD2	2.01	0.41
2:A:327:ARG:O	2:A:331:ILE:HG12	2.20	0.41
2:A:611:LYS:HA	2:A:617:ASP:OD2	2.20	0.41
1:B:271:ARG:HB3	1:B:274:LYS:HB2	2.02	0.41
1:C:324:MET:HE2	1:C:324:MET:HA	2.01	0.41
1:C:343:THR:OG1	1:C:353:LYS:HD3	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
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.41
1:C:106:PHE:CZ	1:C:359:GLN:HG2	2.56	0.41
2:A:65:VAL:HA	2:A:121:LEU:CD2	2.50	0.41
2:A:119:GLY:C	2:A:121:LEU:H	2.27	0.41
2:A:121:LEU:HB3	2:A:125:VAL:HG21	2.01	0.41
2:A:342:LEU:HD23	2:A:342:LEU:HA	1.83	0.41
2:A:530:LEU:C	2:A:530:LEU:HD12	2.46	0.41
2:A:534:HIS:O	2:A:534:HIS:HD2	2.04	0.41
1:B:132:ILE:CD1	1:B:229:ILE:HB	2.50	0.41
1:B:302:ASN:HD21	1:B:306:ALA:H	1.68	0.41
1:B:335:THR:HG23	1:B:338:GLU:O	2.21	0.41
1:B:399:ARG:O	1:B:400:SER:HB2	2.19	0.41
1:C:281:TRP:HB2	1:C:298:LEU:HD23	2.02	0.41
1:C:329:SER:HA	1:C:365:THR:HG22	2.01	0.41
2:A:46:GLN:HB2	2:A:96:ILE:HD13	2.03	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:461:PHE:C	2:A:463:PRO:HD2	2.46	0.41
1:B:342:ILE:HG21	1:B:398:MET:HE1	2.02	0.41
1:C:220:ALA:HB3	1:C:237:LYS:HB3	2.02	0.41
2:A:67:TYR:CD2	2:A:67:TYR:C	2.98	0.41
2:A:189:VAL:HG22	2:A:265:VAL:HG22	2.01	0.41
1:B:259:LYS:HG3	1:B:260:ASP:N	2.36	0.41
1:B:291:THR:O	1:B:293:THR:HG23	2.21	0.41
1:B:125:GLN:HE21	1:C:227:MET:HB3	1.85	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
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

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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:595:LEU:HB3	2:A:653:VAL:HG22	2.03	0.41
2:A:661:LEU:CD1	2:A:679:SER:HB3	2.51	0.41
2:A:834:VAL:HA	2:A:837:VAL:HG22	2.02	0.41
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.55	0.41
1:C:283:LEU:HD23	1:C:283:LEU:HA	1.82	0.41
2:A:201:ILE:HD13	2:A:248:LEU:HB3	2.02	0.41
2:A:356:PHE:HE2	2:A:985:ALA:O	2.04	0.41
2:A:641:THR:H	2:A:644:LYS:HB2	1.86	0.41
2:A:946:MET:HE2	2:A:947:TYR:CE2	2.56	0.41
1:C:357:VAL:HA	1:C:367:LEU:HD12	2.03	0.40
2:A:904:VAL:O	2:A:908:LEU:HG	2.20	0.40
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.36	0.40
2:A:533:LEU:HD22	2:A:1036:LYS:HD2	2.03	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
1:C:108:GLN:HA	1:C:108:GLN:OE1	2.22	0.40
1:C:322:GLU:O	1:C:324:MET:HG2	2.21	0.40
2:A:590:GLN:HG2	2:A:594:LYS:HE3	2.02	0.40
2:A:899:LEU:HA	2:A:899:LEU:HD22	1.90	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:317:LEU:C	1:C:317:LEU:CD1	2.94	0.40
1:C:332:LEU:C	1:C:332:LEU:HD23	2.47	0.40
1:C:353:LYS:HE2	1:C:375:GLU:OE2	2.21	0.40
2:A:359:HIS:CD2	2:A:360:VAL:N	2.90	0.40
2:A:753:GLY:O	2:A:754:ALA:C	2.63	0.40
2:A:960:ASN:HA	2:A:963:THR:O	2.22	0.40
1:B:360:ALA:CB	1:B:365:THR:HG22	2.49	0.40
2:A:421:TRP:O	2:A:421:TRP:HD1	2.04	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 [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%)	284 (89%)	31 (10%)	5 (2%)	7	29
1	C	322/336 (96%)	300 (93%)	19 (6%)	3 (1%)	14	41
2	A	1024/1054 (97%)	923 (90%)	91 (9%)	10 (1%)	12	39
All	All	1666/1726 (96%)	1507 (90%)	141 (8%)	18 (1%)	11	37

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 [i](#)

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%)	6	23
1	C	265/275 (96%)	232 (88%)	33 (12%)	4	18
2	A	847/871 (97%)	757 (89%)	90 (11%)	6	23
All	All	1375/1421 (97%)	1224 (89%)	151 (11%)	6	22

All (151) 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	159	VAL
1	B	167	LEU
1	B	206	THR
1	B	234	VAL
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	307	LEU
1	B	322	GLU
1	B	332	LEU
1	B	335	THR
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

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Mol	Chain	Res	Type
1	C	145	GLN
1	C	150	LEU
1	C	151	LEU
1	C	181	ILE
1	C	185	LEU
1	C	207	ARG
1	C	234	VAL
1	C	247	THR
1	C	257	LEU
1	C	258	VAL
1	C	260	ASP
1	C	268	VAL
1	C	271	ARG
1	C	274	LYS
1	C	283	LEU
1	C	287	VAL
1	C	304	ASP
1	C	317	LEU
1	C	324	MET
1	C	325	LEU
1	C	339	GLN
1	C	351	VAL
1	C	353	LYS
1	C	364	VAL
1	C	365	THR
1	C	367	LEU
1	C	373	GLU
1	C	375	GLU
1	C	382	LEU
1	C	395	LEU
2	A	6	ILE
2	A	34	THR
2	A	36	VAL
2	A	42	LEU
2	A	48	ILE
2	A	51	THR
2	A	59	GLN
2	A	65	VAL
2	A	88	PHE
2	A	105	TRP
2	A	114	LEU
2	A	144	LEU

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Mol	Chain	Res	Type
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	222	ILE
2	A	259	LEU
2	A	260	ARG
2	A	288	VAL
2	A	298	ARG
2	A	322	VAL
2	A	335	ILE
2	A	338	LEU
2	A	343	LEU
2	A	374	LEU
2	A	411	ILE
2	A	412	GLU
2	A	418	LEU
2	A	434	THR
2	A	462	ILE
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	538	THR
2	A	541	LEU
2	A	545	LEU
2	A	547	VAL
2	A	548	LEU
2	A	551	LEU
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	637	ARG
2	A	642	MET

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Mol	Chain	Res	Type
2	A	649	LEU
2	A	660	ASN
2	A	661	LEU
2	A	663	VAL
2	A	672	MET
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	781	GLN
2	A	786	LEU
2	A	789	LEU
2	A	804	ILE
2	A	812	MET
2	A	813	LEU
2	A	882	ILE
2	A	884	PHE
2	A	885	VAL
2	A	899	LEU
2	A	904	VAL
2	A	909	VAL
2	A	945	LEU
2	A	946	MET
2	A	948	LEU
2	A	952	ILE
2	A	955	VAL
2	A	958	LEU
2	A	970	ASP
2	A	999	LEU
2	A	1007	GLU
2	A	1020	MET
2	A	1039	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	120	GLN

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	177	GLN
1	B	202	GLN
1	B	302	ASN
1	B	330	GLN
1	B	390	ASN
1	C	125	GLN
1	C	177	GLN
1	C	263	GLN
1	C	302	ASN
2	A	118	GLN
2	A	151	HIS
2	A	215	GLN
2	A	238	GLN
2	A	279	ASN
2	A	329	GLN
2	A	359	HIS
2	A	413	ASN
2	A	423	HIS
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	651	ASN
2	A	660	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	794	GLN
2	A	795	GLN
2	A	838	HIS
2	A	921	HIS
2	A	950	HIS
2	A	1043	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.18	10 (3%) 51 38	24, 58, 112, 176	0
1	C	324/336 (96%)	0.12	10 (3%) 51 38	25, 58, 110, 174	0
2	A	1028/1054 (97%)	0.97	188 (18%) 3 4	28, 106, 212, 312	0
All	All	1674/1726 (96%)	0.66	208 (12%) 8 9	24, 79, 194, 312	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	15	LEU	11.3
2	A	890	ALA	8.3
2	A	889	LEU	8.1
2	A	450	LEU	6.9
2	A	495	VAL	6.4
2	A	496	VAL	6.3
2	A	17	LEU	6.2
2	A	886	LEU	6.1
2	A	887	LEU	5.5
1	B	386	ASP	5.4
2	A	494	ILE	5.2
1	B	387	SER	5.1
2	A	366	ALA	5.0
2	A	896	GLU	5.0
2	A	406	ALA	4.9
2	A	396	ILE	4.9
2	A	579	GLY	4.8
2	A	883	ILE	4.8
2	A	77	PRO	4.8
2	A	457	ILE	4.6
2	A	355	LEU	4.5
1	C	157	ASP	4.5
2	A	538	THR	4.5

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Mol	Chain	Res	Type	RSRZ
2	A	872	LEU	4.4
2	A	895	GLY	4.2
2	A	484	TYR	4.1
2	A	815	THR	4.1
2	A	972	ALA	4.1
2	A	899	LEU	4.1
2	A	939	GLU	4.1
2	A	973	LEU	4.0
2	A	891	PHE	4.0
2	A	522	ILE	3.9
2	A	480	PHE	3.9
2	A	884	PHE	3.9
2	A	554	LEU	3.9
1	B	157	ASP	3.8
2	A	120	LYS	3.8
2	A	451	PHE	3.8
2	A	392	SER	3.7
2	A	986	MET	3.7
2	A	530	LEU	3.7
2	A	14	PHE	3.7
1	C	255	ALA	3.7
2	A	880	LEU	3.7
2	A	20	ALA	3.6
2	A	935	GLY	3.6
1	C	242	ASP	3.6
2	A	23	LEU	3.6
2	A	528	LEU	3.6
2	A	409	VAL	3.6
2	A	669	ARG	3.6
2	A	6	ILE	3.5
2	A	373	GLY	3.5
2	A	994	GLY	3.5
2	A	124	GLY	3.4
2	A	874	LEU	3.4
2	A	878	MET	3.4
2	A	1000	TRP	3.4
2	A	18	MET	3.4
2	A	22	PHE	3.3
2	A	486	MET	3.3
2	A	71	THR	3.3
2	A	499	ILE	3.3
2	A	35	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	491	LEU	3.3
2	A	942	VAL	3.2
2	A	1039	TRP	3.2
1	B	339	GLN	3.2
2	A	16	VAL	3.2
2	A	353	CYS	3.2
2	A	1036	LYS	3.2
2	A	888	TYR	3.2
2	A	368	ILE	3.2
2	A	363	ALA	3.2
2	A	548	LEU	3.1
2	A	520	PHE	3.1
2	A	401	GLY	3.1
2	A	497	ILE	3.1
2	A	537	LYS	3.1
2	A	1035	TYR	3.1
2	A	870	HIS	3.1
2	A	465	PHE	3.1
2	A	462	ILE	3.1
2	A	10	VAL	3.1
2	A	360	VAL	3.1
2	A	539	THR	3.0
2	A	400	VAL	3.0
2	A	545	LEU	3.0
1	B	242	ASP	3.0
2	A	345	GLU	3.0
2	A	500	LEU	3.0
2	A	873	LYS	3.0
2	A	283	GLU	2.9
2	A	52	SER	2.9
2	A	362	SER	2.9
2	A	354	ALA	2.9
2	A	943	VAL	2.9
2	A	981	VAL	2.9
2	A	901	ILE	2.9
1	C	340	ARG	2.9
2	A	541	LEU	2.9
2	A	552	TRP	2.9
2	A	59	GLN	2.8
2	A	388	ALA	2.8
2	A	82	VAL	2.8
2	A	284	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	A	532	VAL	2.8
2	A	1031	ILE	2.8
2	A	578	PRO	2.8
2	A	369	SER	2.8
2	A	4	TRP	2.7
2	A	720	GLY	2.7
2	A	442	ALA	2.7
2	A	376	ILE	2.7
2	A	439	ILE	2.7
2	A	365	VAL	2.7
2	A	63	ASN	2.7
2	A	990	VAL	2.7
2	A	622	GLU	2.7
2	A	413	ASN	2.7
2	A	969	LEU	2.7
2	A	521	LEU	2.6
2	A	970	ASP	2.6
2	A	563	PRO	2.6
2	A	382	HIS	2.6
1	C	253	SER	2.6
2	A	70	THR	2.6
2	A	871	LYS	2.6
2	A	459	LEU	2.6
2	A	950	HIS	2.5
1	C	339	GLN	2.5
2	A	83	ARG	2.5
2	A	906	PHE	2.5
2	A	553	PRO	2.5
2	A	418	LEU	2.5
2	A	31	ILE	2.5
2	A	448	PRO	2.5
2	A	87	GLN	2.5
2	A	443	SER	2.5
2	A	78	GLY	2.5
2	A	404	VAL	2.5
2	A	551	LEU	2.4
2	A	299	GLU	2.4
2	A	533	LEU	2.4
2	A	1032	PRO	2.4
1	B	214	ILE	2.4
2	A	1037	LEU	2.4
2	A	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	851	LYS	2.4
2	A	946	MET	2.4
2	A	30	THR	2.4
2	A	498	PRO	2.4
2	A	115	ASN	2.4
2	A	73	MET	2.4
2	A	1012	ILE	2.3
2	A	928	THR	2.3
2	A	979	LEU	2.3
2	A	416	LYS	2.3
2	A	481	THR	2.3
2	A	688	THR	2.3
2	A	118	GLN	2.3
2	A	547	VAL	2.3
1	C	105	THR	2.3
2	A	372	LEU	2.3
2	A	952	ILE	2.2
2	A	72	THR	2.2
2	A	379	ILE	2.2
1	B	158	TRP	2.2
2	A	955	VAL	2.2
2	A	279	ASN	2.2
2	A	900	ILE	2.2
2	A	957	SER	2.2
1	B	93	GLY	2.2
2	A	504	TRP	2.2
1	C	306	ALA	2.1
2	A	911	GLY	2.1
2	A	517	LEU	2.1
2	A	879	THR	2.1
2	A	996	LEU	2.1
2	A	273	ARG	2.1
1	C	97	ALA	2.1
2	A	544	ALA	2.1
2	A	1033	ALA	2.1
2	A	502	GLY	2.1
2	A	75	SER	2.1
2	A	332	ASP	2.1
2	A	452	ILE	2.1
2	A	621	LEU	2.1
1	B	271	ARG	2.1
1	B	170	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	703	VAL	2.1
2	A	408	ILE	2.1
2	A	947	TYR	2.1
2	A	57	ALA	2.1
2	A	377	ALA	2.1
2	A	687	GLY	2.1
2	A	378	PHE	2.1
2	A	866	GLU	2.1
2	A	105	TRP	2.0
2	A	81	THR	2.0
1	C	158	TRP	2.0
2	A	26	TRP	2.0
2	A	503	TYR	2.0
2	A	549	THR	2.0
2	A	678	LYS	2.0
2	A	848	VAL	2.0
2	A	826	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CU	A	1048	1/1	0.93	0.09	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.