



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:44 PM UTC

PDB ID : 4DOP / pdb_00004dop
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, R mutant
Authors : Su, C.-C.; Long, F.; Yu, E.
Deposited on : 2012-02-10
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

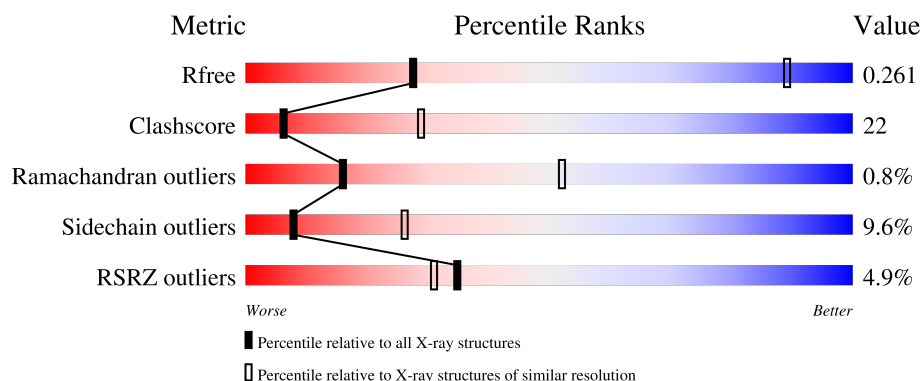
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	413	
1	C	413	
2	A	1054	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12891 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	1031	Total	C	N	O	S	0	0	0
			7942	5137	1330	1438	37			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P38054
A	-5	HIS	-	expression tag	UNP P38054

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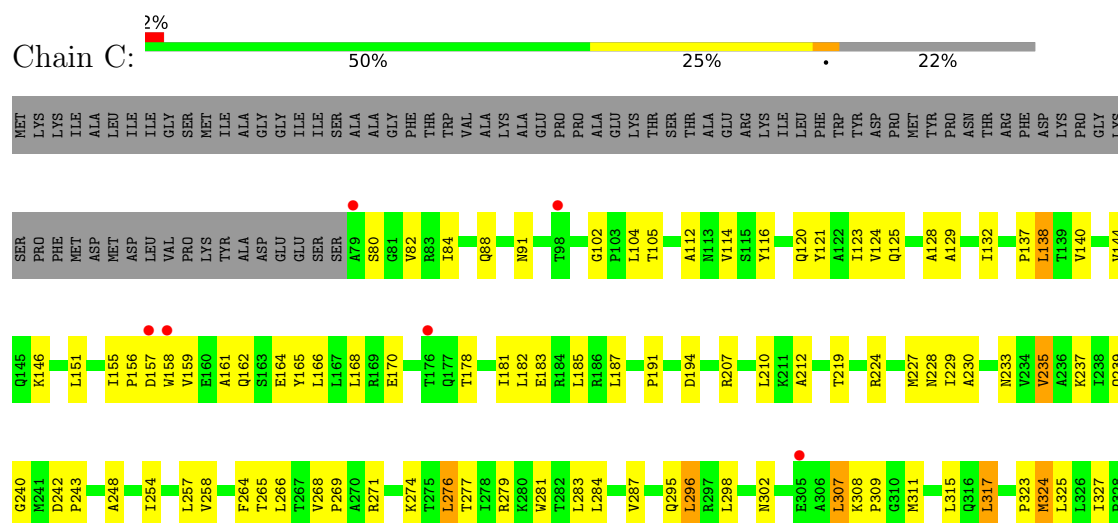
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P38054
A	-3	HIS	-	expression tag	UNP P38054
A	-2	HIS	-	expression tag	UNP P38054
A	-1	HIS	-	expression tag	UNP P38054
A	0	HIS	-	expression tag	UNP P38054
A	669	ALA	ARG	engineered mutation	UNP P38054

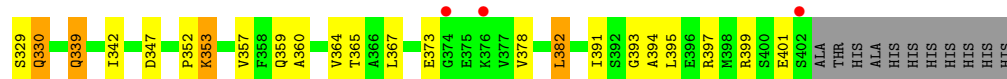
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total O 4 4	0	0
3	C	11	Total O 11 11	0	0
3	A	3	Total O 3 3	0	0

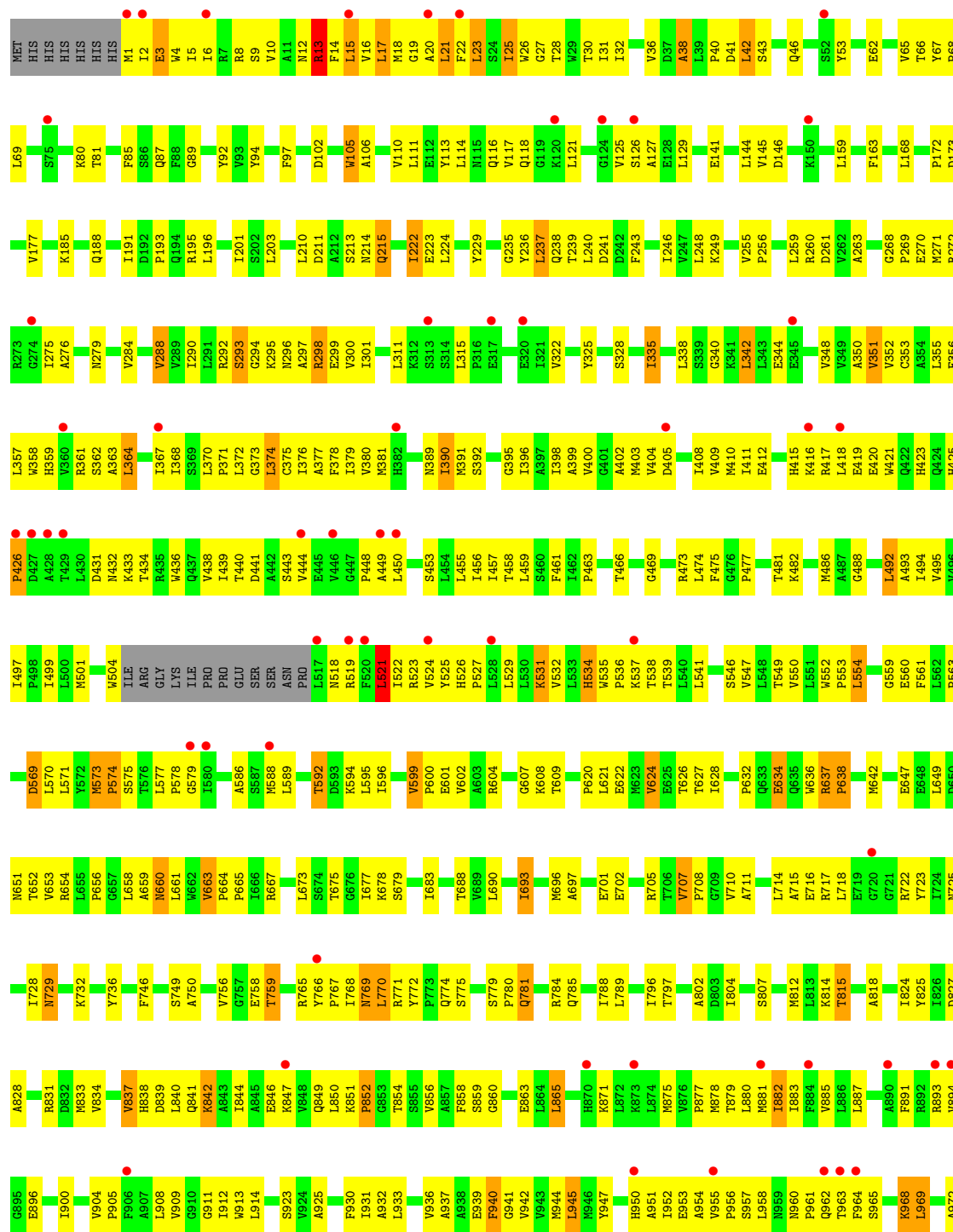
i

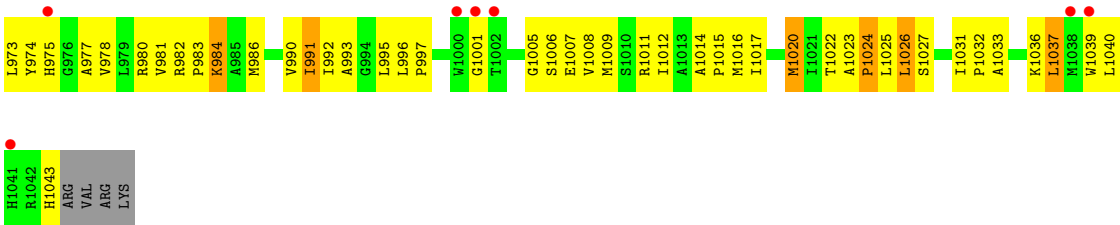
- Molecule 1: Cation efflux system protein CusB





• 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	160.52Å 160.52Å 681.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.31 – 4.20 97.31 – 4.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (97.31-4.20) 99.9 (97.31-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 4.15Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.222 , 0.268 0.212 , 0.261	Depositor DCC
R_{free} test set	1284 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	86.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 150.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12891	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	5/3401 (0.1%)
1	C	0.28	0/2513	0.75	0/3421
2	A	0.29	0/8108	0.76	11/11041 (0.1%)
All	All	0.29	0/13119	0.76	16/17863 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	294	GLY	N-CA-C	6.58	123.77	115.21
2	A	521	LEU	N-CA-C	-6.44	107.27	114.62
1	B	190	MET	CA-C-N	5.86	125.80	119.76
1	B	190	MET	C-N-CA	5.86	125.80	119.76
1	B	381	GLY	N-CA-C	-5.79	105.67	115.34
2	A	577	LEU	CA-C-N	5.63	125.48	119.28
2	A	577	LEU	C-N-CA	5.63	125.48	119.28
2	A	663	VAL	CA-C-N	5.49	123.67	119.66
2	A	663	VAL	C-N-CA	5.49	123.67	119.66
2	A	599	VAL	CA-C-N	5.33	125.04	119.82
2	A	599	VAL	C-N-CA	5.33	125.04	119.82
2	A	707	VAL	CA-C-N	5.30	126.47	119.84
2	A	707	VAL	C-N-CA	5.30	126.47	119.84
2	A	579	GLY	N-CA-C	5.28	120.55	114.16
1	B	271	ARG	CA-C-N	5.19	124.70	119.19
1	B	271	ARG	C-N-CA	5.19	124.70	119.19

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	98	0
1	C	2473	0	2533	84	0
2	A	7942	0	8187	422	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	11	0	0	0	0
All	All	12891	0	13242	582	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 22.

All (582) 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:573:MET:HG2	2:A:678:LYS:NZ	1.80	0.96
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.49	0.94
2:A:696:MET:HG3	2:A:854:THR:HG21	1.50	0.93
2:A:573:MET:SD	2:A:678:LYS:HD2	2.11	0.90
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.52	0.89
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.55	0.89
2:A:459:LEU:HB3	2:A:882:ILE:HD11	1.58	0.84
1:B:117:ASN:HD22	1:B:119:TYR:H	1.23	0.83
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.61	0.82
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.62	0.80
2:A:851:LYS:HB3	2:A:852:PRO:HD2	1.63	0.80
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.63	0.79
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.63	0.79
2:A:550:VAL:HB	2:A:909:VAL:HG13	1.65	0.79
2:A:191:ILE:HD13	2:A:263:ALA:HB2	1.65	0.77
2:A:550:VAL:HG11	2:A:909:VAL:HG22	1.65	0.77
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.67	0.76
1:C:80:SER:HA	1:C:397:ARG:HD2	1.67	0.76
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.69	0.75
1:B:117:ASN:ND2	1:B:119:TYR:H	1.85	0.74
2:A:6:ILE:HD13	2:A:443:SER:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:GLN:HE22	2:A:127:ALA:H	1.35	0.74
1:B:159:VAL:HG23	1:B:204:ILE:HG21	1.70	0.74
1:C:283:LEU:HD23	1:C:296:LEU:HD12	1.69	0.74
2:A:573:MET:HG2	2:A:678:LYS:HZ2	1.52	0.73
1:B:125:GLN:NE2	1:C:228:ASN:H	1.88	0.72
1:B:125:GLN:HE21	1:C:228:ASN:H	1.38	0.71
2:A:391:MET:HE3	2:A:474:LEU:HD11	1.73	0.71
2:A:20:ALA:HA	2:A:23:LEU:HD23	1.71	0.71
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.71	0.71
2:A:529:LEU:O	2:A:532:VAL:HG12	1.92	0.70
2:A:27:GLY:HA3	2:A:375:CYS:HB3	1.72	0.70
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.73	0.70
2:A:784:ARG:HG3	2:A:804:ILE:HD11	1.73	0.70
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.71	0.70
2:A:377:ALA:O	2:A:381:MET:HG3	1.93	0.69
2:A:466:THR:O	2:A:871:LYS:HE2	1.92	0.69
2:A:493:ALA:HA	2:A:497:ILE:HB	1.74	0.69
2:A:609:THR:HG22	2:A:624:VAL:HB	1.75	0.69
2:A:42:LEU:HA	2:A:473:ARG:HD2	1.75	0.68
2:A:80:LYS:HG2	2:A:81:THR:HG23	1.74	0.68
2:A:991:ILE:O	2:A:995:LEU:HB2	1.93	0.68
2:A:573:MET:CG	2:A:678:LYS:HD2	2.23	0.68
2:A:378:PHE:HA	2:A:381:MET:HE2	1.76	0.68
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.76	0.68
2:A:279:ASN:HD21	2:A:604:ARG:HA	1.57	0.68
1:B:360:ALA:HA	1:B:365:THR:HA	1.74	0.67
2:A:980:ARG:O	2:A:984:LYS:HB2	1.94	0.67
1:B:308:LYS:HB2	1:B:311:MET:HE3	1.77	0.66
2:A:357:LEU:HD13	2:A:986:MET:HE1	1.77	0.66
2:A:547:VAL:O	2:A:550:VAL:HG12	1.95	0.66
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.76	0.66
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.30	0.66
2:A:552:TRP:HB3	2:A:553:PRO:HD3	1.76	0.66
2:A:940:PHE:C	2:A:940:PHE:CD2	2.73	0.66
2:A:65:VAL:O	2:A:69:LEU:HB2	1.96	0.66
2:A:977:ALA:HA	2:A:980:ARG:NE	2.10	0.66
2:A:411:ILE:HA	2:A:501:MET:HE1	1.78	0.65
2:A:940:PHE:CE1	2:A:1024:PRO:HA	2.32	0.65
2:A:986:MET:O	2:A:990:VAL:HG22	1.97	0.65
1:C:254:ILE:HG22	1:C:257:LEU:HB2	1.77	0.65
1:C:219:THR:OG1	1:C:237:LYS:HD2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:707:VAL:HG21	2:A:840:LEU:HD23	1.77	0.65
2:A:573:MET:HG2	2:A:678:LYS:HD2	1.78	0.65
2:A:364:LEU:O	2:A:368:ILE:HG12	1.96	0.65
2:A:588:MET:HE2	2:A:658:LEU:HD22	1.77	0.65
1:C:302:ASN:HD21	1:C:307:LEU:H	1.45	0.64
2:A:482:LYS:O	2:A:486:MET:HG2	1.96	0.64
2:A:573:MET:HG2	2:A:678:LYS:CE	2.28	0.64
1:B:280:LYS:HE3	1:B:280:LYS:HA	1.80	0.63
2:A:601:GLU:OE2	2:A:637:ARG:HD3	1.99	0.63
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.79	0.63
2:A:532:VAL:HG23	2:A:539:THR:HG21	1.81	0.63
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.81	0.63
2:A:569:ASP:HB3	2:A:628:ILE:O	1.98	0.63
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.34	0.63
2:A:729:ASN:C	2:A:729:ASN:HD22	2.07	0.63
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.79	0.63
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.79	0.63
2:A:398:ILE:HD11	2:A:482:LYS:HG3	1.82	0.62
2:A:955:VAL:HG12	2:A:956:PRO:HD3	1.81	0.62
2:A:960:ASN:HB2	2:A:961:PRO:HD3	1.81	0.62
2:A:550:VAL:HG21	2:A:909:VAL:HA	1.80	0.62
1:B:385:ILE:HG22	1:B:389:ALA:HB2	1.82	0.62
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.34	0.62
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.80	0.62
1:B:360:ALA:HB2	1:B:365:THR:HG22	1.82	0.62
2:A:891:PHE:HE2	2:A:942:VAL:HG13	1.64	0.62
2:A:696:MET:HE3	2:A:851:LYS:HG3	1.82	0.61
2:A:660:ASN:N	2:A:660:ASN:HD22	1.98	0.61
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.82	0.61
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.81	0.61
2:A:534:HIS:C	2:A:534:HIS:CD2	2.78	0.61
2:A:877:PRO:O	2:A:881:MET:HG2	2.00	0.61
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.83	0.60
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.83	0.60
2:A:696:MET:CE	2:A:851:LYS:HG3	2.31	0.60
2:A:519:ARG:O	2:A:523:ARG:HG3	2.01	0.60
2:A:370:LEU:O	2:A:374:LEU:HB2	2.01	0.60
2:A:418:LEU:HD21	2:A:438:VAL:HG11	1.83	0.60
1:C:327:ILE:HG12	1:C:367:LEU:HD21	1.83	0.59
2:A:338:LEU:HD21	2:A:390:ILE:HG13	1.85	0.59
1:C:279:ARG:NH1	1:C:279:ARG:HB2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2:ILE:H	2:A:2:ILE:HD12	1.68	0.59
2:A:573:MET:HG2	2:A:678:LYS:CD	2.32	0.59
2:A:416:LYS:HD2	2:A:419:GLU:HB3	1.84	0.59
2:A:969:LEU:O	2:A:973:LEU:HD13	2.02	0.59
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.85	0.58
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.84	0.58
2:A:904:VAL:HG12	2:A:937:ALA:HB3	1.84	0.58
2:A:340:GLY:O	2:A:344:GLU:HG3	2.03	0.58
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.84	0.58
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.34	0.58
2:A:188:GLN:HA	2:A:769:ASN:ND2	2.18	0.58
2:A:276:ALA:HB3	2:A:284:VAL:O	2.03	0.58
2:A:995:LEU:O	2:A:1017:ILE:HD11	2.04	0.58
2:A:38:ALA:O	2:A:390:ILE:HG22	2.03	0.58
1:B:110:PHE:CG	1:B:250:ILE:HG12	2.38	0.58
2:A:168:LEU:HB3	2:A:177:VAL:HG21	1.86	0.57
2:A:87:GLN:HG2	2:A:812:MET:HE2	1.86	0.57
2:A:399:ALA:HA	2:A:486:MET:HE2	1.86	0.57
1:C:317:LEU:C	1:C:317:LEU:HD12	2.30	0.57
2:A:2:ILE:HD13	2:A:448:PRO:HB3	1.86	0.57
2:A:573:MET:HG2	2:A:678:LYS:HZ3	1.68	0.57
2:A:940:PHE:C	2:A:940:PHE:HD2	2.09	0.57
2:A:535:TRP:O	2:A:538:THR:HG22	2.05	0.57
2:A:746:PHE:CZ	2:A:788:ILE:HG23	2.40	0.57
2:A:188:GLN:HA	2:A:769:ASN:HD21	1.70	0.57
2:A:912:ILE:HD12	2:A:930:PHE:CZ	2.40	0.57
1:C:342:ILE:HB	1:C:378:VAL:HG12	1.86	0.57
2:A:696:MET:HE1	2:A:849:GLN:O	2.05	0.57
2:A:756:VAL:HG21	2:A:770:LEU:HD22	1.87	0.57
2:A:28:THR:O	2:A:32:ILE:HG13	2.05	0.56
2:A:222:ILE:HG12	2:A:223:GLU:N	2.20	0.56
2:A:141:GLU:HB3	2:A:325:TYR:HB3	1.87	0.56
2:A:410:MET:HE1	2:A:493:ALA:O	2.06	0.56
2:A:893:ARG:HB3	2:A:896:GLU:HB3	1.87	0.56
1:B:390:ASN:HD22	1:B:393:GLY:H	1.53	0.56
2:A:975:HIS:C	2:A:977:ALA:H	2.13	0.56
2:A:4:TRP:O	2:A:8:ARG:HG2	2.06	0.56
2:A:900:ILE:HG23	2:A:941:GLY:HA3	1.88	0.56
1:C:116:TYR:CE2	1:C:309:PRO:HG2	2.40	0.56
2:A:390:ILE:HD12	2:A:1005:GLY:HA3	1.88	0.56
2:A:588:MET:HE1	2:A:658:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:804:ILE:HG13	2:A:804:ILE:O	2.04	0.55
2:A:933:LEU:HB2	2:A:1016:MET:HG2	1.87	0.55
1:B:330:GLN:HA	1:B:330:GLN:HE21	1.71	0.55
1:C:219:THR:HG1	1:C:237:LYS:HD2	1.70	0.55
2:A:488:GLY:O	2:A:492:LEU:HB2	2.07	0.55
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.88	0.55
2:A:351:VAL:O	2:A:355:LEU:HG	2.06	0.55
2:A:449:ALA:O	2:A:453:SER:HB2	2.05	0.55
1:B:220:ALA:HB3	1:B:237:LYS:HB2	1.88	0.55
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.37	0.55
1:C:359:GLN:HG3	1:C:360:ALA:N	2.22	0.55
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.89	0.55
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.87	0.55
1:B:144:VAL:HG21	1:B:238:ILE:HD13	1.88	0.55
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.87	0.55
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.89	0.54
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.88	0.54
1:B:268:VAL:HG23	1:B:271:ARG:H	1.72	0.54
2:A:40:PRO:O	2:A:42:LEU:HG	2.06	0.54
1:B:387:SER:HA	2:A:771:ARG:HH12	1.72	0.54
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.08	0.54
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.30	0.54
1:B:389:ALA:O	1:B:390:ASN:C	2.50	0.54
2:A:53:TYR:O	2:A:89:GLY:HA2	2.08	0.54
2:A:363:ALA:O	2:A:367:ILE:HG13	2.08	0.54
2:A:955:VAL:HA	2:A:958:LEU:HD13	1.90	0.54
2:A:880:LEU:HA	2:A:883:ILE:HG22	1.89	0.54
2:A:972:ALA:HA	2:A:975:HIS:HD2	1.73	0.54
1:B:123:ILE:HD12	1:B:237:LYS:HG3	1.89	0.54
1:B:242:ASP:CB	1:B:243:PRO:HD3	2.37	0.54
1:B:135:VAL:HG12	1:B:225:ALA:HB2	1.89	0.53
2:A:522:ILE:HG12	2:A:981:VAL:HG11	1.90	0.53
1:B:123:ILE:HB	1:C:227:MET:CG	2.38	0.53
2:A:842:LYS:O	2:A:846:GLU:HG2	2.08	0.53
1:C:164:GLU:O	1:C:168:LEU:HD13	2.09	0.53
1:B:155:ILE:HB	1:B:208:PHE:HE1	1.74	0.53
2:A:441:ASP:HA	2:A:444:VAL:HG23	1.89	0.53
1:B:126:ALA:HB2	1:B:229:ILE:HD13	1.91	0.53
2:A:620:PRO:HG2	2:A:622:GLU:HG2	1.91	0.53
2:A:459:LEU:HB3	2:A:882:ILE:CD1	2.34	0.53
1:C:102:GLY:O	1:C:323:PRO:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:SER:HA	2:A:12:ASN:ND2	2.24	0.53
2:A:421:TRP:HD1	2:A:421:TRP:O	1.92	0.53
2:A:436:TRP:CD1	2:A:436:TRP:C	2.87	0.53
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.35	0.52
2:A:248:LEU:HD11	2:A:259:LEU:HA	1.91	0.52
2:A:882:ILE:HD13	2:A:882:ILE:C	2.35	0.52
2:A:239:THR:HG22	2:A:241:ASP:H	1.72	0.52
2:A:301:ILE:HD12	2:A:328:SER:HB3	1.91	0.52
1:B:180:GLY:O	1:B:184:ARG:HG3	2.09	0.52
1:B:156:PRO:O	1:B:159:VAL:HG12	2.09	0.52
2:A:955:VAL:N	2:A:956:PRO:CD	2.72	0.52
1:C:325:LEU:HD12	1:C:325:LEU:H	1.73	0.52
2:A:338:LEU:HG	2:A:390:ILE:HA	1.91	0.52
2:A:474:LEU:HD23	2:A:475:PHE:CE1	2.45	0.52
1:B:266:LEU:HD13	1:B:267:THR:N	2.25	0.52
1:B:223:LEU:HD11	1:B:235:VAL:HA	1.90	0.52
1:C:324:MET:HE2	1:C:324:MET:HA	1.92	0.52
2:A:759:THR:HG22	2:A:768:ILE:HD11	1.91	0.52
2:A:977:ALA:O	2:A:981:VAL:HG23	2.10	0.52
2:A:391:MET:HE1	2:A:1008:VAL:HG11	1.91	0.52
2:A:904:VAL:N	2:A:905:PRO:CD	2.73	0.52
1:B:143:LYS:HD2	1:B:216:GLY:O	2.10	0.51
2:A:546:SER:O	2:A:549:THR:HG22	2.10	0.51
2:A:710:VAL:HA	2:A:828:ALA:HB2	1.92	0.51
2:A:214:ASN:OD1	2:A:237:LEU:HB2	2.09	0.51
2:A:891:PHE:CE2	2:A:942:VAL:HG13	2.44	0.51
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.09	0.51
1:B:259:LYS:HG3	1:B:260:ASP:N	2.25	0.51
2:A:964:PHE:CE2	2:A:1043:HIS:HB3	2.46	0.51
2:A:361:ARG:HA	2:A:364:LEU:HB2	1.92	0.51
1:B:124:VAL:HB	1:B:235:VAL:HG22	1.92	0.51
2:A:844:ILE:HD12	2:A:858:PHE:HZ	1.76	0.51
1:B:340:ARG:HB3	1:B:354:ARG:HA	1.92	0.51
2:A:214:ASN:H	2:A:215:GLN:NE2	2.09	0.51
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.92	0.51
2:A:342:LEU:HD21	2:A:396:ILE:HG22	1.93	0.51
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.10	0.51
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.37	0.51
1:C:156:PRO:O	1:C:159:VAL:HG22	2.11	0.51
2:A:522:ILE:HG23	2:A:526:HIS:HE2	1.75	0.51
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:850:LEU:HD21	2:A:856:VAL:HG23	1.94	0.50
1:C:128:ALA:HB3	1:C:155:ILE:HG21	1.93	0.50
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.46	0.50
2:A:746:PHE:O	2:A:750:ALA:HB3	2.11	0.50
1:B:384:LEU:HD12	1:B:384:LEU:N	2.26	0.50
1:C:80:SER:HB3	1:C:401:GLU:OE2	2.11	0.50
2:A:16:VAL:HG11	2:A:495:VAL:HG12	1.93	0.50
2:A:534:HIS:O	2:A:535:TRP:C	2.55	0.50
1:B:385:ILE:HG13	2:A:272:ARG:H	1.77	0.50
2:A:359:HIS:HB3	2:A:362:SER:OG	2.12	0.50
2:A:392:SER:O	2:A:481:THR:HG21	2.11	0.50
2:A:725:ASN:O	2:A:804:ILE:HA	2.12	0.50
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.77	0.50
1:C:391:ILE:C	1:C:393:GLY:H	2.19	0.50
2:A:1:MET:O	2:A:5:ILE:HG13	2.12	0.50
1:C:138:LEU:HD21	1:C:144:VAL:HG11	1.94	0.50
1:B:336:GLY:HA3	2:A:775:SER:HB2	1.94	0.50
2:A:19:GLY:O	2:A:23:LEU:HB3	2.12	0.50
2:A:26:TRP:O	2:A:30:THR:HG23	2.12	0.50
2:A:121:LEU:HB3	2:A:125:VAL:CG2	2.42	0.50
2:A:111:LEU:HD13	2:A:129:LEU:HD22	1.94	0.49
2:A:878:MET:O	2:A:882:ILE:HG22	2.11	0.49
2:A:932:ALA:O	2:A:936:VAL:HG23	2.12	0.49
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.73	0.49
1:B:169:ARG:HE	1:B:169:ARG:HA	1.77	0.49
2:A:21:LEU:O	2:A:25:ILE:HG22	2.12	0.49
1:B:391:ILE:HG12	2:A:774:GLN:OE1	2.12	0.49
2:A:405:ASP:OD2	2:A:991:ILE:HG12	2.12	0.49
2:A:596:ILE:HG12	2:A:653:VAL:HG21	1.93	0.49
2:A:697:ALA:HA	2:A:824:ILE:HD11	1.93	0.49
2:A:5:ILE:HA	2:A:8:ARG:HG3	1.94	0.49
2:A:390:ILE:HD12	2:A:1005:GLY:CA	2.43	0.49
2:A:458:THR:HA	2:A:482:LYS:NZ	2.27	0.49
2:A:42:LEU:HD12	2:A:42:LEU:H	1.77	0.49
2:A:952:ILE:C	2:A:957:SER:HB3	2.37	0.49
1:B:153:LEU:H	1:B:153:LEU:HD23	1.76	0.49
1:B:324:MET:HE1	1:B:358:PHE:CG	2.48	0.49
1:C:166:LEU:O	1:C:170:GLU:HG2	2.12	0.49
2:A:23:LEU:HD12	2:A:23:LEU:O	2.13	0.49
2:A:14:PHE:O	2:A:17:LEU:HB3	2.12	0.49
2:A:113:TYR:HA	2:A:116:GLN:HE21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASP:CB	1:C:243:PRO:HD3	2.33	0.49
2:A:421:TRP:O	2:A:421:TRP:CD1	2.66	0.49
2:A:482:LYS:HD3	2:A:482:LYS:C	2.38	0.49
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.94	0.49
2:A:592:THR:O	2:A:596:ILE:HG13	2.13	0.49
2:A:596:ILE:HD13	2:A:628:ILE:HD11	1.94	0.49
2:A:550:VAL:HG23	2:A:913:TRP:CD1	2.48	0.49
2:A:947:TYR:O	2:A:951:ALA:HB2	2.12	0.49
1:B:121:TYR:CG	1:C:224:ARG:HD3	2.48	0.48
1:C:302:ASN:ND2	1:C:307:LEU:H	2.11	0.48
2:A:338:LEU:O	2:A:342:LEU:HB2	2.12	0.48
2:A:399:ALA:O	2:A:403:MET:HG3	2.12	0.48
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.95	0.48
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.43	0.48
2:A:1020:MET:HE3	2:A:1020:MET:HA	1.95	0.48
2:A:356:PHE:HD2	2:A:986:MET:CB	2.27	0.48
2:A:526:HIS:N	2:A:527:PRO:CD	2.77	0.48
2:A:683:ILE:HB	2:A:824:ILE:HB	1.95	0.48
2:A:944:MET:HE2	2:A:1027:SER:O	2.13	0.48
1:B:117:ASN:HD22	1:B:117:ASN:C	2.21	0.48
2:A:945:LEU:HD13	2:A:945:LEU:O	2.14	0.48
2:A:40:PRO:O	2:A:41:ASP:C	2.56	0.48
2:A:173:ASP:HB2	2:A:300:VAL:CG2	2.44	0.48
2:A:270:GLU:HG2	2:A:271:MET:H	1.79	0.48
2:A:431:ASP:CG	2:A:432:ASN:H	2.21	0.48
2:A:900:ILE:HD12	2:A:941:GLY:O	2.14	0.48
2:A:925:ALA:O	2:A:1012:ILE:HG13	2.14	0.48
1:B:84:ILE:HG22	1:C:91:ASN:OD1	2.14	0.48
1:C:158:TRP:O	1:C:162:GLN:HG3	2.13	0.48
2:A:270:GLU:HG2	2:A:271:MET:N	2.28	0.48
2:A:522:ILE:HG23	2:A:526:HIS:NE2	2.29	0.48
2:A:784:ARG:HG3	2:A:804:ILE:CD1	2.44	0.48
1:B:390:ASN:ND2	1:B:393:GLY:H	2.12	0.48
1:C:360:ALA:HB2	1:C:365:THR:HG22	1.96	0.48
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.96	0.48
2:A:2:ILE:HD12	2:A:2:ILE:N	2.28	0.47
2:A:550:VAL:O	2:A:553:PRO:HD2	2.14	0.47
2:A:736:TYR:CE1	2:A:796:ILE:HG21	2.49	0.47
1:B:324:MET:HE1	1:B:358:PHE:CD2	2.49	0.47
2:A:661:LEU:HD21	2:A:663:VAL:HG13	1.96	0.47
1:B:124:VAL:O	1:B:235:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:ILE:HG12	2:A:494:ILE:HG13	1.96	0.47
2:A:27:GLY:O	2:A:31:ILE:HG22	2.14	0.47
2:A:368:ILE:O	2:A:372:LEU:HD13	2.14	0.47
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.96	0.47
1:B:178:THR:O	1:B:182:LEU:HB2	2.15	0.47
1:C:394:ALA:HA	1:C:397:ARG:NH1	2.30	0.47
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.49	0.47
1:C:279:ARG:HB2	1:C:279:ARG:HH11	1.79	0.47
2:A:408:ILE:HG13	2:A:409:VAL:N	2.29	0.47
2:A:574:PRO:HD2	2:A:624:VAL:HG22	1.95	0.47
2:A:911:GLY:HA3	2:A:930:PHE:HE2	1.80	0.47
1:B:85:ASP:HA	1:B:86:PRO:HD3	1.78	0.47
1:B:99:VAL:HG22	1:B:327:ILE:HG22	1.95	0.47
1:C:114:VAL:O	1:C:309:PRO:HA	2.14	0.47
1:C:264:PHE:HB3	1:C:315:LEU:HD11	1.97	0.47
2:A:6:ILE:HG21	2:A:443:SER:HB3	1.97	0.47
2:A:715:ALA:HB2	2:A:824:ILE:HG12	1.97	0.47
2:A:833:MET:O	2:A:837:VAL:HG12	2.15	0.47
2:A:213:SER:O	2:A:237:LEU:HD13	2.14	0.47
2:A:951:ALA:HB1	2:A:972:ALA:O	2.14	0.47
2:A:458:THR:HA	2:A:482:LYS:HZ3	1.79	0.47
2:A:461:PHE:CE2	2:A:932:ALA:HB2	2.49	0.47
2:A:571:LEU:CD1	2:A:665:PRO:HA	2.45	0.47
2:A:574:PRO:HA	2:A:659:ALA:O	2.15	0.47
2:A:846:GLU:HG3	2:A:847:LYS:HG3	1.97	0.47
1:B:93:GLY:HA3	2:A:146:ASP:O	2.15	0.47
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.15	0.47
2:A:408:ILE:HD12	2:A:986:MET:HE2	1.97	0.47
2:A:463:PRO:CB	2:A:875:MET:HG3	2.45	0.47
2:A:589:LEU:HD13	2:A:609:THR:HG23	1.95	0.47
2:A:837:VAL:O	2:A:841:GLN:HG3	2.14	0.47
1:B:217:VAL:HG21	1:B:241:MET:HE2	1.96	0.46
1:B:339:GLN:OE1	1:B:339:GLN:N	2.47	0.46
1:C:284:LEU:HB2	1:C:295:GLN:HB2	1.97	0.46
2:A:550:VAL:C	2:A:553:PRO:HD2	2.40	0.46
2:A:419:GLU:O	2:A:423:HIS:HD2	1.97	0.46
2:A:859:SER:HA	2:A:863:GLU:HB2	1.97	0.46
1:B:386:ASP:HB2	2:A:269:PRO:O	2.16	0.46
2:A:702:GLU:HA	2:A:705:ARG:HH21	1.80	0.46
1:B:264:PHE:CE2	1:B:317:LEU:HD22	2.50	0.46
2:A:1036:LYS:O	2:A:1036:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ILE:HG12	2:A:774:GLN:CD	2.40	0.46
2:A:402:ALA:HB3	2:A:486:MET:HE1	1.95	0.46
2:A:433:LYS:HA	2:A:436:TRP:HB3	1.96	0.46
1:B:121:TYR:HE1	1:B:123:ILE:HD11	1.81	0.46
1:B:259:LYS:HE3	1:B:259:LYS:HB2	1.81	0.46
1:C:121:TYR:HE1	1:C:237:LYS:HD3	1.81	0.46
1:C:125:GLN:HG2	1:C:233:ASN:O	2.14	0.46
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.98	0.46
1:C:352:PRO:O	1:C:353:LYS:HG3	2.16	0.46
2:A:678:LYS:HE2	2:A:825:TYR:CD2	2.51	0.46
1:B:121:TYR:CE1	1:B:123:ILE:HD11	2.50	0.46
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.97	0.46
2:A:647:GLU:O	2:A:651:ASN:HB2	2.16	0.46
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.97	0.46
1:C:308:LYS:HB2	1:C:311:MET:HE3	1.96	0.46
2:A:537:LYS:HD3	2:A:1037:LEU:HD11	1.98	0.46
2:A:550:VAL:CB	2:A:909:VAL:HG13	2.41	0.46
2:A:693:ILE:HD11	2:A:718:LEU:HD22	1.98	0.46
2:A:728:ILE:HA	2:A:802:ALA:HB2	1.97	0.46
2:A:785:GLN:HA	2:A:797:THR:HB	1.98	0.46
1:B:296:LEU:C	1:B:296:LEU:HD23	2.41	0.46
2:A:758:GLU:HA	2:A:766:TYR:O	2.16	0.46
2:A:759:THR:HG23	2:A:766:TYR:HB2	1.98	0.46
2:A:952:ILE:O	2:A:952:ILE:HG22	2.16	0.46
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.44	0.45
2:A:769:ASN:HD22	2:A:769:ASN:N	2.15	0.45
2:A:13:ARG:HA	2:A:499:ILE:HD13	1.98	0.45
2:A:395:GLY:O	2:A:398:ILE:HG12	2.16	0.45
2:A:459:LEU:C	2:A:461:PHE:H	2.24	0.45
2:A:525:TYR:OH	2:A:980:ARG:NH2	2.49	0.45
2:A:887:LEU:HD13	2:A:900:ILE:HB	1.98	0.45
2:A:930:PHE:CE1	2:A:1015:PRO:HB3	2.51	0.45
1:B:183:GLU:O	1:B:187:LEU:HG	2.16	0.45
1:B:207:ARG:O	1:B:207:ARG:HG3	2.13	0.45
2:A:348:VAL:HG12	2:A:993:ALA:HB1	1.98	0.45
2:A:418:LEU:HD12	2:A:439:ILE:HD11	1.98	0.45
2:A:844:ILE:HD12	2:A:858:PHE:CZ	2.51	0.45
2:A:42:LEU:HD21	2:A:474:LEU:HD13	1.98	0.45
2:A:453:SER:OG	2:A:939:GLU:HA	2.15	0.45
2:A:474:LEU:O	2:A:477:PRO:HD2	2.16	0.45
2:A:637:ARG:HB3	2:A:638:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:675:THR:HG21	2:A:860:GLY:O	2.16	0.45
1:C:266:LEU:HB3	1:C:276:LEU:HD12	1.97	0.45
2:A:421:TRP:HE1	2:A:425:HIS:CD2	2.34	0.45
1:C:395:LEU:HB3	1:C:399:ARG:HH12	1.82	0.45
2:A:2:ILE:O	2:A:6:ILE:HG13	2.15	0.45
2:A:18:MET:HA	2:A:21:LEU:HB3	1.99	0.45
1:C:230:ALA:H	1:C:233:ASN:ND2	2.15	0.45
1:C:329:SER:HA	1:C:365:THR:HG23	1.99	0.45
2:A:195:ARG:HD3	2:A:261:ASP:O	2.17	0.45
2:A:297:ALA:O	2:A:301:ILE:HG13	2.16	0.45
2:A:463:PRO:HB2	2:A:875:MET:HG3	1.99	0.45
2:A:831:ARG:HH22	2:A:839:ASP:CG	2.24	0.45
2:A:875:MET:CE	2:A:931:ILE:HG21	2.47	0.45
1:B:387:SER:HB2	2:A:271:MET:HG3	1.98	0.45
2:A:38:ALA:O	2:A:389:ASN:HB2	2.16	0.45
2:A:298:ARG:NE	2:A:328:SER:HB2	2.32	0.45
2:A:701:GLU:HG2	2:A:705:ARG:HH22	1.80	0.45
1:C:397:ARG:O	1:C:401:GLU:HG3	2.17	0.44
2:A:944:MET:HE1	2:A:1032:PRO:HG3	1.99	0.44
2:A:118:GLN:HE22	2:A:127:ALA:N	2.11	0.44
2:A:301:ILE:CD1	2:A:328:SER:HB3	2.46	0.44
2:A:350:ALA:HA	2:A:353:CYS:SG	2.58	0.44
2:A:554:LEU:CD2	2:A:912:ILE:HG12	2.48	0.44
2:A:716:GLU:OE1	2:A:814:LYS:HE3	2.17	0.44
2:A:3:GLU:CD	2:A:3:GLU:H	2.25	0.44
1:B:121:TYR:CD1	1:C:224:ARG:HD3	2.52	0.44
2:A:559:GLY:H	2:A:834:VAL:HG12	1.81	0.44
1:C:151:LEU:HD11	1:C:210:LEU:HD12	2.00	0.44
1:C:156:PRO:O	1:C:157:ASP:C	2.60	0.44
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.47	0.44
2:A:6:ILE:O	2:A:10:VAL:HG23	2.17	0.44
2:A:292:ARG:O	2:A:293:SER:C	2.58	0.44
2:A:561:PHE:HA	2:A:865:LEU:HG	1.99	0.44
1:B:288:ASP:O	1:B:292:ARG:N	2.50	0.44
1:C:298:LEU:HD11	1:C:315:LEU:HD22	1.99	0.44
1:C:330:GLN:O	1:C:382:LEU:HD12	2.18	0.44
2:A:116:GLN:H	2:A:116:GLN:HG2	1.65	0.44
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.17	0.44
2:A:420:GLU:HG3	2:A:421:TRP:N	2.33	0.44
2:A:711:ALA:HB3	2:A:827:ASP:O	2.18	0.44
2:A:723:TYR:HB2	2:A:807:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:118:GLN:NE2	2:A:126:SER:HA	2.33	0.44
2:A:288:VAL:HG22	2:A:290:ILE:HD12	2.00	0.44
2:A:969:LEU:O	2:A:969:LEU:HD12	2.18	0.44
1:C:183:GLU:O	1:C:187:LEU:HG	2.18	0.43
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.37	0.43
1:C:146:LYS:HA	1:C:212:ALA:O	2.18	0.43
2:A:196:LEU:HD22	2:A:201:ILE:O	2.17	0.43
2:A:781:GLN:CD	2:A:781:GLN:H	2.26	0.43
1:B:383:PHE:C	1:B:384:LEU:HD12	2.43	0.43
1:C:88:GLN:HE21	2:A:654:ARG:HG3	1.82	0.43
1:C:120:GLN:NE2	1:C:243:PRO:HD2	2.32	0.43
2:A:492:LEU:HD22	2:A:492:LEU:HA	1.81	0.43
2:A:571:LEU:HD11	2:A:665:PRO:HA	2.00	0.43
2:A:940:PHE:CE1	2:A:984:LYS:HE3	2.54	0.43
1:C:191:PRO:HG2	1:C:194:ASP:OD2	2.19	0.43
2:A:541:LEU:HD13	2:A:541:LEU:C	2.44	0.43
2:A:595:LEU:HD23	2:A:595:LEU:HA	1.86	0.43
2:A:661:LEU:CD2	2:A:663:VAL:HG13	2.48	0.43
1:B:396:GLU:HG2	1:B:399:ARG:HH21	1.83	0.43
1:B:287:VAL:CG1	1:B:294:LEU:HD23	2.47	0.43
2:A:550:VAL:CG1	2:A:909:VAL:HG22	2.43	0.43
2:A:965:SER:OG	2:A:968:LYS:HB3	2.19	0.43
1:B:104:LEU:HB2	1:B:321:SER:OG	2.19	0.43
1:C:132:ILE:CD1	1:C:229:ILE:HB	2.48	0.43
2:A:526:HIS:HB3	2:A:974:TYR:OH	2.18	0.43
2:A:834:VAL:HG22	2:A:838:HIS:NE2	2.33	0.43
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.43
1:C:84:ILE:HG21	2:A:656:PRO:HG3	2.01	0.43
2:A:42:LEU:HD12	2:A:42:LEU:N	2.33	0.43
2:A:461:PHE:CD1	2:A:482:LYS:HD2	2.53	0.43
2:A:677:ILE:HG22	2:A:679:SER:H	1.82	0.43
2:A:1036:LYS:O	2:A:1040:LEU:HG	2.19	0.43
1:B:334:ASP:OD2	1:B:339:GLN:HB3	2.19	0.43
1:C:181:ILE:O	1:C:185:LEU:HD13	2.18	0.43
2:A:573:MET:HE3	2:A:573:MET:HB2	1.68	0.43
2:A:636:TRP:CD1	2:A:636:TRP:N	2.87	0.43
2:A:891:PHE:CE1	2:A:945:LEU:HD12	2.54	0.43
1:B:340:ARG:HD2	1:B:395:LEU:HD13	1.99	0.43
1:C:121:TYR:CE1	1:C:237:LYS:HD3	2.54	0.43
1:C:254:ILE:HD11	2:A:797:THR:CG2	2.49	0.43
2:A:21:LEU:C	2:A:21:LEU:HD13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:HIS:HB3	2:A:974:TYR:CZ	2.54	0.43
1:B:385:ILE:HG23	1:B:385:ILE:O	2.19	0.42
2:A:940:PHE:CE2	2:A:944:MET:HG3	2.54	0.42
1:B:298:LEU:N	1:B:298:LEU:HD23	2.34	0.42
1:C:268:VAL:HA	1:C:269:PRO:HD3	1.85	0.42
2:A:240:LEU:HD23	2:A:240:LEU:HA	1.85	0.42
2:A:325:TYR:HB2	2:A:627:THR:HG21	2.00	0.42
2:A:348:VAL:O	2:A:352:VAL:HG23	2.19	0.42
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.46	0.42
2:A:522:ILE:CG1	2:A:981:VAL:HG11	2.48	0.42
2:A:575:SER:O	2:A:714:LEU:HD22	2.19	0.42
1:B:390:ASN:HA	2:A:774:GLN:HE22	1.85	0.42
2:A:185:LYS:O	2:A:767:PRO:HD2	2.19	0.42
2:A:469:GLY:O	2:A:473:ARG:HG3	2.18	0.42
2:A:904:VAL:O	2:A:908:LEU:HG	2.19	0.42
2:A:110:VAL:O	2:A:114:LEU:HB2	2.19	0.42
2:A:376:ILE:O	2:A:380:VAL:HG23	2.19	0.42
2:A:534:HIS:CD2	2:A:534:HIS:O	2.72	0.42
2:A:715:ALA:CB	2:A:824:ILE:HG12	2.49	0.42
1:B:322:GLU:O	1:B:324:MET:HG3	2.20	0.42
2:A:222:ILE:CD1	2:A:224:LEU:HG	2.49	0.42
2:A:311:LEU:O	2:A:315:LEU:HG	2.19	0.42
2:A:718:LEU:HD12	2:A:718:LEU:HA	1.84	0.42
1:B:291:THR:O	1:B:293:THR:HG23	2.19	0.42
1:C:367:LEU:N	1:C:367:LEU:HD22	2.35	0.42
2:A:295:LYS:HA	2:A:295:LYS:HD3	1.88	0.42
2:A:531:LYS:O	2:A:534:HIS:HB3	2.19	0.42
1:B:125:GLN:HG2	1:B:233:ASN:O	2.19	0.42
1:C:161:ALA:HB3	1:C:185:LEU:HD11	2.01	0.42
2:A:62:GLU:HA	2:A:66:THR:HB	2.00	0.42
2:A:67:TYR:N	2:A:68:PRO:HD2	2.34	0.42
2:A:411:ILE:HA	2:A:501:MET:CE	2.47	0.42
2:A:421:TRP:HE3	2:A:438:VAL:HB	1.84	0.42
2:A:933:LEU:HD23	2:A:1016:MET:HA	2.02	0.42
2:A:534:HIS:O	2:A:534:HIS:HD2	2.02	0.42
2:A:770:LEU:O	2:A:771:ARG:HB2	2.18	0.42
2:A:97:PHE:CZ	2:A:106:ALA:HB1	2.55	0.42
2:A:172:PRO:O	2:A:173:ASP:HB2	2.20	0.42
1:B:132:ILE:HD11	1:B:229:ILE:HB	2.01	0.42
2:A:729:ASN:HB3	2:A:732:LYS:HB2	2.01	0.42
2:A:1025:LEU:HD23	2:A:1025:LEU:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.20	0.41
1:B:389:ALA:O	1:B:391:ILE:N	2.53	0.41
2:A:114:LEU:HD12	2:A:114:LEU:HA	1.95	0.41
1:B:280:LYS:HE3	1:B:281:TRP:H	1.84	0.41
1:B:302:ASN:HD21	1:B:306:ALA:N	2.19	0.41
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.72	0.41
2:A:275:ILE:O	2:A:608:LYS:HA	2.20	0.41
2:A:375:CYS:O	2:A:379:ILE:HG13	2.20	0.41
2:A:992:ILE:O	2:A:996:LEU:HB2	2.20	0.41
2:A:1016:MET:O	2:A:1020:MET:HB2	2.20	0.41
2:A:15:LEU:HD22	2:A:15:LEU:HA	1.92	0.41
2:A:404:VAL:O	2:A:408:ILE:HG12	2.19	0.41
2:A:535:TRP:C	2:A:537:LYS:H	2.28	0.41
2:A:599:VAL:HG12	2:A:601:GLU:H	1.86	0.41
2:A:972:ALA:HA	2:A:975:HIS:CD2	2.55	0.41
2:A:992:ILE:HD11	2:A:1020:MET:O	2.20	0.41
1:B:159:VAL:HG13	1:B:160:GLU:N	2.36	0.41
2:A:188:GLN:NE2	2:A:268:GLY:HA3	2.35	0.41
2:A:193:PRO:HG3	2:A:772:TYR:CD2	2.54	0.41
2:A:578:PRO:HG2	2:A:717:ARG:HB2	2.02	0.41
2:A:904:VAL:HG22	2:A:905:PRO:HD3	2.03	0.41
1:B:110:PHE:CD1	1:B:250:ILE:HG12	2.56	0.41
1:C:129:ALA:O	1:C:155:ILE:HG23	2.20	0.41
2:A:214:ASN:HB2	2:A:237:LEU:HD22	2.03	0.41
2:A:535:TRP:NE1	2:A:537:LYS:HB3	2.35	0.41
1:C:395:LEU:O	1:C:399:ARG:HG3	2.20	0.41
2:A:1020:MET:HA	2:A:1020:MET:CE	2.51	0.41
1:C:112:ALA:HB2	1:C:248:ALA:HB2	2.02	0.41
2:A:418:LEU:CD2	2:A:438:VAL:HG11	2.51	0.41
2:A:456:ILE:HG23	2:A:883:ILE:HD13	2.02	0.41
2:A:574:PRO:CD	2:A:624:VAL:HG22	2.51	0.41
2:A:22:PHE:O	2:A:25:ILE:HG23	2.21	0.41
2:A:159:LEU:O	2:A:163:PHE:HB3	2.20	0.41
2:A:494:ILE:HG12	2:A:494:ILE:O	2.21	0.41
2:A:911:GLY:HA3	2:A:930:PHE:CE2	2.56	0.41
1:B:350:PHE:O	1:B:351:VAL:HG13	2.20	0.41
1:C:120:GLN:OE1	1:C:240:GLY:HA3	2.21	0.41
1:C:124:VAL:O	1:C:235:VAL:HG13	2.21	0.41
1:C:266:LEU:HD23	1:C:266:LEU:HA	1.93	0.41
2:A:243:PHE:O	2:A:246:ILE:HG13	2.21	0.41
2:A:373:GLY:HA2	2:A:376:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:560:GLU:HG3	2:A:923:SER:HB3	2.02	0.41
2:A:574:PRO:HD2	2:A:624:VAL:O	2.21	0.41
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.50	0.41
2:A:962:GLN:HG3	2:A:963:THR:N	2.34	0.41
1:C:391:ILE:C	1:C:393:GLY:N	2.79	0.41
2:A:440:THR:O	2:A:440:THR:HG22	2.21	0.41
1:B:84:ILE:HG22	1:C:91:ASN:CG	2.46	0.40
2:A:36:VAL:HG21	2:A:335:ILE:HG12	2.02	0.40
2:A:296:ASN:HB3	2:A:299:GLU:CB	2.51	0.40
2:A:535:TRP:O	2:A:537:LYS:N	2.54	0.40
2:A:769:ASN:HD22	2:A:769:ASN:H	1.69	0.40
2:A:815:THR:HG22	2:A:818:ALA:HA	2.03	0.40
2:A:945:LEU:HD22	2:A:945:LEU:HA	1.96	0.40
2:A:664:PRO:HA	2:A:665:PRO:HD3	1.99	0.40
1:B:307:LEU:HD22	1:B:307:LEU:H	1.85	0.40
1:C:161:ALA:CB	1:C:185:LEU:HD11	2.51	0.40
2:A:46:GLN:OE1	2:A:94:TYR:HD2	2.04	0.40
2:A:431:ASP:CG	2:A:432:ASN:N	2.80	0.40
2:A:553:PRO:HB2	2:A:912:ILE:HG22	2.02	0.40
2:A:1031:ILE:N	2:A:1032:PRO:CD	2.85	0.40
2:A:522:ILE:HD13	2:A:978:VAL:HG23	2.04	0.40
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.85	0.40
1:C:360:ALA:CB	1:C:365:THR:HG22	2.52	0.40
2:A:23:LEU:HD12	2:A:23:LEU:C	2.46	0.40
2:A:255:VAL:HA	2:A:256:PRO:HD3	1.87	0.40
2:A:390:ILE:O	2:A:390:ILE:HG12	2.16	0.40
2:A:632:PRO:C	2:A:634:GLU:H	2.29	0.40
2:A:933:LEU:HD13	2:A:933:LEU:C	2.47	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	320/413 (78%)	281 (88%)	36 (11%)	3 (1%)	14	49
1	C	322/413 (78%)	300 (93%)	21 (6%)	1 (0%)	36	71
2	A	1027/1054 (97%)	922 (90%)	95 (9%)	10 (1%)	12	47
All	All	1669/1880 (89%)	1503 (90%)	152 (9%)	14 (1%)	16	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	GLU
2	A	638	PRO
1	B	337	SER
1	B	390	ASN
2	A	894	VAL
2	A	574	PRO
2	A	13	ARG
2	A	238	GLN
1	C	137	PRO
2	A	38	ALA
2	A	235	GLY
2	A	852	PRO
2	A	1024	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	263/338 (78%)	242 (92%)	21 (8%)	11	32
1	C	265/338 (78%)	238 (90%)	27 (10%)	7	24
2	A	849/871 (98%)	765 (90%)	84 (10%)	7	25
All	All	1377/1547 (89%)	1245 (90%)	132 (10%)	8	26

All (132) 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	168	LEU
1	B	169	ARG
1	B	183	GLU
1	B	185	LEU
1	B	207	ARG
1	B	223	LEU
1	B	235	VAL
1	B	241	MET
1	B	280	LYS
1	B	282	THR
1	B	287	VAL
1	B	307	LEU
1	B	322	GLU
1	B	351	VAL
1	B	357	VAL
1	B	378	VAL
1	B	388	GLU
1	B	396	GLU
1	C	82	VAL
1	C	104	LEU
1	C	105	THR
1	C	138	LEU
1	C	140	VAL
1	C	178	THR
1	C	182	LEU
1	C	207	ARG
1	C	235	VAL
1	C	239	GLN
1	C	258	VAL
1	C	265	THR
1	C	271	ARG
1	C	276	LEU
1	C	277	THR
1	C	287	VAL
1	C	296	LEU
1	C	307	LEU
1	C	317	LEU
1	C	324	MET
1	C	330	GLN
1	C	339	GLN

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Mol	Chain	Res	Type
1	C	347	ASP
1	C	353	LYS
1	C	364	VAL
1	C	373	GLU
1	C	382	LEU
2	A	3	GLU
2	A	13	ARG
2	A	15	LEU
2	A	17	LEU
2	A	21	LEU
2	A	23	LEU
2	A	25	ILE
2	A	42	LEU
2	A	105	TRP
2	A	117	VAL
2	A	144	LEU
2	A	145	VAL
2	A	203	LEU
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	236	TYR
2	A	237	LEU
2	A	249	LYS
2	A	260	ARG
2	A	288	VAL
2	A	293	SER
2	A	298	ARG
2	A	322	VAL
2	A	335	ILE
2	A	342	LEU
2	A	351	VAL
2	A	358	TRP
2	A	364	LEU
2	A	374	LEU
2	A	390	ILE
2	A	400	VAL
2	A	412	GLU
2	A	415	HIS
2	A	417	ARG
2	A	434	THR

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Mol	Chain	Res	Type
2	A	455	LEU
2	A	457	ILE
2	A	492	LEU
2	A	521	LEU
2	A	524	VAL
2	A	531	LYS
2	A	534	HIS
2	A	554	LEU
2	A	569	ASP
2	A	573	MET
2	A	592	THR
2	A	602	VAL
2	A	621	LEU
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	642	MET
2	A	660	ASN
2	A	667	ARG
2	A	688	THR
2	A	693	ILE
2	A	722	ARG
2	A	729	ASN
2	A	749	SER
2	A	759	THR
2	A	765	ARG
2	A	769	ASN
2	A	770	LEU
2	A	781	GLN
2	A	789	LEU
2	A	815	THR
2	A	837	VAL
2	A	842	LYS
2	A	865	LEU
2	A	879	THR
2	A	882	ILE
2	A	885	VAL
2	A	940	PHE
2	A	945	LEU
2	A	968	LYS
2	A	969	LEU
2	A	984	LYS

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Mol	Chain	Res	Type
2	A	991	ILE
2	A	1020	MET
2	A	1026	LEU
2	A	1037	LEU
2	A	1039	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	117	ASN
1	B	125	GLN
1	B	177	GLN
1	B	302	ASN
1	B	330	GLN
1	B	359	GLN
1	B	390	ASN
1	C	88	GLN
1	C	177	GLN
1	C	233	ASN
1	C	263	GLN
1	C	302	ASN
2	A	116	GLN
2	A	118	GLN
2	A	151	HIS
2	A	198	GLN
2	A	215	GLN
2	A	238	GLN
2	A	244	ASN
2	A	279	ASN
2	A	329	GLN
2	A	359	HIS
2	A	423	HIS
2	A	470	GLN
2	A	534	HIS
2	A	629	GLN
2	A	633	GLN
2	A	635	GLN
2	A	660	ASN
2	A	668	ASN
2	A	729	ASN
2	A	744	GLN

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Mol	Chain	Res	Type
2	A	769	ASN
2	A	795	GLN
2	A	838	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](#)

There are no ligands in this entry.

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	322/413 (77%)	0.34	10 (3%)	51 39	36, 86, 147, 228	0
1	C	324/413 (78%)	0.28	9 (2%)	55 42	35, 88, 138, 216	0
2	A	1031/1054 (97%)	0.51	63 (6%)	27 27	30, 110, 226, 401	0
All	All	1677/1880 (89%)	0.44	82 (4%)	35 31	30, 99, 210, 401	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	GLY	4.7
1	C	79	ALA	4.0
2	A	446	VAL	3.9
2	A	873	LYS	3.6
1	C	98	THR	3.5
2	A	405	ASP	3.5
2	A	1	MET	3.5
2	A	360	VAL	3.4
2	A	528	LEU	3.4
2	A	429	THR	3.3
2	A	126	SER	3.2
2	A	588	MET	3.1
2	A	1001	GLY	3.1
2	A	579	GLY	3.1
2	A	870	HIS	3.1
2	A	517	LEU	3.1
2	A	520	PHE	3.0
2	A	2	ILE	2.9
2	A	22	PHE	2.9
2	A	382	HIS	2.9
2	A	120	LYS	2.9
1	B	79	ALA	2.9
1	C	176	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	386	ASP	2.9
2	A	427	ASP	2.9
2	A	367	ILE	2.8
2	A	963	THR	2.8
2	A	426	PRO	2.8
1	C	157	ASP	2.8
2	A	893	ARG	2.8
2	A	345	GLU	2.8
2	A	428	ALA	2.7
2	A	890	ALA	2.7
1	B	170	GLU	2.7
2	A	537	LYS	2.7
2	A	955	VAL	2.7
2	A	720	GLY	2.6
2	A	975	HIS	2.6
2	A	894	VAL	2.6
2	A	15	LEU	2.6
2	A	1038	MET	2.6
2	A	881	MET	2.5
1	C	305	GLU	2.5
2	A	320	GLU	2.5
1	B	392	SER	2.5
2	A	449	ALA	2.5
2	A	313	SER	2.4
2	A	418	LEU	2.4
2	A	450	LEU	2.4
2	A	1039	TRP	2.4
2	A	962	GLN	2.4
2	A	317	GLU	2.3
1	C	402	SER	2.3
2	A	75	SER	2.3
2	A	1041	HIS	2.3
2	A	524	VAL	2.3
1	B	318	ASN	2.2
2	A	847	LYS	2.2
1	B	93	GLY	2.2
2	A	580	ILE	2.2
2	A	150	LYS	2.2
1	C	376	LYS	2.2
2	A	1002	THR	2.2
2	A	950	HIS	2.2
2	A	906	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	157	ASP	2.2
2	A	20	ALA	2.2
2	A	444	VAL	2.1
2	A	964	PHE	2.1
2	A	274	GLY	2.1
2	A	416	LYS	2.1
1	C	158	TRP	2.1
2	A	52	SER	2.1
2	A	766	TYR	2.0
2	A	6	ILE	2.0
1	B	349	ARG	2.0
2	A	884	PHE	2.0
2	A	124	GLY	2.0
1	B	158	TRP	2.0
1	C	374	GLY	2.0
2	A	519	ARG	2.0
2	A	1000	TRP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.