



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:14 am GMT

PDB ID : 4DNT
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

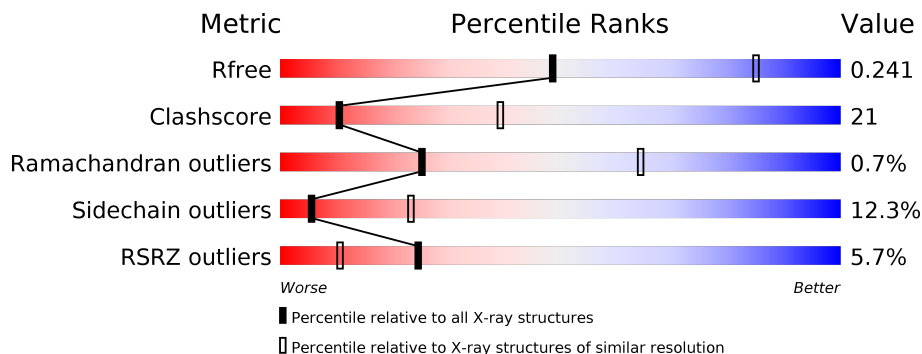
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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

Mol	Chain	Length	Quality of chain
1	B	413	<div> <div style="width: 9%; background-color: red;"></div> <div style="width: 53%; background-color: green;"></div> <div style="width: 21%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 15%; background-color: grey;"></div> </div> <div>53% 21% • 22%</div>
1	C	413	<div> <div style="width: 54%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 22%; background-color: grey;"></div> </div> <div>54% 22% • 22%</div>
2	A	1054	<div> <div style="width: 9%; background-color: red;"></div> <div style="width: 54%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>9% 54% 37% 6% •</div>

2 Entry composition

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
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
			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

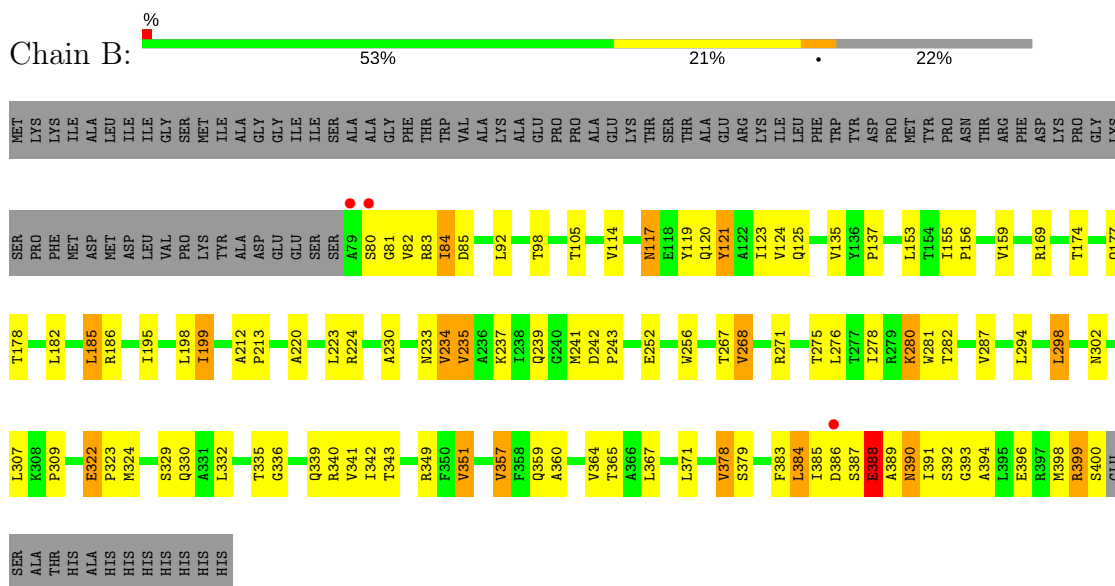
- Molecule 3 is water.

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

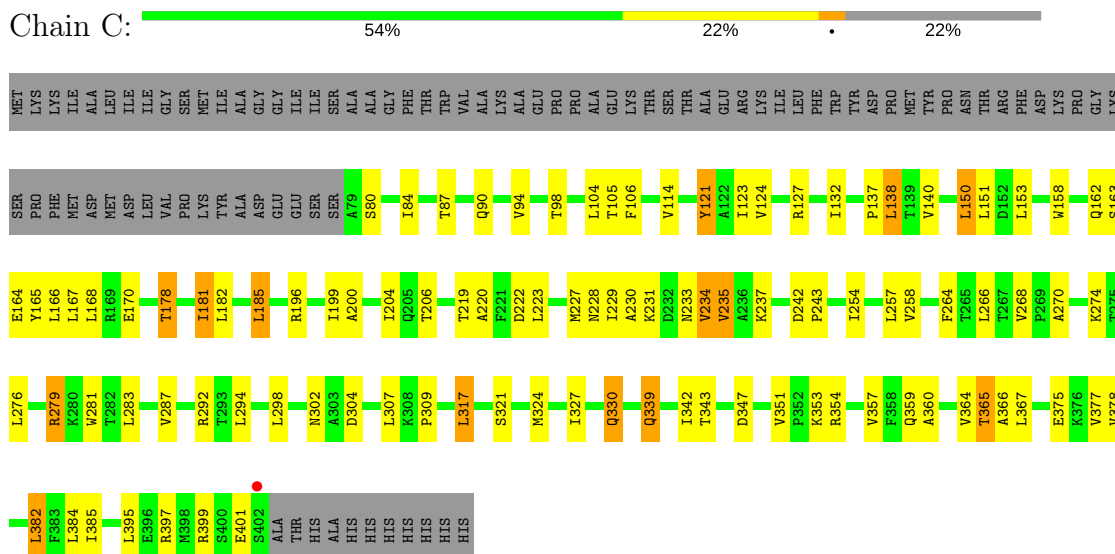
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

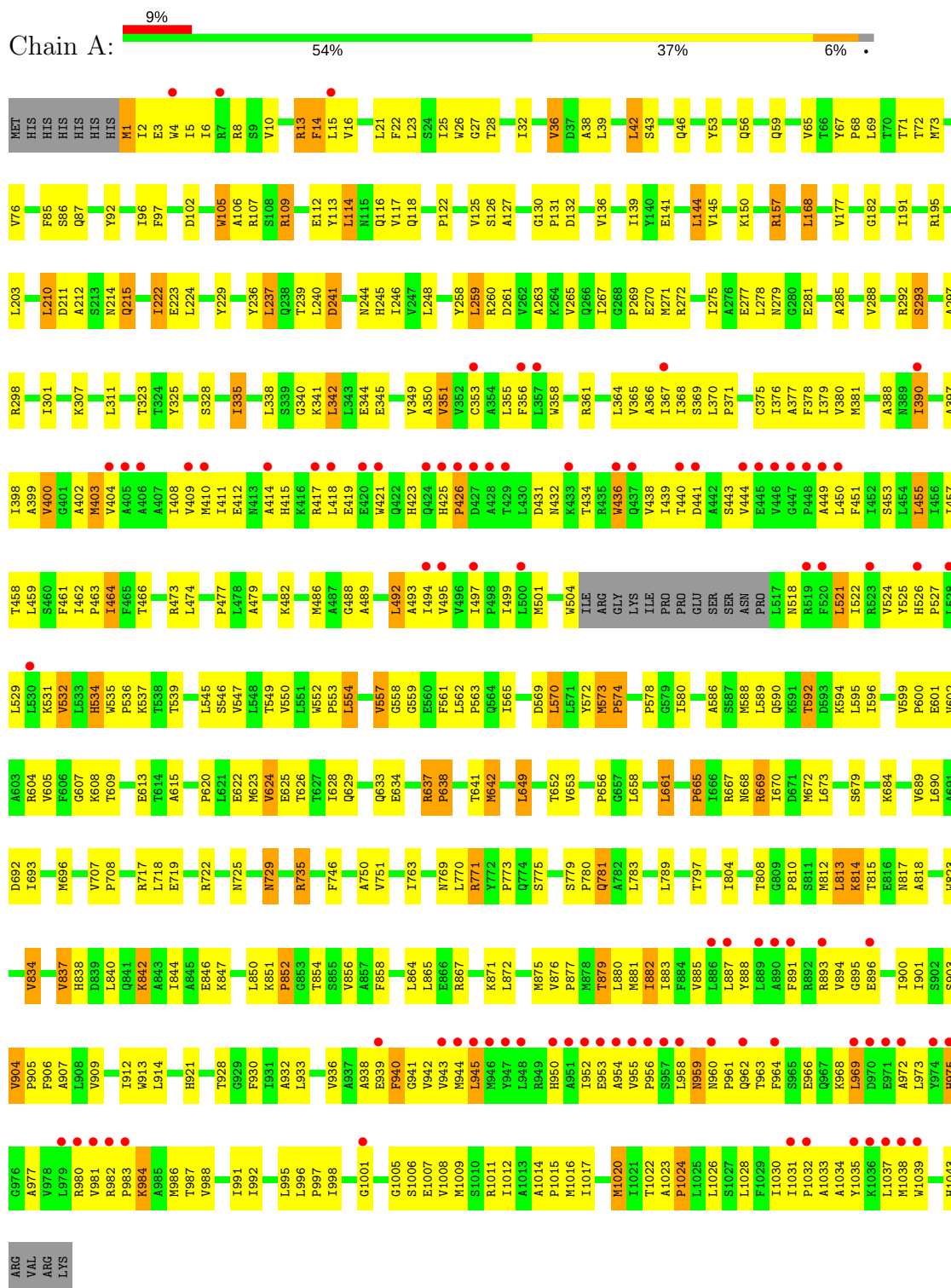
• Molecule 1: Cation efflux system protein CusB



• 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	159.64Å 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)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.219 , 0.244 0.213 , 0.241	Depositor DCC
R_{free} test set	3095 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12895	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage'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	0.23	0/2498	0.45	1/3401 (0.0%)
1	C	0.22	0/2513	0.43	0/3421
2	A	0.21	0/8111	0.42	0/11044
All	All	0.22	0/13122	0.43	1/17866 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLU	N-CA-C	5.12	124.83	111.00

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	91	0
1	C	2473	0	2533	78	0
2	A	7945	0	8196	395	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	539	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 21.

All (539) 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:HH21	2:A:735:ARG:HG2	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
2:A:574:PRO:HG2	2:A:624:VAL:CG1	2.05	0.86
1:C:359:GLN:HG3	1:C:360:ALA:H	1.39	0.86
2:A:13:ARG:HH11	2:A:436:TRP:HZ3	0.86	0.85
2:A:14:PHE:CD2	2:A:14:PHE:O	2.30	0.84
1:B:388:GLU:OE1	1:B:388:GLU:HA	1.77	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
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:588:MET:HE2	2:A:658:LEU:HD13	1.63	0.81
2:A:888:TYR:OH	2:A:894:VAL:HG23	1.81	0.80
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:A:888:TYR:OH	2:A:894:VAL:CG2	2.36	0.72
1:B:120:GLN:HE22	1:B:243:PRO:HD2	1.52	0.72
2:A:536:PRO:HB3	2:A:1033:ALA:HB1	1.70	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: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:HD2	2:A:14:PHE:O	1.69	0.70
2:A:850:LEU:HD21	2:A:856:VAL:HG23	1.74	0.70
1:C:254:ILE:HD11	2:A:797:THR:HG21	1.74	0.70
1:C:106:PHE:HE2	1:C:359:GLN:HG2	1.56	0.70
1:C:165:TYR:HB2	1:C:181:ILE:CG2	2.21	0.69
2:A:2:ILE:HD12	2:A:2:ILE:H	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
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
2:A:13:ARG:C	2:A:13:ARG:HD2	2.13	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:117:ASN:ND2	1:B:119:TYR:H	1.92	0.67
1:B:174:THR:H	1:B:177:GLN:NE2	1.92	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:B:84:ILE:HD11	2:A:594:LYS:HD2	1.75	0.67
1:C:268:VAL:HG13	1:C:276:LEU:HD11	1.76	0.67
2:A:118:GLN:NE2	2:A:127:ALA:H	1.89	0.67
2:A:27:GLY:HA3	2:A:375:CYS:HB3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:B:280:LYS:HE3	1.78	0.65
1:B:384:LEU:HD23	1:B:394:ALA:HB3	1.78	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
2:A:980:ARG:O	2:A:984:LYS:HB2	1.96	0.64
1:B:342:ILE:HB	1:B:378:VAL:HG13	1.78	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: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:361:ARG:O	2:A:365:VAL:HG23	1.99	0.63
2:A:574:PRO:HB2	2:A:658:LEU:CD1	2.24	0.63
2:A:356:PHE:HD2	2:A:986:MET:HB3	1.62	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:351:VAL:O	2:A:355:LEU:HG	2.00	0.62
2:A:888:TYR:CE2	2:A:894:VAL:CG2	2.83	0.62
2:A:888:TYR:CZ	2:A:894:VAL:CG2	2.80	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: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:940:PHE:CD2	2:A:940:PHE:C	2.73	0.61
2:A:85:PHE:CE1	2:A:814:LYS:HD3	2.36	0.61
2:A:620:PRO:HB2	2:A:622:GLU:HG2	1.83	0.61
1:B:220:ALA:HB3	1:B:237:LYS:HB3	1.83	0.61
2:A:1023:ALA:HB3	2:A:1024:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:345:GLU:HG2	2:A:997:PRO:HG2	1.83	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:C:317:LEU:C	1:C:317:LEU:HD12	2.22	0.60
2:A:6:ILE:O	2:A:10:VAL:HG23	2.02	0.60
2:A:6:ILE:HD13	2:A:443:SER:HB3	1.82	0.60
1:B:123:ILE:HB	1:C:227:MET:CG	2.31	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: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
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
2:A:13:ARG:C	2:A:13:ARG:CD	2.70	0.59
1:B:252:GLU:HG3	1:C:270:ALA:HB2	1.85	0.59
2:A:410:MET:HE1	2:A:493:ALA:O	2.03	0.58
2:A:377:ALA:O	2:A:381:MET:HG3	2.03	0.58
2:A:1001:GLY:HA2	2:A:1006:SER:HB2	1.84	0.58
2:A:975:HIS:C	2:A:977:ALA:H	2.07	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
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
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:572:TYR:HB3	2:A:626:THR:OG1	2.05	0.56
2:A:550:VAL:HB	2:A:909:VAL:HG23	1.86	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:411:ILE:HG12	2:A:501:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ILE:HD12	1:B:398:MET:HE1	1.87	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
2:A:954:ALA:HB3	2:A:956:PRO:HD2	1.88	0.56
1:B:220:ALA:HB3	1:B:237:LYS:CB	2.35	0.56
2:A:940:PHE:HA	2:A:943:VAL:HG22	1.87	0.56
1:B:384:LEU:N	1:B:384:LEU:HD12	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
1:B:386:ASP:HB2	2:A:269:PRO:O	2.07	0.55
2:A:707:VAL:HG13	2:A:708:PRO:HD2	1.89	0.55
2:A:1009:MET:HA	2:A:1012:ILE:HG22	1.88	0.55
1:B:121:TYR:OH	1:B:237:LYS:HE2	2.06	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
1:B:117:ASN:HD22	1:B:117:ASN:C	2.10	0.55
2:A:464:ILE:HG13	2:A:875:MET:HE1	1.87	0.54
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: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
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
1:B:223:LEU:C	1:B:224:ARG:HD2	2.29	0.53
1:B:256:TRP:HE1	1:B:359:GLN:NE2	2.06	0.53
2:A:1022:THR:O	2:A:1026:LEU:HB2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:464:ILE:CD1	2:A:928:THR:HG23	2.39	0.53
1:C:266:LEU:HB3	1:C:276:LEU:HD12	1.91	0.53
2:A:888:TYR:HH	2:A:894:VAL:HG23	1.73	0.53
2:A:549:THR:HG23	2:A:913:TRP:HE1	1.74	0.53
2:A:67:TYR:N	2:A:68:PRO:HD2	2.23	0.53
2:A:623:MET:CE	2:A:625:GLU:HG3	2.39	0.53
2:A:1031:ILE:HB	2:A:1032:PRO:HD3	1.90	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
1:B:80:SER:HB3	1:B:82:VAL:HG12	1.91	0.52
2:A:661:LEU:HD11	2:A:679:SER:HB3	1.90	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:623:MET:HE3	2:A:625:GLU:HG3	1.91	0.52
2:A:893:ARG:HB3	2:A:896:GLU:HB2	1.91	0.52
2:A:307:LYS:O	2:A:311:LEU:HG	2.10	0.52
2:A:436:TRP:C	2:A:436:TRP:CD1	2.82	0.52
1:B:387:SER:HA	2:A:771:ARG:HH12	1.75	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
2:A:1026:LEU:O	2:A:1030:ILE:HG12	2.09	0.52
2:A:912:ILE:HD12	2:A:930:PHE:CZ	2.45	0.52
1:B:342:ILE:HB	1:B:378:VAL:CG1	2.39	0.52
2:A:907:ALA:HB2	2:A:1023:ALA:HB2	1.93	0.51
2:A:883:ILE:HD11	2:A:938:ALA:HB1	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
1:C:123:ILE:HG12	1:C:237:LYS:HG3	1.92	0.51
2:A:376:ILE:HD13	2:A:488:GLY:HA2	1.92	0.51
2:A:604:ARG:HB2	2:A:629:GLN:HE21	1.75	0.51
2:A:464:ILE:HD11	2:A:928:THR:HG23	1.91	0.51
2:A:607:GLY:HA2	2:A:626:THR:HG22	1.93	0.51
2:A:279:ASN:ND2	2:A:605:VAL:H	2.08	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:896:GLU:OE1	2:A:945:LEU:HD11	2.07	0.51
1:C:281:TRP:CB	1:C:298:LEU:HD23	2.41	0.51
1:C:230:ALA:H	1:C:233:ASN:ND2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:191:ILE:O	2:A:773:PRO:HD3	2.11	0.51
2:A:378:PHE:HA	2:A:381:MET:HE2	1.93	0.50
2:A:425:HIS:HB3	2:A:426:PRO:CD	2.41	0.50
2:A:969:LEU:HD12	2:A:969:LEU:O	2.12	0.50
2:A:944:MET:SD	2:A:980:ARG:HD2	2.50	0.50
2:A:534:HIS:C	2:A:534:HIS:CD2	2.84	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
2:A:3:GLU:CD	2:A:3:GLU:H	2.15	0.50
2:A:1014:ALA:HB3	2:A:1015:PRO:HD3	1.94	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
1:B:385:ILE:HA	2:A:272:ARG:HH11	1.76	0.50
2:A:950:HIS:HA	2:A:953:GLU:HB2	1.93	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
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
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:42:LEU:HA	2:A:473:ARG:HD2	1.93	0.49
2:A:729:ASN:HD22	2:A:729:ASN:C	2.14	0.49
2:A:390:ILE:HD11	2:A:1008:VAL:HG12	1.94	0.49
2:A:418:LEU:HD12	2:A:439:ILE:HD11	1.95	0.49
2:A:56:GLN:HA	2:A:56:GLN:OE1	2.13	0.49
2:A:940:PHE:HD2	2:A:940:PHE:C	2.13	0.49
2:A:240:LEU:HD22	2:A:265:VAL:HG12	1.94	0.49
2:A:414:ALA:HB1	2:A:439:ILE:HD12	1.94	0.49
2:A:403:MET:HB3	2:A:489:ALA:HB2	1.93	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
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: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
2:A:668:ASN:O	2:A:672:MET:HG3	2.13	0.49
1:B:123:ILE:CD1	1:B:237:LYS:HG3	2.43	0.49
1:B:123:ILE:HB	1:C:227:MET:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:872:LEU:HA	2:A:875:MET:HB3	1.95	0.48
2:A:553:PRO:HB2	2:A:912:ILE:CG2	2.43	0.48
1:B:278:ILE:HG21	1:B:298:LEU:HD13	1.95	0.48
2:A:400:VAL:HA	2:A:403:MET:HG3	1.95	0.48
2:A:599:VAL:HG21	2:A:649:LEU:HD12	1.95	0.48
2:A:559:GLY:O	2:A:834:VAL:HB	2.14	0.48
2:A:894:VAL:HG12	2:A:895:GLY:N	2.28	0.48
2:A:896:GLU:OE1	2:A:945:LEU:HD12	2.12	0.48
1:B:83:ARG:CZ	1:C:90:GLN:HB3	2.43	0.48
1:B:385:ILE:HG13	2:A:272:ARG:H	1.77	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: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:449:ALA:O	2:A:453:SER:HB2	2.14	0.48
2:A:959:ASN:ND2	2:A:968:LYS:HD3	2.28	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:938:ALA:O	2:A:942:VAL:HG23	2.14	0.48
1:B:242:ASP:O	1:B:302:ASN:HB3	2.14	0.48
2:A:376:ILE:HG21	2:A:488:GLY:HA3	1.96	0.48
2:A:959:ASN:N	2:A:959:ASN:OD1	2.46	0.48
1:B:388:GLU:O	1:B:389:ALA:C	2.52	0.48
1:C:395:LEU:O	1:C:399:ARG:HG3	2.14	0.48
2:A:553:PRO:HB2	2:A:912:ILE:HG22	1.96	0.48
2:A:945:LEU:O	2:A:945:LEU:HD13	2.13	0.48
2:A:988:VAL:HG21	2:A:1024:PRO:HB3	1.96	0.48
1:C:279:ARG:HH11	1:C:279:ARG:HB2	1.78	0.48
2:A:459:LEU:C	2:A:461:PHE:H	2.17	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: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
1:C:342:ILE:HB	1:C:378:VAL:CG1	2.44	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
1:C:264:PHE:HE1	1:C:281:TRP:CE2	2.32	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
2:A:1:MET:O	2:A:5:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:904:VAL:N	2:A:905:PRO:CD	2.77	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
1:C:167:LEU:HD12	1:C:167:LEU:C	2.35	0.47
2:A:68:PRO:O	2:A:72:THR:HG23	2.15	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:494:ILE:HG23	2:A:495:VAL:HG23	1.95	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:268:VAL:HG23	1:B:271:ARG:H	1.79	0.47
2:A:356:PHE:HD2	2:A:986:MET:CB	2.27	0.47
2:A:834:VAL:HG22	2:A:838:HIS:CD2	2.50	0.47
2:A:554:LEU:CD2	2:A:912:ILE:HG12	2.45	0.47
1:B:153:LEU:H	1:B:153:LEU:HD23	1.80	0.47
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
1:B:280:LYS:HA	1:B:280:LYS:CE	2.44	0.46
2:A:474:LEU:O	2:A:477:PRO:HD2	2.14	0.46
2:A:361:ARG:HB3	2:A:504:TRP:HB3	1.96	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
2:A:403:MET:H	2:A:403:MET:HG2	1.39	0.46
1:B:336:GLY:HA3	2:A:775:SER:HB2	1.98	0.46
1:B:223:LEU:O	1:B:224:ARG:HD2	2.16	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
2:A:122:PRO:HB2	2:A:125:VAL:CG1	2.45	0.46
2:A:425:HIS:CB	2:A:426:PRO:HD2	2.45	0.46
2:A:421:TRP:CE3	2:A:438:VAL:HB	2.50	0.46
2:A:531:LYS:O	2:A:534:HIS:HB3	2.16	0.46
1:C:138:LEU:HD23	1:C:150:LEU:HD12	1.97	0.46
2:A:240:LEU:HD21	2:A:267:ILE:HD11	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD21	2:A:278:LEU:HD23	1.98	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
2:A:340:GLY:O	2:A:344:GLU:HG3	2.16	0.45
1:C:153:LEU:HD12	1:C:229:ILE:HG21	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
2:A:73:MET:HA	2:A:76:VAL:HG23	1.98	0.45
2:A:888:TYR:HE2	2:A:894:VAL:HG22	1.82	0.45
1:C:94:VAL:HG21	1:C:385:ILE:HD11	1.97	0.45
2:A:964:PHE:HZ	2:A:1043:HIS:HB3	1.81	0.45
2:A:376:ILE:O	2:A:380:VAL:HG23	2.16	0.45
2:A:633:GLN:HE21	2:A:633:GLN:HB2	1.61	0.45
2:A:408:ILE:HD12	2:A:986:MET:HG3	1.98	0.45
1:C:330:GLN:O	1:C:382:LEU:HD12	2.17	0.45
1:C:281:TRP:HB2	1:C:298:LEU:HD23	1.98	0.45
2:A:525:TYR:OH	2:A:1028:LEU:HB3	2.17	0.45
2:A:46:GLN:HG3	2:A:96:ILE:HD13	1.98	0.45
2:A:781:GLN:H	2:A:781:GLN:CD	2.19	0.45
1:B:185:LEU:HA	1:B:185:LEU:HD12	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:995:LEU:HD11	2:A:1016:MET:HE3	1.98	0.45
2:A:6:ILE:HG12	2:A:494:ILE:HG13	1.99	0.45
2:A:588:MET:HE2	2:A:658:LEU:HD22	1.99	0.45
2:A:109:ARG:HD3	2:A:109:ARG:HA	1.85	0.45
2:A:39:LEU:HD23	2:A:390:ILE:HG23	1.99	0.45
2:A:493:ALA:HA	2:A:497:ILE:CB	2.36	0.45
1:B:322:GLU:O	1:B:324:MET:HG3	2.16	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
2:A:940:PHE:CZ	2:A:1024:PRO:HA	2.52	0.45
2:A:22:PHE:HA	2:A:25:ILE:HG22	1.99	0.45
2:A:2:ILE:N	2:A:2:ILE:HD12	2.28	0.45
2:A:909:VAL:O	2:A:913:TRP:HD1	2.00	0.45
1:B:153:LEU:N	1:B:153:LEU:HD23	2.32	0.45
1:B:92:LEU:HD13	2:A:281:GLU:O	2.17	0.45
2:A:592:THR:O	2:A:596:ILE:HG13	2.17	0.44
1:C:223:LEU:HD12	1:C:235:VAL:HB	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:HG22	1:C:254:ILE:O	2.17	0.44
2:A:222:ILE:HG12	2:A:223:GLU:N	2.33	0.44
2:A:402:ALA:HB3	2:A:486:MET:HE1	1.98	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
2:A:930:PHE:CZ	2:A:1015:PRO:HB3	2.52	0.44
2:A:580:ILE:HG22	2:A:622:GLU:CB	2.48	0.44
1:B:390:ASN:HD22	1:B:393:GLY:H	1.64	0.44
1:B:92:LEU:HD11	2:A:281:GLU:HG3	1.99	0.44
1:B:384:LEU:HD23	1:B:394:ALA:CB	2.46	0.44
2:A:97:PHE:CE1	2:A:106:ALA:HB1	2.53	0.44
2:A:212:ALA:C	2:A:215:GLN:HE22	2.21	0.44
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:210:LEU:HD22	2:A:246:ILE:HD12	2.00	0.43
2:A:141:GLU:HB3	2:A:325:TYR:HB3	2.00	0.43
2:A:642:MET:HA	2:A:642:MET:HE3	2.00	0.43
2:A:718:LEU:HD12	2:A:718:LEU:HA	1.91	0.43
1:B:120:GLN:HE22	1:B:243:PRO:CD	2.25	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
1:C:84:ILE:HG21	2:A:656:PRO:HG3	2.00	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:880:LEU:HD23	2:A:880:LEU:HA	1.85	0.43
2:A:882:ILE:C	2:A:882:ILE:HD13	2.39	0.43
2:A:940:PHE:HE2	2:A:944:MET:HG3	1.82	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:CD1	2:A:421:TRP:O	2.72	0.43
2:A:431:ASP:CG	2:A:432:ASN:H	2.22	0.43
1:C:274:LYS:HE2	1:C:274:LYS:HB3	1.75	0.43
2:A:195:ARG:HD3	2:A:261:ASP:O	2.18	0.43
1:C:234:VAL:HG22	1:C:234:VAL:O	2.18	0.43
2:A:1009:MET:O	2:A:1012:ILE:HG22	2.18	0.43
2:A:814:LYS:HE3	2:A:823:TRP:CH2	2.54	0.43
1:B:234:VAL:HG22	1:B:234:VAL:O	2.19	0.43
1:B:378:VAL:HG21	1:B:383:PHE:CE2	2.54	0.43
2:A:345:GLU:OE2	2:A:998:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:O	1:C:168:LEU:HD13	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
1:C:384:LEU:HD21	2:A:588:MET:HE1	2.01	0.42
2:A:996:LEU:N	2:A:997:PRO:CD	2.82	0.42
2:A:16:VAL:HG11	2:A:495:VAL:O	2.18	0.42
2:A:952:ILE:HG22	2:A:952:ILE:O	2.19	0.42
1:C:162:GLN:HG2	1:C:185:LEU:HD21	2.01	0.42
2:A:492:LEU:HA	2:A:492:LEU:HD22	1.86	0.42
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:B:195:ILE:O	1:B:198:LEU:HB3	2.19	0.42
2:A:595:LEU:CB	2:A:653:VAL:HG22	2.49	0.42
1:C:196:ARG:O	1:C:199:ILE:HG12	2.19	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
1:C:281:TRP:HB3	1:C:298:LEU:HD23	2.02	0.42
2:A:342:LEU:HD21	2:A:397:ALA:HA	2.02	0.42
2:A:26:TRP:CE3	2:A:379:ILE:HD13	2.55	0.42
2:A:975:HIS:C	2:A:977:ALA:N	2.73	0.42
2:A:367:ILE:C	2:A:369:SER:H	2.23	0.42
2:A:497:ILE:O	2:A:501:MET:HG2	2.20	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:O	1:C:317:LEU:HD12	2.19	0.42
2:A:139:ILE:HG23	2:A:301:ILE:HD11	2.00	0.42
2:A:596:ILE:HG12	2:A:653:VAL:HG21	2.02	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:1007:GLU:O	2:A:1011:ARG:HD3	2.20	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
1:C:167:LEU:HA	1:C:170:GLU:CG	2.50	0.42
1:C:279:ARG:NH1	1:C:279:ARG:HB2	2.35	0.42
2:A:930:PHE:CE2	2:A:1015:PRO:HB3	2.55	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: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:525:TYR:OH	2:A:980:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:SER:HB3	1:C:401:GLU:OE2	2.19	0.41
2:A:87:GLN:HG2	2:A:812:MET:HG3	2.02	0.41
1:B:114:VAL:HG12	1:B:309:PRO:HA	2.00	0.41
2:A:578:PRO:CG	2:A:717:ARG:HB2	2.51	0.41
2:A:842:LYS:O	2:A:846:GLU:HG2	2.20	0.41
1:B:195:ILE:O	1:B:199:ILE:HG23	2.19	0.41
2:A:21:LEU:HD13	2:A:21:LEU:C	2.41	0.41
1:C:384:LEU:HD11	2:A:588:MET:HE3	2.03	0.41
1:C:127:ARG:O	1:C:231:LYS:HD3	2.20	0.41
2:A:239:THR:HG22	2:A:241:ASP:N	2.29	0.41
2:A:292:ARG:O	2:A:293:SER:C	2.58	0.41
2:A:2:ILE:CD1	2:A:2:ILE:H	2.29	0.41
2:A:574:PRO:CG	2:A:624:VAL:HG13	2.42	0.41
2:A:624:VAL:O	2:A:624:VAL:HG22	2.19	0.41
1:B:322:GLU:OE1	1:B:322:GLU:HA	2.20	0.41
1:C:151:LEU:C	1:C:151:LEU:HD12	2.41	0.41
2:A:157:ARG:HG2	2:A:182:GLY:HA3	2.01	0.41
1:B:174:THR:HB	1:B:177:GLN:HG3	2.03	0.41
1:C:165:TYR:CE2	1:C:178:THR:HG23	2.55	0.41
2:A:1032:PRO:C	2:A:1034:ALA:H	2.24	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: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:458:THR:HG22	2:A:486:MET:HB2	2.03	0.41
2:A:2:ILE:O	2:A:6:ILE:HG13	2.21	0.41
1:C:114:VAL:HG12	1:C:309:PRO:HA	2.03	0.41
2:A:210:LEU:HD22	2:A:246:ILE:CD1	2.51	0.41
2:A:67:TYR:O	2:A:71:THR:HG23	2.21	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
2:A:462:ILE:N	2:A:463:PRO:CD	2.84	0.40
2:A:275:ILE:CD1	2:A:586:ALA:HB2	2.45	0.40
2:A:86:SER:HB2	2:A:813:LEU:HB2	2.03	0.40
2:A:969:LEU:O	2:A:973:LEU:HD13	2.21	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: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:HE3	2:A:150:LYS:HB2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:408:ILE:HD12	2:A:986:MET:HE2	2.03	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:240:LEU:HA	2:A:240:LEU:HD23	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
1:B:360:ALA:HB2	1:B:365:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	320/413 (78%)	297 (93%)	20 (6%)	3 (1%)	20	60
1	C	322/413 (78%)	309 (96%)	12 (4%)	1 (0%)	44	79
2	A	1027/1054 (97%)	942 (92%)	77 (8%)	8 (1%)	22	62
All	All	1669/1880 (89%)	1548 (93%)	109 (6%)	12 (1%)	25	64

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 ⓘ

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%)	227 (86%)	36 (14%)	4	19
1	C	265/338 (78%)	234 (88%)	31 (12%)	6	26
2	A	849/871 (98%)	747 (88%)	102 (12%)	6	24
All	All	1377/1547 (89%)	1208 (88%)	169 (12%)	5	23

All (169) 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	121	TYR
1	B	135	VAL
1	B	159	VAL
1	B	169	ARG
1	B	185	LEU
1	B	199	ILE
1	B	234	VAL
1	B	235	VAL
1	B	239	GLN
1	B	241	MET
1	B	267	THR
1	B	268	VAL
1	B	275	THR
1	B	276	LEU

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Mol	Chain	Res	Type
1	B	280	LYS
1	B	282	THR
1	B	298	LEU
1	B	322	GLU
1	B	330	GLN
1	B	340	ARG
1	B	349	ARG
1	B	351	VAL
1	B	357	VAL
1	B	364	VAL
1	B	367	LEU
1	B	378	VAL
1	B	379	SER
1	B	384	LEU
1	B	388	GLU
1	B	392	SER
1	B	396	GLU
1	B	399	ARG
1	C	98	THR
1	C	104	LEU
1	C	105	THR
1	C	121	TYR
1	C	138	LEU
1	C	140	VAL
1	C	150	LEU
1	C	178	THR
1	C	181	ILE
1	C	182	LEU
1	C	185	LEU
1	C	234	VAL
1	C	235	VAL
1	C	258	VAL
1	C	279	ARG
1	C	283	LEU
1	C	292	ARG
1	C	304	ASP
1	C	317	LEU
1	C	330	GLN
1	C	339	GLN
1	C	343	THR
1	C	347	ASP
1	C	351	VAL

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Mol	Chain	Res	Type
1	C	353	LYS
1	C	354	ARG
1	C	364	VAL
1	C	365	THR
1	C	375	GLU
1	C	377	VAL
1	C	382	LEU
2	A	1	MET
2	A	13	ARG
2	A	15	LEU
2	A	23	LEU
2	A	36	VAL
2	A	42	LEU
2	A	53	TYR
2	A	59	GLN
2	A	105	TRP
2	A	109	ARG
2	A	114	LEU
2	A	117	VAL
2	A	126	SER
2	A	144	LEU
2	A	145	VAL
2	A	157	ARG
2	A	168	LEU
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	241	ASP
2	A	259	LEU
2	A	260	ARG
2	A	288	VAL
2	A	293	SER
2	A	298	ARG
2	A	323	THR
2	A	335	ILE
2	A	342	LEU
2	A	351	VAL
2	A	358	TRP

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Mol	Chain	Res	Type
2	A	390	ILE
2	A	400	VAL
2	A	403	MET
2	A	412	GLU
2	A	415	HIS
2	A	417	ARG
2	A	436	TRP
2	A	455	LEU
2	A	457	ILE
2	A	464	ILE
2	A	492	LEU
2	A	521	LEU
2	A	524	VAL
2	A	532	VAL
2	A	534	HIS
2	A	545	LEU
2	A	554	LEU
2	A	557	VAL
2	A	570	LEU
2	A	573	MET
2	A	592	THR
2	A	602	VAL
2	A	624	VAL
2	A	634	GLU
2	A	637	ARG
2	A	641	THR
2	A	642	MET
2	A	649	LEU
2	A	661	LEU
2	A	667	ARG
2	A	669	ARG
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

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Mol	Chain	Res	Type
2	A	808	THR
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	904	VAL
2	A	940	PHE
2	A	945	LEU
2	A	959	ASN
2	A	966	GLU
2	A	969	LEU
2	A	975	HIS
2	A	984	LYS
2	A	987	THR
2	A	1020	MET
2	A	1035	TYR
2	A	1037	LEU
2	A	1038	MET
2	A	1039	TRP

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

Mol	Chain	Res	Type
1	B	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	233	ASN
1	C	302	ASN

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Mol	Chain	Res	Type
2	A	87	GLN
2	A	116	GLN
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	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	729	ASN
2	A	744	GLN
2	A	769	ASN
2	A	795	GLN
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 carbohydrates 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%)	-0.03	3 (0%)	84 69	26, 53, 97, 153	0
1	C	324/413 (78%)	0.01	1 (0%)	93 86	31, 54, 100, 142	0
2	A	1031/1054 (97%)	0.38	91 (8%)	11 4	26, 77, 184, 278	0
All	All	1677/1880 (89%)	0.23	95 (5%)	24 11	26, 65, 166, 278	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	427	ASP	6.0
2	A	429	THR	5.7
2	A	948	LEU	5.2
2	A	1001	GLY	5.1
2	A	890	ALA	5.0
2	A	1035	TYR	4.7
2	A	954	ALA	4.6
2	A	428	ALA	4.5
2	A	980	ARG	4.5
2	A	494	ILE	4.5
2	A	449	ALA	4.5
2	A	444	VAL	4.4
2	A	448	PRO	4.4
2	A	1036	LYS	4.3
2	A	971	GLU	4.3
2	A	7	ARG	4.2
2	A	891	PHE	4.2
2	A	889	LEU	4.1
2	A	946	MET	4.1
2	A	418	LEU	4.1
2	A	410	MET	4.1
2	A	960	ASN	4.0
2	A	981	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
2	A	436	TRP	3.8
2	A	357	LEU	3.8
2	A	446	VAL	3.8
2	A	421	TRP	3.7
2	A	975	HIS	3.7
2	A	426	PRO	3.7
2	A	950	HIS	3.6
2	A	1038	MET	3.5
2	A	953	GLU	3.5
2	A	445	GLU	3.4
2	A	520	PHE	3.4
2	A	943	VAL	3.4
2	A	1039	TRP	3.3
2	A	433	LYS	3.3
2	A	970	ASP	3.3
2	A	896	GLU	3.3
1	B	79	ALA	3.2
2	A	519	ARG	3.2
2	A	979	LEU	3.2
2	A	406	ALA	3.2
2	A	530	LEU	3.2
2	A	972	ALA	3.2
2	A	437	GLN	3.1
2	A	939	GLU	3.1
2	A	887	LEU	3.1
2	A	955	VAL	3.1
2	A	450	LEU	3.1
2	A	964	PHE	3.0
2	A	947	TYR	3.0
2	A	4	TRP	2.9
2	A	956	PRO	2.9
2	A	983	PRO	2.9
2	A	958	LEU	2.9
2	A	353	CYS	2.8
2	A	424	GLN	2.8
2	A	526	HIS	2.8
2	A	495	VAL	2.7
1	C	402	SER	2.7
2	A	417	ARG	2.6
2	A	523	ARG	2.6
2	A	447	GLY	2.6
2	A	893	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	951	ALA	2.6
2	A	425	HIS	2.5
2	A	528	LEU	2.5
1	B	80	SER	2.5
2	A	390	ILE	2.4
2	A	405	ALA	2.4
2	A	1031	ILE	2.4
2	A	497	ILE	2.4
2	A	441	ASP	2.3
2	A	500	LEU	2.3
2	A	15	LEU	2.3
2	A	440	THR	2.3
2	A	952	ILE	2.3
2	A	969	LEU	2.3
2	A	945	LEU	2.3
2	A	1037	LEU	2.2
1	B	386	ASP	2.2
2	A	420	GLU	2.2
2	A	404	VAL	2.2
2	A	409	VAL	2.2
2	A	414	ALA	2.2
2	A	944	MET	2.2
2	A	982	ARG	2.2
2	A	974	TYR	2.1
2	A	886	LEU	2.1
2	A	957	SER	2.1
2	A	1032	PRO	2.1
2	A	356	PHE	2.0
2	A	962	GLN	2.0
2	A	367	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.