



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:57 PM UTC

PDB ID : 4DNT / pdb_00004dnt
Title : Crystal structure of the CusBA heavy-metal efflux complex from Escherichia coli, mutant
Authors : Su, C.-C.; Long, F.; Yu, E.
Deposited on : 2012-02-09
Resolution : 3.10 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

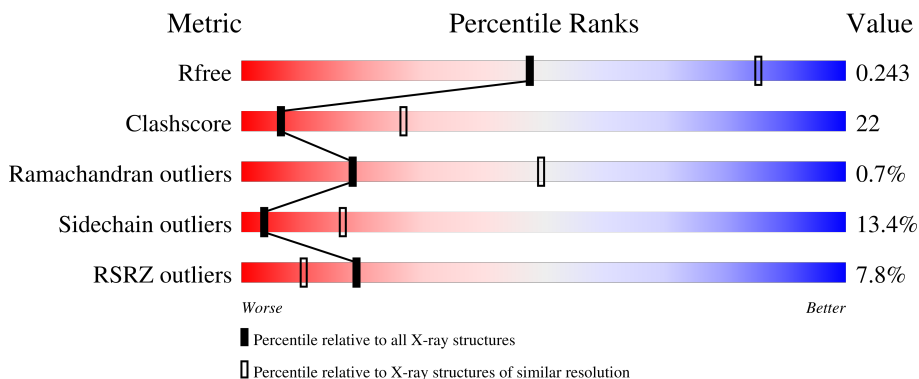
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	 3% 51% 22% 5% 22%
1	C	413	 2% 53% 21% 5% 22%
2	A	1054	 11% 53% 38% 7% .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12895 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	1031	Total	C	N	O	S	0	0	0
			7945	5139	1333	1436	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	405	ALA	ASP	engineered mutation	UNP P38054

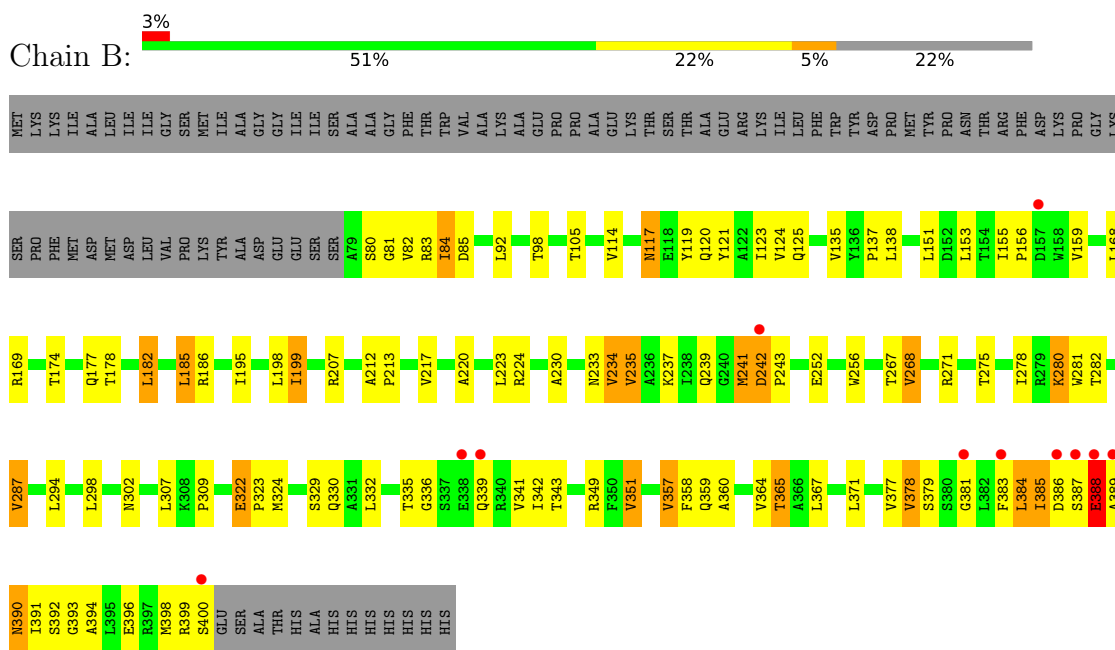
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total O 4 4	0	0
3	C	10	Total O 10 10	0	0
3	A	5	Total O 5 5	0	0

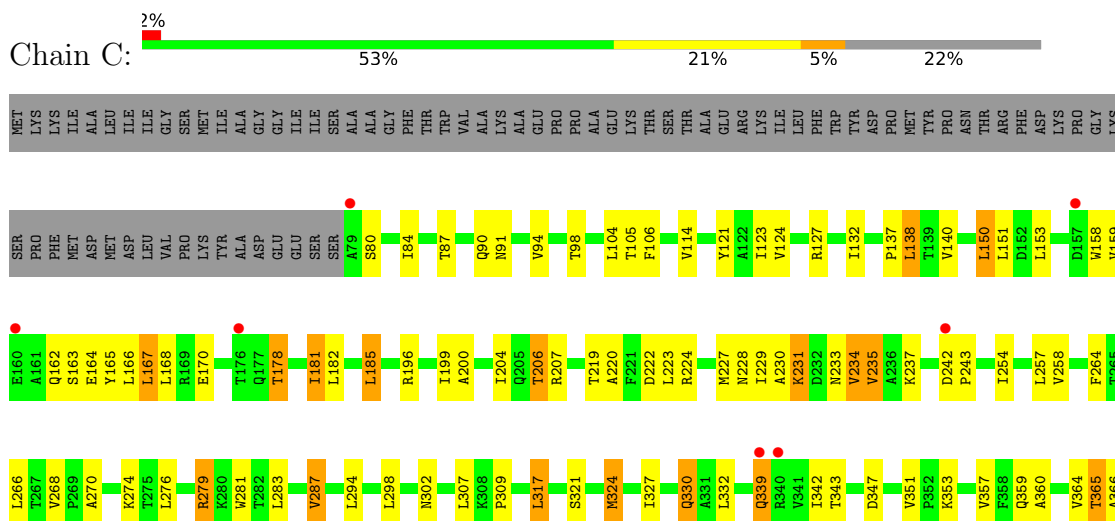
3 Residue-property plots

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

• Molecule 1: Cation efflux system protein CusB



• Molecule 1: Cation efflux system protein CusB



S1006	E1007	V1008	M1009	R1010	I1011	A1012	A1013	A1014	P1015	M1016	I1017	M1020	I1021	T1022	A1023	P1024	L1025	L1026	S1027	L1028	F1029	I1030	I1031	P1032	A1033	A1034	Y1035	K1036	L1037	M1038	W1039	L1040	H1041	R1042	H1043	ARG	VAL	ARG	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	159.64Å 159.64Å 681.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.33 – 3.10 107.33 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (107.33-3.10) 99.9 (107.33-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.13Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.219 , 0.244 0.217 , 0.243	Depositor DCC
R_{free} test set	3098 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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](#)

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	0.30	0/2498	0.77	4/3401 (0.1%)
1	C	0.29	0/2513	0.75	0/3421
2	A	0.29	0/8111	0.78	8/11044 (0.1%)
All	All	0.29	0/13122	0.77	12/17866 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLU	N-CA-C	6.58	124.83	110.80
2	A	577	LEU	CA-C-N	6.14	125.63	119.24
2	A	577	LEU	C-N-CA	6.14	125.63	119.24
2	A	707	VAL	CA-C-N	5.73	127.00	119.84
2	A	707	VAL	C-N-CA	5.73	127.00	119.84
1	B	381	GLY	N-CA-C	-5.62	105.95	115.34
2	A	958	LEU	N-CA-C	-5.19	107.11	113.50
2	A	521	LEU	N-CA-C	-5.18	107.62	114.04
1	B	242	ASP	CA-C-N	-5.07	113.50	119.84
1	B	242	ASP	C-N-CA	-5.07	113.50	119.84
2	A	53	TYR	CA-C-N	5.04	125.32	119.93
2	A	53	TYR	C-N-CA	5.04	125.32	119.93

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	96	0
1	C	2473	0	2533	81	0
2	A	7945	0	8196	418	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	10	0	0	0	0
All	All	12895	0	13251	570	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 (570) 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:13:ARG:HB2	2:A:499:ILE:CD1	1.72	1.18
2:A:13:ARG:HD2	2:A:13:ARG:O	1.52	1.08
2:A:696:MET:HG3	2:A:854:THR:HG21	1.34	1.07
2:A:735:ARG:HG2	2:A:735:ARG:HH21	1.18	1.06
2:A:896:GLU:OE1	2:A:945:LEU:HG	1.55	1.06
2:A:574:PRO:HB2	2:A:658:LEU:HD11	1.38	1.04
2:A:118:GLN:HE22	2:A:127:ALA:H	1.07	1.02
2:A:13:ARG:CB	2:A:499:ILE:HD13	1.92	0.99
1:C:165:TYR:HB2	1:C:181:ILE:HG21	1.45	0.96
2:A:13:ARG:NH1	2:A:436:TRP:HZ3	1.63	0.96
2:A:13:ARG:HB2	2:A:499:ILE:HD13	0.96	0.95
2:A:896:GLU:OE1	2:A:945:LEU:CD1	2.20	0.90
2:A:888:TYR:CZ	2:A:894:VAL:HG23	2.07	0.89
2:A:896:GLU:OE1	2:A:945:LEU:CG	2.20	0.89
2:A:493:ALA:HA	2:A:497:ILE:HB	1.51	0.89
1:C:359:GLN:HG3	1:C:360:ALA:H	1.39	0.86
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.05	0.86
2:A:13:ARG:HH11	2:A:436:TRP:HZ3	0.86	0.85
1:B:388:GLU:OE1	1:B:388:GLU:HA	1.77	0.84
2:A:14:PHE:O	2:A:14:PHE:CD2	2.30	0.84
2:A:570:LEU:HA	2:A:665:PRO:HD3	1.58	0.83
2:A:459:LEU:HB3	2:A:882:ILE:HD11	1.60	0.83
2:A:464:ILE:HG13	2:A:875:MET:HE1	1.59	0.82
1:B:117:ASN:HD22	1:B:119:TYR:H	1.28	0.82
1:B:242:ASP:HB3	1:B:243:PRO:HD3	1.62	0.82
1:B:174:THR:H	1:B:177:GLN:HE21	1.25	0.81
2:A:735:ARG:HH21	2:A:735:ARG:CG	1.91	0.81
2:A:888:TYR:OH	2:A:894:VAL:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LYS:HE3	1:B:281:TRP:H	1.47	0.80
1:C:242:ASP:HB3	1:C:243:PRO:HD3	1.64	0.79
1:C:302:ASN:HD21	1:C:307:LEU:H	1.27	0.79
1:C:163:SER:HB3	1:C:204:ILE:HD11	1.64	0.79
2:A:43:SER:HB2	2:A:673:LEU:HD23	1.65	0.79
1:C:359:GLN:HG3	1:C:360:ALA:N	1.95	0.79
1:B:125:GLN:HE21	1:C:228:ASN:H	1.32	0.77
2:A:569:ASP:HB2	2:A:628:ILE:O	1.85	0.77
2:A:995:LEU:HD21	2:A:1016:MET:HE3	1.65	0.76
2:A:574:PRO:HG2	2:A:624:VAL:HG13	1.65	0.76
2:A:409:VAL:HB	2:A:450:LEU:HD11	1.68	0.76
2:A:588:MET:HE2	2:A:658:LEU:HD22	1.69	0.75
1:B:82:VAL:HG11	2:A:652:THR:HG23	1.69	0.75
2:A:239:THR:HG22	2:A:241:ASP:H	1.52	0.75
2:A:13:ARG:O	2:A:13:ARG:CD	2.32	0.75
2:A:275:ILE:HD13	2:A:586:ALA:HB2	1.68	0.74
1:B:342:ILE:HD12	1:B:398:MET:HE1	1.70	0.73
1:C:106:PHE:CE2	1:C:359:GLN:HG2	2.24	0.73
2:A:425:HIS:HB3	2:A:426:PRO:HD2	1.71	0.73
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.52	0.72
2:A:888:TYR:OH	2:A:894:VAL:CG2	2.36	0.72
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.70	0.72
2:A:13:ARG:HD2	2:A:13:ARG:C	2.13	0.72
2:A:36:VAL:HG21	2:A:335:ILE:HG12	1.71	0.72
2:A:518:ASN:HA	2:A:521:LEU:HD21	1.70	0.72
1:B:387:SER:HB2	2:A:271:MET:HB2	1.72	0.71
1:B:385:ILE:HG22	1:B:389:ALA:HB2	1.70	0.71
2:A:378:PHE:HA	2:A:381:MET:HE2	1.72	0.71
2:A:735:ARG:HG2	2:A:735:ARG:NH2	1.98	0.71
2:A:960:ASN:HB2	2:A:961:PRO:HD3	1.73	0.71
2:A:977:ALA:HA	2:A:980:ARG:NE	2.05	0.70
2:A:982:ARG:HB3	2:A:983:PRO:HD3	1.74	0.70
2:A:14:PHE:O	2:A:14:PHE:HD2	1.69	0.70
2:A:850:LEU:HD21	2:A:856:VAL:HG23	1.74	0.70
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.56	0.70
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.74	0.70
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.21	0.69
2:A:2:ILE:H	2:A:2:ILE:HD12	1.55	0.69
2:A:940:PHE:CE1	2:A:1024:PRO:HA	2.28	0.69
1:B:125:GLN:NE2	1:C:228:ASN:H	1.90	0.69
2:A:574:PRO:HG2	2:A:624:VAL:HG11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD11	1:B:339:GLN:HB2	1.76	0.68
1:B:388:GLU:OE1	1:B:388:GLU:CA	2.41	0.68
1:B:117:ASN:ND2	1:B:119:TYR:H	1.92	0.67
2:A:279:ASN:HD21	2:A:604:ARG:HA	1.58	0.67
2:A:804:ILE:HG13	2:A:804:ILE:O	1.93	0.67
1:B:174:THR:H	1:B:177:GLN:NE2	1.92	0.67
1:B:84:ILE:HD11	2:A:594:LYS:HD2	1.75	0.67
2:A:191:ILE:HD13	2:A:263:ALA:HB2	1.77	0.67
2:A:846:GLU:HG3	2:A:847:LYS:HG3	1.75	0.67
1:C:268:VAL:HG13	1:C:276:LEU:HD11	1.76	0.67
2:A:27:GLY:HA3	2:A:375:CYS:HB3	1.76	0.67
2:A:118:GLN:NE2	2:A:127:ALA:H	1.89	0.67
2:A:707:VAL:HG21	2:A:840:LEU:HD23	1.76	0.67
1:C:254:ILE:HG22	1:C:257:LEU:HB2	1.75	0.66
1:B:84:ILE:HG12	1:B:85:ASP:N	2.09	0.66
2:A:466:THR:O	2:A:871:LYS:HE2	1.94	0.66
2:A:904:VAL:HG22	2:A:905:PRO:HD3	1.77	0.66
2:A:940:PHE:C	2:A:940:PHE:CD2	2.73	0.66
2:A:844:ILE:HD12	2:A:858:PHE:HZ	1.61	0.66
2:A:991:ILE:O	2:A:995:LEU:HB2	1.95	0.66
2:A:399:ALA:O	2:A:403:MET:HG2	1.97	0.65
2:A:546:SER:O	2:A:549:THR:HG22	1.96	0.65
1:B:280:LYS:HE3	1:B:280:LYS:HA	1.78	0.65
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.78	0.65
1:C:317:LEU:C	1:C:317:LEU:HD12	2.22	0.65
2:A:42:LEU:HD13	2:A:670:ILE:HD13	1.79	0.65
2:A:955:VAL:HG12	2:A:956:PRO:HD3	1.78	0.65
1:B:342:ILE:HB	1:B:378:VAL:HG13	1.78	0.64
2:A:980:ARG:O	2:A:984:LYS:HB2	1.96	0.64
2:A:370:LEU:HB2	2:A:371:PRO:HD3	1.77	0.64
1:B:335:THR:HG22	1:B:391:ILE:HD12	1.80	0.64
1:B:386:ASP:O	1:B:388:GLU:N	2.25	0.64
2:A:4:TRP:O	2:A:8:ARG:HG3	1.98	0.64
1:B:242:ASP:HB3	1:B:243:PRO:CD	2.28	0.64
1:B:341:VAL:HG21	1:B:371:LEU:HD11	1.80	0.63
2:A:13:ARG:CD	2:A:13:ARG:C	2.70	0.63
2:A:13:ARG:CB	2:A:499:ILE:CD1	2.65	0.63
2:A:36:VAL:CG2	2:A:335:ILE:HG12	2.27	0.63
2:A:690:LEU:HD22	2:A:718:LEU:HD23	1.80	0.63
2:A:356:PHE:HD2	2:A:986:MET:HB3	1.62	0.63
2:A:361:ARG:O	2:A:365:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:574:PRO:HB2	2:A:658:LEU:CD1	2.24	0.63
2:A:975:HIS:C	2:A:977:ALA:H	2.07	0.63
2:A:391:MET:HE3	2:A:474:LEU:HD11	1.80	0.63
2:A:411:ILE:HA	2:A:501:MET:HE1	1.80	0.63
1:B:399:ARG:O	1:B:400:SER:HB2	1.99	0.62
2:A:907:ALA:HB1	2:A:933:LEU:HD11	1.82	0.62
2:A:87:GLN:HE21	2:A:812:MET:HE2	1.63	0.62
2:A:351:VAL:O	2:A:355:LEU:HG	2.00	0.62
2:A:888:TYR:CZ	2:A:894:VAL:CG2	2.80	0.62
2:A:888:TYR:CE2	2:A:894:VAL:CG2	2.83	0.62
1:C:384:LEU:HD21	2:A:588:MET:HE3	1.81	0.62
2:A:482:LYS:O	2:A:486:MET:HG2	1.99	0.62
2:A:851:LYS:HB3	2:A:852:PRO:HD2	1.82	0.62
2:A:955:VAL:HA	2:A:958:LEU:HD13	1.81	0.61
1:B:324:MET:HE1	1:B:358:PHE:CG	2.34	0.61
1:C:219:THR:OG1	1:C:237:LYS:HD2	2.00	0.61
2:A:962:GLN:HG3	2:A:963:THR:N	2.15	0.61
2:A:940:PHE:CE1	2:A:984:LYS:HE3	2.35	0.61
2:A:85:PHE:CE1	2:A:814:LYS:HD3	2.36	0.61
1:B:220:ALA:HB3	1:B:237:LYS:HB3	1.83	0.61
2:A:620:PRO:HB2	2:A:622:GLU:HG2	1.83	0.61
2:A:345:GLU:HG2	2:A:997:PRO:HG2	1.83	0.61
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.81	0.61
2:A:122:PRO:HB2	2:A:125:VAL:HG13	1.83	0.61
2:A:547:VAL:O	2:A:550:VAL:HG12	2.00	0.61
2:A:964:PHE:CZ	2:A:1043:HIS:HB3	2.36	0.60
2:A:574:PRO:HD2	2:A:624:VAL:HG22	1.83	0.60
1:B:123:ILE:HB	1:C:227:MET:CG	2.31	0.60
2:A:6:ILE:HD13	2:A:443:SER:HB3	1.82	0.60
2:A:6:ILE:O	2:A:10:VAL:HG23	2.02	0.60
2:A:552:TRP:HB3	2:A:553:PRO:HD3	1.82	0.60
2:A:573:MET:O	2:A:661:LEU:HB3	2.02	0.60
2:A:357:LEU:HD13	2:A:986:MET:HE1	1.83	0.60
2:A:85:PHE:HB2	2:A:92:TYR:HB2	1.83	0.60
1:C:242:ASP:HB3	1:C:243:PRO:CD	2.32	0.59
1:B:117:ASN:HD22	1:B:117:ASN:C	2.10	0.59
2:A:43:SER:HB2	2:A:673:LEU:CD2	2.32	0.59
2:A:995:LEU:O	2:A:1017:ILE:HD11	2.02	0.59
2:A:13:ARG:NH1	2:A:436:TRP:CZ3	2.53	0.59
1:B:252:GLU:HG3	1:C:270:ALA:HB2	1.85	0.59
2:A:377:ALA:O	2:A:381:MET:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.84	0.58
1:B:186:ARG:NH2	1:C:206:THR:HG21	2.18	0.58
1:B:174:THR:N	1:B:177:GLN:HE21	1.99	0.58
1:B:223:LEU:C	1:B:224:ARG:HD2	2.29	0.58
2:A:601:GLU:OE2	2:A:637:ARG:HD3	2.03	0.58
2:A:535:TRP:O	2:A:537:LYS:N	2.37	0.58
2:A:553:PRO:O	2:A:557:VAL:HG22	2.03	0.58
1:B:81:GLY:HA2	1:C:87:THR:HG21	1.84	0.58
2:A:402:ALA:HB3	2:A:486:MET:HE1	1.86	0.57
1:B:302:ASN:HD21	1:B:307:LEU:H	1.51	0.57
2:A:940:PHE:CE2	2:A:944:MET:HG3	2.38	0.57
2:A:364:LEU:O	2:A:368:ILE:HG12	2.04	0.57
2:A:992:ILE:O	2:A:996:LEU:HB2	2.04	0.57
2:A:38:ALA:O	2:A:390:ILE:HG22	2.05	0.57
1:C:360:ALA:HB2	1:C:365:THR:HB	1.85	0.57
2:A:589:LEU:HD13	2:A:609:THR:HG23	1.86	0.56
2:A:888:TYR:CE2	2:A:894:VAL:HG22	2.40	0.56
2:A:436:TRP:CD1	2:A:436:TRP:C	2.82	0.56
2:A:550:VAL:HB	2:A:909:VAL:HG23	1.86	0.56
2:A:572:TYR:HB3	2:A:626:THR:OG1	2.05	0.56
2:A:224:LEU:HB2	2:A:229:TYR:CE1	2.40	0.56
2:A:13:ARG:O	2:A:14:PHE:CB	2.52	0.56
2:A:441:ASP:HA	2:A:444:VAL:HG23	1.87	0.56
2:A:877:PRO:O	2:A:881:MET:HG2	2.05	0.56
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.35	0.56
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.88	0.56
2:A:940:PHE:HA	2:A:943:VAL:HG22	1.87	0.56
1:B:384:LEU:HD12	1:B:384:LEU:N	2.21	0.55
1:C:166:LEU:O	1:C:170:GLU:HG2	2.06	0.55
2:A:214:ASN:HB2	2:A:237:LEU:HD22	1.88	0.55
2:A:455:LEU:HD13	2:A:459:LEU:HD13	1.89	0.55
2:A:390:ILE:HD11	2:A:1008:VAL:CG1	2.36	0.55
2:A:534:HIS:C	2:A:534:HIS:CD2	2.84	0.55
1:B:386:ASP:HB2	2:A:269:PRO:O	2.07	0.55
2:A:3:GLU:CD	2:A:3:GLU:H	2.15	0.55
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.89	0.55
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.06	0.55
2:A:1009:MET:HA	2:A:1012:ILE:HG22	1.88	0.55
2:A:940:PHE:C	2:A:940:PHE:HD2	2.13	0.55
2:A:113:TYR:HA	2:A:116:GLN:HE21	1.72	0.55
2:A:526:HIS:HA	2:A:529:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:453:SER:OG	2:A:939:GLU:HG2	2.07	0.54
1:C:324:MET:HB2	1:C:366:ALA:HB1	1.89	0.54
2:A:729:ASN:C	2:A:729:ASN:HD22	2.14	0.54
2:A:418:LEU:HD21	2:A:438:VAL:HG11	1.89	0.54
2:A:746:PHE:O	2:A:750:ALA:HB3	2.08	0.54
2:A:390:ILE:HD12	2:A:1005:GLY:HA3	1.90	0.54
2:A:13:ARG:O	2:A:14:PHE:HB3	2.08	0.54
2:A:214:ASN:H	2:A:215:GLN:NE2	2.06	0.54
2:A:735:ARG:CG	2:A:735:ARG:NH2	2.60	0.54
2:A:779:SER:HB2	2:A:780:PRO:HD2	1.89	0.54
2:A:341:LYS:O	2:A:345:GLU:HG3	2.08	0.53
2:A:684:LYS:HG2	2:A:823:TRP:CD1	2.43	0.53
2:A:888:TYR:CE2	2:A:894:VAL:HG23	2.42	0.53
1:B:256:TRP:HE1	1:B:359:GLN:NE2	2.06	0.53
2:A:368:ILE:O	2:A:368:ILE:HG22	2.08	0.53
2:A:900:ILE:HD12	2:A:941:GLY:O	2.08	0.53
2:A:65:VAL:O	2:A:69:LEU:HB2	2.07	0.53
2:A:876:VAL:HB	2:A:877:PRO:HD3	1.90	0.53
2:A:1022:THR:O	2:A:1026:LEU:HB2	2.08	0.53
2:A:637:ARG:HB3	2:A:638:PRO:HD2	1.90	0.53
2:A:844:ILE:HD12	2:A:858:PHE:CZ	2.42	0.53
2:A:991:ILE:HG21	2:A:1020:MET:SD	2.48	0.53
1:C:266:LEU:HB3	1:C:276:LEU:HD12	1.91	0.53
2:A:464:ILE:CD1	2:A:928:THR:HG23	2.39	0.53
2:A:888:TYR:HH	2:A:894:VAL:HG23	1.73	0.53
2:A:67:TYR:N	2:A:68:PRO:HD2	2.23	0.53
2:A:549:THR:HG23	2:A:913:TRP:HE1	1.74	0.53
2:A:623:MET:CE	2:A:625:GLU:HG3	2.39	0.53
1:B:388:GLU:O	1:B:389:ALA:C	2.52	0.53
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.91	0.52
2:A:880:LEU:HA	2:A:883:ILE:HG22	1.91	0.52
2:A:932:ALA:O	2:A:936:VAL:HG23	2.09	0.52
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.90	0.52
2:A:661:LEU:HD11	2:A:679:SER:HB3	1.90	0.52
2:A:14:PHE:CD2	2:A:14:PHE:C	2.86	0.52
2:A:459:LEU:C	2:A:461:PHE:H	2.17	0.52
2:A:28:THR:O	2:A:32:ILE:HG13	2.09	0.52
2:A:977:ALA:O	2:A:981:VAL:HG23	2.09	0.52
2:A:459:LEU:HB3	2:A:882:ILE:CD1	2.36	0.52
2:A:461:PHE:CE2	2:A:932:ALA:HB2	2.45	0.52
2:A:893:ARG:HB3	2:A:896:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:SER:HA	2:A:771:ARG:HH12	1.75	0.52
2:A:307:LYS:O	2:A:311:LEU:HG	2.10	0.52
2:A:398:ILE:HB	2:A:1016:MET:HE1	1.91	0.52
2:A:900:ILE:O	2:A:903:SER:HB3	2.10	0.52
2:A:964:PHE:CE2	2:A:1043:HIS:HB3	2.44	0.52
2:A:689:VAL:HG12	2:A:692:ASP:H	1.74	0.52
1:B:342:ILE:HB	1:B:378:VAL:CG1	2.39	0.52
2:A:912:ILE:HD12	2:A:930:PHE:CZ	2.45	0.52
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.09	0.52
2:A:883:ILE:HD11	2:A:938:ALA:HB1	1.92	0.51
2:A:907:ALA:HB2	2:A:1023:ALA:HB2	1.93	0.51
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.92	0.51
2:A:522:ILE:HG23	2:A:526:HIS:CD2	2.46	0.51
2:A:563:PRO:HG3	2:A:1011:ARG:HG2	1.91	0.51
2:A:357:LEU:CD1	2:A:986:MET:HE1	2.40	0.51
2:A:376:ILE:HD13	2:A:488:GLY:HA2	1.92	0.51
2:A:464:ILE:HD11	2:A:928:THR:HG23	1.91	0.51
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.75	0.51
1:C:167:LEU:C	1:C:167:LEU:HD12	2.35	0.51
2:A:410:MET:HE1	2:A:493:ALA:O	2.11	0.51
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.93	0.51
1:B:230:ALA:H	1:B:233:ASN:ND2	2.09	0.51
1:B:322:GLU:HG3	1:B:323:PRO:HD2	1.92	0.51
2:A:279:ASN:ND2	2:A:605:VAL:H	2.08	0.51
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.41	0.51
2:A:896:GLU:OE1	2:A:945:LEU:HD11	2.07	0.51
1:C:230:ALA:H	1:C:233:ASN:ND2	2.08	0.51
2:A:191:ILE:O	2:A:773:PRO:HD3	2.11	0.51
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.41	0.50
2:A:944:MET:SD	2:A:980:ARG:HD2	2.50	0.50
2:A:969:LEU:HD12	2:A:969:LEU:O	2.12	0.50
1:C:342:ILE:O	1:C:378:VAL:HG12	2.11	0.50
2:A:270:GLU:HG2	2:A:271:MET:H	1.76	0.50
1:B:385:ILE:HA	2:A:272:ARG:HH11	1.76	0.50
2:A:398:ILE:HD11	2:A:482:LYS:HG3	1.93	0.50
2:A:563:PRO:O	2:A:565:ILE:HD12	2.11	0.50
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.94	0.50
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.93	0.50
2:A:781:GLN:CD	2:A:781:GLN:H	2.19	0.50
2:A:864:LEU:HD22	2:A:867:ARG:HH12	1.77	0.50
2:A:725:ASN:O	2:A:804:ILE:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:CD1	1:C:229:ILE:HB	2.42	0.49
1:C:397:ARG:O	1:C:401:GLU:HG3	2.12	0.49
2:A:144:LEU:HB2	2:A:285:ALA:O	2.12	0.49
2:A:366:ALA:HB1	2:A:404:VAL:HG23	1.95	0.49
2:A:42:LEU:HA	2:A:473:ARG:HD2	1.93	0.49
2:A:56:GLN:OE1	2:A:56:GLN:HA	2.13	0.49
2:A:390:ILE:HD11	2:A:1008:VAL:HG12	1.94	0.49
2:A:408:ILE:HD12	2:A:986:MET:HE2	1.93	0.49
2:A:418:LEU:HD12	2:A:439:ILE:HD11	1.95	0.49
1:B:280:LYS:HE3	1:B:281:TRP:N	2.23	0.49
1:B:329:SER:HA	1:B:365:THR:HG23	1.95	0.49
1:B:339:GLN:HG3	1:B:357:VAL:HG22	1.93	0.49
2:A:240:LEU:HD22	2:A:265:VAL:HG12	1.94	0.49
2:A:403:MET:HB3	2:A:489:ALA:HB2	1.93	0.49
2:A:414:ALA:HB1	2:A:439:ILE:HD12	1.94	0.49
2:A:529:LEU:O	2:A:532:VAL:HG12	2.13	0.49
2:A:569:ASP:HB3	2:A:629:GLN:HA	1.94	0.49
2:A:955:VAL:N	2:A:956:PRO:CD	2.75	0.49
2:A:972:ALA:HA	2:A:975:HIS:HD2	1.77	0.49
2:A:940:PHE:CE1	2:A:984:LYS:CE	2.95	0.49
2:A:984:LYS:CA	2:A:984:LYS:HE2	2.43	0.49
1:B:123:ILE:HB	1:C:227:MET:HG2	1.93	0.49
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.43	0.49
2:A:668:ASN:O	2:A:672:MET:HG3	2.13	0.49
2:A:872:LEU:HA	2:A:875:MET:HB3	1.95	0.48
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.95	0.48
2:A:553:PRO:HB2	2:A:912:ILE:CG2	2.43	0.48
1:B:83:ARG:CZ	1:C:90:GLN:HB3	2.43	0.48
2:A:212:ALA:C	2:A:215:GLN:HE22	2.21	0.48
2:A:400:VAL:HA	2:A:403:MET:HG3	1.95	0.48
2:A:559:GLY:O	2:A:834:VAL:HB	2.14	0.48
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.95	0.48
2:A:896:GLU:OE1	2:A:945:LEU:HD12	2.12	0.48
1:B:385:ILE:HG13	2:A:272:ARG:H	1.77	0.48
1:C:106:PHE:CE1	1:C:321:SER:HB3	2.48	0.48
1:C:167:LEU:HA	1:C:170:GLU:HG2	1.94	0.48
2:A:277:GLU:OE2	2:A:590:GLN:HG3	2.14	0.48
2:A:906:PHE:CD1	2:A:1026:LEU:HD23	2.48	0.48
1:B:287:VAL:HG12	1:B:294:LEU:HD23	1.95	0.48
1:C:242:ASP:O	1:C:302:ASN:HB3	2.14	0.48
2:A:449:ALA:O	2:A:453:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:894:VAL:HG12	2:A:895:GLY:N	2.28	0.48
2:A:959:ASN:ND2	2:A:968:LYS:HD3	2.28	0.48
1:B:242:ASP:O	1:B:302:ASN:HB3	2.14	0.48
2:A:938:ALA:O	2:A:942:VAL:HG23	2.14	0.48
1:C:395:LEU:O	1:C:399:ARG:HG3	2.14	0.48
2:A:376:ILE:HG21	2:A:488:GLY:HA3	1.96	0.48
2:A:882:ILE:HD13	2:A:882:ILE:C	2.39	0.48
2:A:959:ASN:N	2:A:959:ASN:OD1	2.46	0.48
1:C:279:ARG:HH11	1:C:279:ARG:HB2	1.78	0.48
2:A:431:ASP:CG	2:A:432:ASN:H	2.22	0.48
2:A:553:PRO:HB2	2:A:912:ILE:HG22	1.96	0.48
2:A:945:LEU:HD13	2:A:945:LEU:O	2.13	0.48
2:A:988:VAL:HG21	2:A:1024:PRO:HB3	1.96	0.48
1:B:117:ASN:HD21	1:B:119:TYR:HB2	1.79	0.47
1:C:287:VAL:HB	1:C:294:LEU:HD23	1.96	0.47
2:A:751:VAL:O	2:A:771:ARG:HD2	2.14	0.47
2:A:893:ARG:HB3	2:A:896:GLU:CB	2.43	0.47
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.44	0.47
1:C:264:PHE:HE1	1:C:281:TRP:CE2	2.32	0.47
2:A:109:ARG:O	2:A:112:GLU:HG2	2.14	0.47
2:A:887:LEU:HD13	2:A:900:ILE:HB	1.96	0.47
2:A:131:PRO:HD2	2:A:615:ALA:HB3	1.95	0.47
2:A:608:LYS:HE2	2:A:625:GLU:HB2	1.96	0.47
2:A:837:VAL:HA	2:A:840:LEU:HD12	1.95	0.47
1:B:124:VAL:HB	1:B:235:VAL:HG22	1.96	0.47
1:B:186:ARG:HH22	1:C:206:THR:HG21	1.78	0.47
1:B:360:ALA:HA	1:B:365:THR:HA	1.96	0.47
2:A:1:MET:O	2:A:5:ILE:HG13	2.15	0.47
2:A:399:ALA:HA	2:A:486:MET:HE2	1.95	0.47
2:A:904:VAL:N	2:A:905:PRO:CD	2.77	0.47
1:B:120:GLN:NE2	1:B:243:PRO:HD2	2.23	0.47
1:C:106:PHE:HE1	1:C:321:SER:HB3	1.79	0.47
2:A:68:PRO:O	2:A:72:THR:HG23	2.15	0.47
2:A:446:VAL:HB	2:A:946:MET:HE1	1.96	0.47
2:A:494:ILE:HG23	2:A:495:VAL:HG23	1.95	0.47
1:B:268:VAL:HG23	1:B:271:ARG:H	1.79	0.47
2:A:297:ALA:O	2:A:301:ILE:HG13	2.15	0.47
2:A:350:ALA:HA	2:A:353:CYS:SG	2.55	0.47
1:B:153:LEU:H	1:B:153:LEU:HD23	1.80	0.47
2:A:356:PHE:HD2	2:A:986:MET:CB	2.27	0.47
2:A:554:LEU:CD2	2:A:912:ILE:HG12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.50	0.47
2:A:975:HIS:C	2:A:977:ALA:N	2.73	0.47
2:A:367:ILE:C	2:A:369:SER:H	2.23	0.47
1:B:280:LYS:HA	1:B:280:LYS:CE	2.44	0.46
2:A:210:LEU:HA	2:A:246:ILE:HD13	1.97	0.46
2:A:390:ILE:HD12	2:A:1005:GLY:CA	2.44	0.46
2:A:880:LEU:HD22	2:A:901:ILE:HD11	1.97	0.46
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.96	0.46
2:A:474:LEU:O	2:A:477:PRO:HD2	2.14	0.46
2:A:573:MET:O	2:A:661:LEU:CB	2.63	0.46
1:B:387:SER:HB3	2:A:271:MET:HG3	1.98	0.46
1:B:223:LEU:O	1:B:224:ARG:HD2	2.16	0.46
1:B:336:GLY:HA3	2:A:775:SER:HB2	1.98	0.46
2:A:403:MET:HG2	2:A:403:MET:H	1.39	0.46
2:A:270:GLU:HG2	2:A:271:MET:N	2.30	0.46
2:A:463:PRO:HB3	2:A:875:MET:HG3	1.98	0.46
2:A:891:PHE:CE1	2:A:945:LEU:HD12	2.49	0.46
1:C:138:LEU:HD23	1:C:150:LEU:HD12	1.97	0.46
2:A:21:LEU:C	2:A:21:LEU:HD13	2.41	0.46
2:A:122:PRO:HB2	2:A:125:VAL:CG1	2.45	0.46
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.50	0.46
2:A:425:HIS:CB	2:A:426:PRO:HD2	2.45	0.46
2:A:531:LYS:O	2:A:534:HIS:HB3	2.16	0.46
1:B:155:ILE:HA	1:B:156:PRO:HD3	1.78	0.46
1:B:223:LEU:HD12	1:B:235:VAL:HA	1.98	0.46
2:A:240:LEU:HD21	2:A:267:ILE:HD11	1.97	0.46
2:A:292:ARG:O	2:A:293:SER:C	2.58	0.46
2:A:338:LEU:HG	2:A:390:ILE:HA	1.98	0.46
2:A:526:HIS:N	2:A:527:PRO:CD	2.79	0.46
2:A:879:THR:HA	2:A:882:ILE:HG22	1.98	0.46
1:B:92:LEU:HD21	2:A:278:LEU:HD23	1.98	0.46
1:C:151:LEU:C	1:C:151:LEU:HD12	2.41	0.46
1:B:212:ALA:HA	1:B:213:PRO:HD3	1.82	0.46
1:B:302:ASN:ND2	1:B:307:LEU:H	2.13	0.46
1:C:153:LEU:HD12	1:C:229:ILE:HG21	1.98	0.45
2:A:340:GLY:O	2:A:344:GLU:HG3	2.16	0.45
2:A:1032:PRO:C	2:A:1034:ALA:H	2.24	0.45
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.97	0.45
2:A:73:MET:HA	2:A:76:VAL:HG23	1.98	0.45
2:A:431:ASP:H	2:A:434:THR:HB	1.81	0.45
2:A:440:THR:HG22	2:A:440:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:888:TYR:HE2	2:A:894:VAL:HG22	1.82	0.45
1:C:330:GLN:O	1:C:382:LEU:HD12	2.17	0.45
2:A:376:ILE:O	2:A:380:VAL:HG23	2.16	0.45
2:A:408:ILE:HD12	2:A:986:MET:HG3	1.98	0.45
2:A:633:GLN:HE21	2:A:633:GLN:HB2	1.61	0.45
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.81	0.45
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.98	0.45
1:B:185:LEU:HD12	1:B:185:LEU:HA	1.76	0.45
1:C:165:TYR:HE2	1:C:178:THR:HG23	1.82	0.45
1:C:339:GLN:HG3	1:C:357:VAL:HG23	1.97	0.45
2:A:46:GLN:HG3	2:A:96:ILE:HD13	1.98	0.45
2:A:525:TYR:OH	2:A:1028:LEU:HB3	2.17	0.45
2:A:6:ILE:HG12	2:A:494:ILE:HG13	1.99	0.45
1:B:322:GLU:O	1:B:324:MET:HG3	2.16	0.45
2:A:39:LEU:HD23	2:A:390:ILE:HG23	1.99	0.45
2:A:109:ARG:HD3	2:A:109:ARG:HA	1.85	0.45
2:A:493:ALA:HA	2:A:497:ILE:CB	2.36	0.45
2:A:132:ASP:O	2:A:293:SER:OG	2.35	0.45
2:A:572:TYR:CZ	2:A:574:PRO:HB3	2.52	0.45
1:B:92:LEU:HD13	2:A:281:GLU:O	2.17	0.45
1:B:153:LEU:HD23	1:B:153:LEU:N	2.32	0.45
2:A:2:ILE:HD12	2:A:2:ILE:N	2.28	0.45
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.99	0.45
2:A:909:VAL:O	2:A:913:TRP:HD1	2.00	0.45
2:A:940:PHE:CZ	2:A:1024:PRO:HA	2.52	0.45
1:C:223:LEU:HD12	1:C:235:VAL:HB	1.99	0.44
2:A:592:THR:O	2:A:596:ILE:HG13	2.17	0.44
1:C:254:ILE:HG22	1:C:254:ILE:O	2.17	0.44
2:A:168:LEU:HB3	2:A:177:VAL:HG21	2.00	0.44
2:A:248:LEU:HD11	2:A:259:LEU:HA	1.99	0.44
2:A:391:MET:HE1	2:A:1008:VAL:HG11	1.99	0.44
2:A:918:MET:HE3	2:A:999:LEU:HD21	1.99	0.44
2:A:623:MET:HE3	2:A:625:GLU:HG3	1.99	0.44
2:A:421:TRP:HE3	2:A:438:VAL:HB	1.82	0.44
2:A:580:ILE:HG22	2:A:622:GLU:HB2	1.98	0.44
2:A:599:VAL:HA	2:A:600:PRO:HD3	1.84	0.44
1:B:92:LEU:HD11	2:A:281:GLU:HG3	1.99	0.44
1:B:390:ASN:HD22	1:B:393:GLY:H	1.64	0.44
2:A:580:ILE:HG22	2:A:622:GLU:CB	2.48	0.44
2:A:930:PHE:CZ	2:A:1015:PRO:HB3	2.52	0.44
1:B:384:LEU:HD23	1:B:394:ALA:CB	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.53	0.44
2:A:12:ASN:O	2:A:13:ARG:C	2.61	0.43
2:A:42:LEU:HD13	2:A:670:ILE:CD1	2.46	0.43
2:A:578:PRO:HG2	2:A:717:ARG:HB2	2.00	0.43
2:A:141:GLU:HB3	2:A:325:TYR:HB3	2.00	0.43
2:A:210:LEU:HD22	2:A:246:ILE:HD12	2.00	0.43
1:B:120:GLN:HE22	1:B:243:PRO:CD	2.25	0.43
2:A:718:LEU:HD12	2:A:718:LEU:HA	1.91	0.43
1:C:84:ILE:HG21	2:A:656:PRO:HG3	2.00	0.43
2:A:349:VAL:HG11	2:A:404:VAL:HG11	2.00	0.43
2:A:561:PHE:CD2	2:A:562:LEU:HG	2.53	0.43
2:A:900:ILE:HG23	2:A:941:GLY:HA3	2.00	0.43
2:A:345:GLU:O	2:A:349:VAL:HG23	2.18	0.43
2:A:451:PHE:O	2:A:455:LEU:HB2	2.19	0.43
2:A:535:TRP:O	2:A:536:PRO:C	2.60	0.43
2:A:880:LEU:HA	2:A:880:LEU:HD23	1.85	0.43
2:A:940:PHE:HE2	2:A:944:MET:HG3	1.82	0.43
1:C:274:LYS:HB3	1:C:274:LYS:HE2	1.75	0.43
2:A:102:ASP:HB3	2:A:105:TRP:HB3	1.99	0.43
2:A:131:PRO:CD	2:A:615:ALA:HB3	2.49	0.43
2:A:421:TRP:O	2:A:421:TRP:CD1	2.72	0.43
1:C:234:VAL:O	1:C:234:VAL:HG22	2.18	0.43
2:A:195:ARG:HD3	2:A:261:ASP:O	2.18	0.43
1:B:234:VAL:O	1:B:234:VAL:HG22	2.19	0.43
1:B:378:VAL:HG21	1:B:383:PHE:CE2	2.54	0.43
1:C:223:LEU:C	1:C:224:ARG:HD2	2.43	0.43
2:A:814:LYS:HE3	2:A:823:TRP:CH2	2.54	0.43
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.18	0.43
1:C:164:GLU:O	1:C:168:LEU:HD13	2.19	0.43
2:A:345:GLU:OE2	2:A:998:ILE:HG23	2.19	0.43
1:C:220:ALA:HB3	1:C:237:LYS:HB2	2.01	0.43
2:A:532:VAL:HG23	2:A:539:THR:HG21	2.01	0.42
2:A:623:MET:HE1	2:A:625:GLU:HG3	2.00	0.42
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.42
1:C:162:GLN:HG2	1:C:185:LEU:HD21	2.01	0.42
1:C:317:LEU:C	1:C:317:LEU:CD1	2.91	0.42
2:A:16:VAL:HG11	2:A:495:VAL:O	2.18	0.42
2:A:952:ILE:O	2:A:952:ILE:HG22	2.19	0.42
2:A:492:LEU:HD22	2:A:492:LEU:HA	1.86	0.42
1:B:84:ILE:HG22	1:C:91:ASN:CG	2.43	0.42
1:B:195:ILE:O	1:B:198:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:558:GLY:HA3	2:A:921:HIS:HD2	1.83	0.42
2:A:599:VAL:HG21	2:A:649:LEU:CD1	2.50	0.42
1:C:196:ARG:O	1:C:199:ILE:HG12	2.19	0.42
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.49	0.42
1:C:281:TRP:HB3	1:C:298:LEU:HD23	2.02	0.42
2:A:719:GLU:HA	2:A:810:PRO:HA	2.02	0.42
2:A:817:ASN:O	2:A:818:ALA:HB3	2.20	0.42
2:A:944:MET:HE2	2:A:1027:SER:O	2.19	0.42
2:A:26:TRP:CE3	2:A:379:ILE:HD13	2.55	0.42
2:A:342:LEU:HD21	2:A:397:ALA:HA	2.02	0.42
1:B:343:THR:OG1	1:B:351:VAL:HG23	2.20	0.42
1:C:158:TRP:O	1:C:162:GLN:HG3	2.20	0.42
1:C:317:LEU:HD12	1:C:317:LEU:O	2.19	0.42
2:A:497:ILE:O	2:A:501:MET:HG2	2.20	0.42
1:B:178:THR:O	1:B:182:LEU:HB2	2.19	0.42
1:C:222:ASP:OD2	1:C:234:VAL:HG13	2.20	0.42
1:C:327:ILE:CD1	1:C:367:LEU:HD21	2.50	0.42
2:A:139:ILE:HG23	2:A:301:ILE:HD11	2.00	0.42
2:A:535:TRP:C	2:A:537:LYS:N	2.76	0.42
2:A:596:ILE:HG12	2:A:653:VAL:HG21	2.02	0.42
2:A:1020:MET:HE3	2:A:1020:MET:HA	2.01	0.42
1:C:167:LEU:HA	1:C:170:GLU:CG	2.50	0.42
1:C:279:ARG:HB2	1:C:279:ARG:NH1	2.35	0.42
2:A:114:LEU:HD12	2:A:114:LEU:HA	1.85	0.42
2:A:814:LYS:HE3	2:A:823:TRP:CZ2	2.54	0.42
2:A:1007:GLU:O	2:A:1011:ARG:HD3	2.20	0.42
2:A:1025:LEU:HD23	2:A:1025:LEU:C	2.45	0.42
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.55	0.41
1:C:80:SER:HB3	1:C:401:GLU:OE2	2.19	0.41
2:A:244:ASN:O	2:A:258:TYR:HB3	2.19	0.41
2:A:419:GLU:O	2:A:423:HIS:HD2	2.02	0.41
2:A:525:TYR:OH	2:A:980:ARG:NH2	2.53	0.41
2:A:834:VAL:HG22	2:A:838:HIS:NE2	2.35	0.41
2:A:914:LEU:HD23	2:A:1014:ALA:O	2.20	0.41
2:A:944:MET:HE3	2:A:944:MET:HB3	1.98	0.41
1:B:114:VAL:HG12	1:B:309:PRO:HA	2.00	0.41
1:B:151:LEU:HD12	1:B:151:LEU:C	2.45	0.41
2:A:87:GLN:HG2	2:A:812:MET:HG3	2.02	0.41
2:A:875:MET:HE2	2:A:931:ILE:HG13	2.02	0.41
1:B:195:ILE:O	1:B:199:ILE:HG23	2.19	0.41
2:A:578:PRO:CG	2:A:717:ARG:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:842:LYS:O	2:A:846:GLU:HG2	2.20	0.41
2:A:1041:HIS:C	2:A:1043:HIS:H	2.28	0.41
1:C:127:ARG:O	1:C:231:LYS:HD3	2.20	0.41
1:B:322:GLU:HA	1:B:322:GLU:OE1	2.20	0.41
2:A:2:ILE:H	2:A:2:ILE:CD1	2.29	0.41
2:A:239:THR:HG22	2:A:241:ASP:N	2.29	0.41
2:A:574:PRO:CG	2:A:624:VAL:HG13	2.42	0.41
2:A:624:VAL:HG22	2:A:624:VAL:O	2.19	0.41
1:B:174:THR:HB	1:B:177:GLN:HG3	2.03	0.41
2:A:157:ARG:HG2	2:A:182:GLY:HA3	2.01	0.41
2:A:619:ALA:HB1	2:A:623:MET:HE2	2.02	0.41
2:A:630:LEU:HD13	2:A:642:MET:HE1	2.01	0.41
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.55	0.41
2:A:933:LEU:HD13	2:A:933:LEU:C	2.45	0.41
2:A:1041:HIS:C	2:A:1043:HIS:N	2.78	0.41
1:C:114:VAL:HG12	1:C:309:PRO:HA	2.03	0.41
1:C:330:GLN:CD	1:C:330:GLN:H	2.28	0.41
2:A:2:ILE:O	2:A:6:ILE:HG13	2.21	0.41
2:A:36:VAL:HG23	2:A:388:ALA:HB3	2.03	0.41
2:A:42:LEU:H	2:A:42:LEU:HD12	1.86	0.41
2:A:136:VAL:HG22	2:A:669:ARG:HB3	2.03	0.41
2:A:245:HIS:HA	2:A:258:TYR:CD2	2.56	0.41
2:A:458:THR:HG22	2:A:486:MET:HB2	2.03	0.41
2:A:67:TYR:O	2:A:71:THR:HG23	2.21	0.41
2:A:210:LEU:HD22	2:A:246:ILE:CD1	2.51	0.41
2:A:463:PRO:CB	2:A:875:MET:HG3	2.50	0.41
2:A:933:LEU:HB2	2:A:1016:MET:HG2	2.02	0.41
2:A:962:GLN:HG3	2:A:963:THR:H	1.86	0.41
1:B:324:MET:HE1	1:B:358:PHE:CD2	2.55	0.40
1:C:121:TYR:CE1	1:C:237:LYS:HD3	2.56	0.40
1:C:199:ILE:HG13	1:C:200:ALA:N	2.35	0.40
2:A:86:SER:HB2	2:A:813:LEU:HB2	2.03	0.40
2:A:275:ILE:CD1	2:A:586:ALA:HB2	2.45	0.40
2:A:462:ILE:N	2:A:463:PRO:CD	2.84	0.40
2:A:588:MET:CE	2:A:658:LEU:HD13	2.51	0.40
2:A:969:LEU:O	2:A:973:LEU:HD13	2.21	0.40
2:A:532:VAL:CG2	2:A:539:THR:HG21	2.51	0.40
2:A:107:ARG:NH1	2:A:130:GLY:O	2.53	0.40
2:A:150:LYS:HB2	2:A:150:LYS:HE3	1.83	0.40
2:A:301:ILE:HG21	2:A:328:SER:HB3	2.02	0.40
2:A:364:LEU:HD23	2:A:367:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:904:VAL:C	2:A:906:PHE:H	2.29	0.40
1:C:124:VAL:O	1:C:235:VAL:HG13	2.21	0.40
1:C:302:ASN:ND2	1:C:307:LEU:HB2	2.36	0.40
2:A:222:ILE:HG12	2:A:223:GLU:N	2.33	0.40
1:B:217:VAL:CG2	1:B:241:MET:HE2	2.52	0.40
1:B:360:ALA:HB2	1:B:365:THR:HG22	2.03	0.40
2:A:240:LEU:HD23	2:A:240:LEU:HA	1.95	0.40
2:A:461:PHE:HE1	2:A:479:ALA:HA	1.85	0.40
2:A:595:LEU:HB3	2:A:653:VAL:HG22	2.02	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%)	297 (93%)	20 (6%)	3 (1%)	14	44
1	C	322/413 (78%)	309 (96%)	12 (4%)	1 (0%)	36	67
2	A	1027/1054 (97%)	942 (92%)	77 (8%)	8 (1%)	16	47
All	All	1669/1880 (89%)	1548 (93%)	109 (6%)	12 (1%)	18	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	638	PRO
2	A	574	PRO
2	A	613	GLU
1	B	388	GLU
1	B	390	ASN
2	A	14	PHE
2	A	426	PRO
2	A	1024	PRO

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Mol	Chain	Res	Type
2	A	665	PRO
1	B	137	PRO
1	C	137	PRO
2	A	852	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	263/338 (78%)	224 (85%)	39 (15%)	3	13
1	C	265/338 (78%)	230 (87%)	35 (13%)	4	17
2	A	849/871 (98%)	739 (87%)	110 (13%)	4	18
All	All	1377/1547 (89%)	1193 (87%)	184 (13%)	4	17

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	98	THR
1	B	105	THR
1	B	117	ASN
1	B	135	VAL
1	B	138	LEU
1	B	159	VAL
1	B	168	LEU
1	B	169	ARG
1	B	182	LEU
1	B	185	LEU
1	B	199	ILE
1	B	207	ARG
1	B	234	VAL
1	B	235	VAL
1	B	239	GLN
1	B	241	MET
1	B	267	THR

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Mol	Chain	Res	Type
1	B	268	VAL
1	B	275	THR
1	B	280	LYS
1	B	282	THR
1	B	287	VAL
1	B	322	GLU
1	B	330	GLN
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	364	VAL
1	B	365	THR
1	B	367	LEU
1	B	377	VAL
1	B	378	VAL
1	B	379	SER
1	B	384	LEU
1	B	385	ILE
1	B	388	GLU
1	B	392	SER
1	B	396	GLU
1	C	98	THR
1	C	104	LEU
1	C	105	THR
1	C	138	LEU
1	C	140	VAL
1	C	150	LEU
1	C	159	VAL
1	C	167	LEU
1	C	178	THR
1	C	181	ILE
1	C	182	LEU
1	C	185	LEU
1	C	206	THR
1	C	207	ARG
1	C	231	LYS
1	C	234	VAL
1	C	235	VAL
1	C	258	VAL
1	C	279	ARG
1	C	283	LEU
1	C	287	VAL

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Mol	Chain	Res	Type
1	C	317	LEU
1	C	324	MET
1	C	330	GLN
1	C	332	LEU
1	C	339	GLN
1	C	343	THR
1	C	347	ASP
1	C	351	VAL
1	C	353	LYS
1	C	364	VAL
1	C	365	THR
1	C	377	VAL
1	C	378	VAL
1	C	382	LEU
2	A	1	MET
2	A	3	GLU
2	A	13	ARG
2	A	15	LEU
2	A	17	LEU
2	A	23	LEU
2	A	31	ILE
2	A	36	VAL
2	A	42	LEU
2	A	59	GLN
2	A	105	TRP
2	A	114	LEU
2	A	117	VAL
2	A	120	LYS
2	A	125	VAL
2	A	126	SER
2	A	129	LEU
2	A	144	LEU
2	A	145	VAL
2	A	168	LEU
2	A	190	VAL
2	A	203	LEU
2	A	210	LEU
2	A	211	ASP
2	A	215	GLN
2	A	222	ILE
2	A	237	LEU
2	A	241	ASP

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Mol	Chain	Res	Type
2	A	259	LEU
2	A	260	ARG
2	A	288	VAL
2	A	293	SER
2	A	298	ARG
2	A	300	VAL
2	A	322	VAL
2	A	323	THR
2	A	335	ILE
2	A	342	LEU
2	A	351	VAL
2	A	358	TRP
2	A	390	ILE
2	A	400	VAL
2	A	403	MET
2	A	411	ILE
2	A	412	GLU
2	A	417	ARG
2	A	436	TRP
2	A	455	LEU
2	A	457	ILE
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	545	LEU
2	A	554	LEU
2	A	557	VAL
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	641	THR
2	A	642	MET
2	A	649	LEU

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Mol	Chain	Res	Type
2	A	661	LEU
2	A	693	ILE
2	A	722	ARG
2	A	729	ASN
2	A	735	ARG
2	A	763	ILE
2	A	769	ASN
2	A	770	LEU
2	A	771	ARG
2	A	781	GLN
2	A	783	LEU
2	A	789	LEU
2	A	808	THR
2	A	812	MET
2	A	813	LEU
2	A	814	LYS
2	A	815	THR
2	A	834	VAL
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	894	VAL
2	A	904	VAL
2	A	933	LEU
2	A	940	PHE
2	A	945	LEU
2	A	948	LEU
2	A	959	ASN
2	A	966	GLU
2	A	969	LEU
2	A	984	LYS
2	A	987	THR
2	A	1020	MET
2	A	1026	LEU
2	A	1037	LEU
2	A	1038	MET
2	A	1039	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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	233	ASN
1	B	302	ASN
1	B	330	GLN
1	B	359	GLN
1	B	390	ASN
1	C	125	GLN
1	C	177	GLN
1	C	228	ASN
1	C	263	GLN
1	C	302	ASN
1	C	330	GLN
2	A	46	GLN
2	A	59	GLN
2	A	87	GLN
2	A	116	GLN
2	A	118	GLN
2	A	215	GLN
2	A	238	GLN
2	A	279	ASN
2	A	329	GLN
2	A	337	ASN
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	699	GLN
2	A	725	ASN
2	A	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
2	A	838	HIS
2	A	921	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%)	-0.02	11 (3%) 48 28	26, 53, 97, 153	0
1	C	324/413 (78%)	-0.03	7 (2%) 62 41	31, 54, 100, 142	0
2	A	1031/1054 (97%)	0.52	113 (10%) 10 5	26, 77, 184, 278	0
All	All	1677/1880 (89%)	0.31	131 (7%) 19 10	26, 65, 166, 278	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	ASP	5.7
2	A	1001	GLY	5.6
2	A	409	VAL	5.6
2	A	979	LEU	5.4
2	A	15	LEU	5.0
2	A	884	PHE	4.9
2	A	14	PHE	4.9
2	A	520	PHE	4.6
1	C	157	ASP	4.6
2	A	413	ASN	4.5
1	B	157	ASP	4.2
2	A	972	ALA	4.2
2	A	6	ILE	4.1
2	A	2	ILE	4.0
1	B	388	GLU	3.9
2	A	517	LEU	3.9
2	A	890	ALA	3.8
2	A	956	PRO	3.8
2	A	1038	MET	3.8
1	B	387	SER	3.7
2	A	446	VAL	3.7
1	B	383	PHE	3.7
2	A	873	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	A	22	PHE	3.7
2	A	20	ALA	3.7
2	A	1035	TYR	3.6
2	A	484	TYR	3.4
1	C	242	ASP	3.3
2	A	975	HIS	3.3
2	A	405	ALA	3.3
2	A	895	GLY	3.3
2	A	480	PHE	3.3
1	C	339	GLN	3.3
1	B	400	SER	3.2
2	A	416	LYS	3.2
2	A	889	LEU	3.1
2	A	4	TRP	3.0
2	A	429	THR	3.0
2	A	948	LEU	3.0
2	A	947	TYR	3.0
2	A	10	VAL	3.0
2	A	444	VAL	3.0
2	A	896	GLU	3.0
2	A	891	PHE	3.0
2	A	946	MET	3.0
2	A	450	LEU	2.9
2	A	428	ALA	2.9
2	A	888	TYR	2.9
1	B	339	GLN	2.9
2	A	1039	TRP	2.9
2	A	410	MET	2.9
2	A	981	VAL	2.9
2	A	919	GLY	2.9
2	A	623	MET	2.9
2	A	637	ARG	2.8
1	C	79	ALA	2.8
2	A	360	VAL	2.8
2	A	957	SER	2.8
2	A	887	LEU	2.8
2	A	373	GLY	2.7
2	A	448	PRO	2.7
2	A	980	ARG	2.7
1	B	242	ASP	2.7
2	A	883	ILE	2.6
2	A	950	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	459	LEU	2.6
2	A	955	VAL	2.6
2	A	564	GLN	2.6
2	A	886	LEU	2.6
2	A	870	HIS	2.6
2	A	954	ALA	2.6
2	A	535	TRP	2.5
2	A	390	ILE	2.5
2	A	432	ASN	2.5
2	A	486	MET	2.5
1	B	389	ALA	2.5
2	A	407	ALA	2.5
2	A	426	PRO	2.5
2	A	537	LYS	2.5
2	A	18	MET	2.5
2	A	906	PHE	2.5
2	A	470	GLN	2.5
2	A	443	SER	2.4
1	B	381	GLY	2.4
1	C	176	THR	2.4
2	A	943	VAL	2.4
2	A	226	GLU	2.4
2	A	1002	THR	2.4
2	A	528	LEU	2.4
2	A	498	PRO	2.4
2	A	547	VAL	2.4
2	A	497	ILE	2.3
1	B	338	GLU	2.3
2	A	935	GLY	2.3
2	A	901	ILE	2.3
2	A	878	MET	2.3
2	A	530	LEU	2.3
2	A	903	SER	2.3
2	A	1031	ILE	2.3
2	A	436	TRP	2.3
2	A	30	THR	2.3
2	A	958	LEU	2.3
1	C	340	ARG	2.3
2	A	504	TRP	2.3
2	A	451	PHE	2.3
2	A	418	LEU	2.2
2	A	964	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	401	GLY	2.2
2	A	430	LEU	2.2
2	A	415	HIS	2.2
2	A	435	ARG	2.2
2	A	406	ALA	2.2
2	A	951	ALA	2.2
2	A	398	ILE	2.2
2	A	898	LEU	2.2
2	A	897	ALA	2.2
2	A	368	ILE	2.1
2	A	545	LEU	2.1
2	A	874	LEU	2.1
2	A	1042	ARG	2.1
2	A	293	SER	2.1
1	C	160	GLU	2.1
2	A	902	SER	2.0
2	A	372	LEU	2.0
2	A	495	VAL	2.0
2	A	457	ILE	2.0
2	A	353	CYS	2.0
2	A	687	GLY	2.0
2	A	7	ARG	2.0
2	A	524	VAL	2.0
2	A	969	LEU	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.