



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:56 pm BST

PDB ID : 5YIL  
Title : Hoisting-loop in bacterial multidrug exporter AcrB is a highly flexible hinge that enables the large motion of the subdomains  
Authors : Zwama, M.; Sakurai, K.; Hayashi, K.; Nakashima, R.; Kitagawa, K.; Nishino, K.; Yamaguchi, A.  
Deposited on : 2017-10-05  
Resolution : 3.00 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

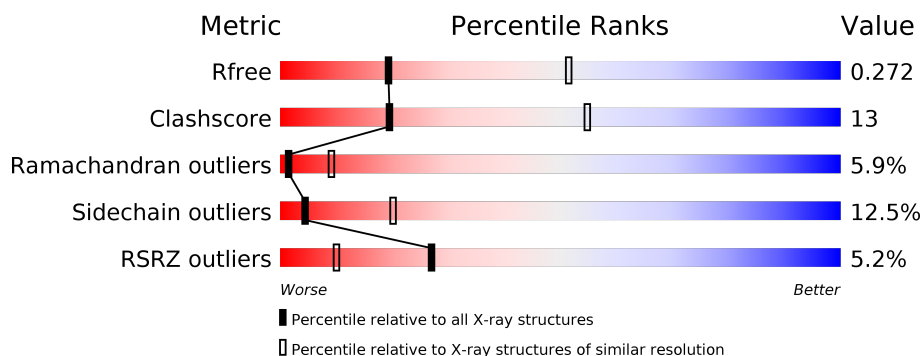
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	A	1050	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div> </div>
1	B	1050	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>••</div> </div> </div>
1	C	1050	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>33%</div> <div>6%</div> <div>••</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23566 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1041	Total	C	N	O	S	0	0	0
			7918	5091	1310	1473	44			
1	B	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			
1	C	1030	Total	C	N	O	S	0	0	0
			7824	5037	1290	1453	44			

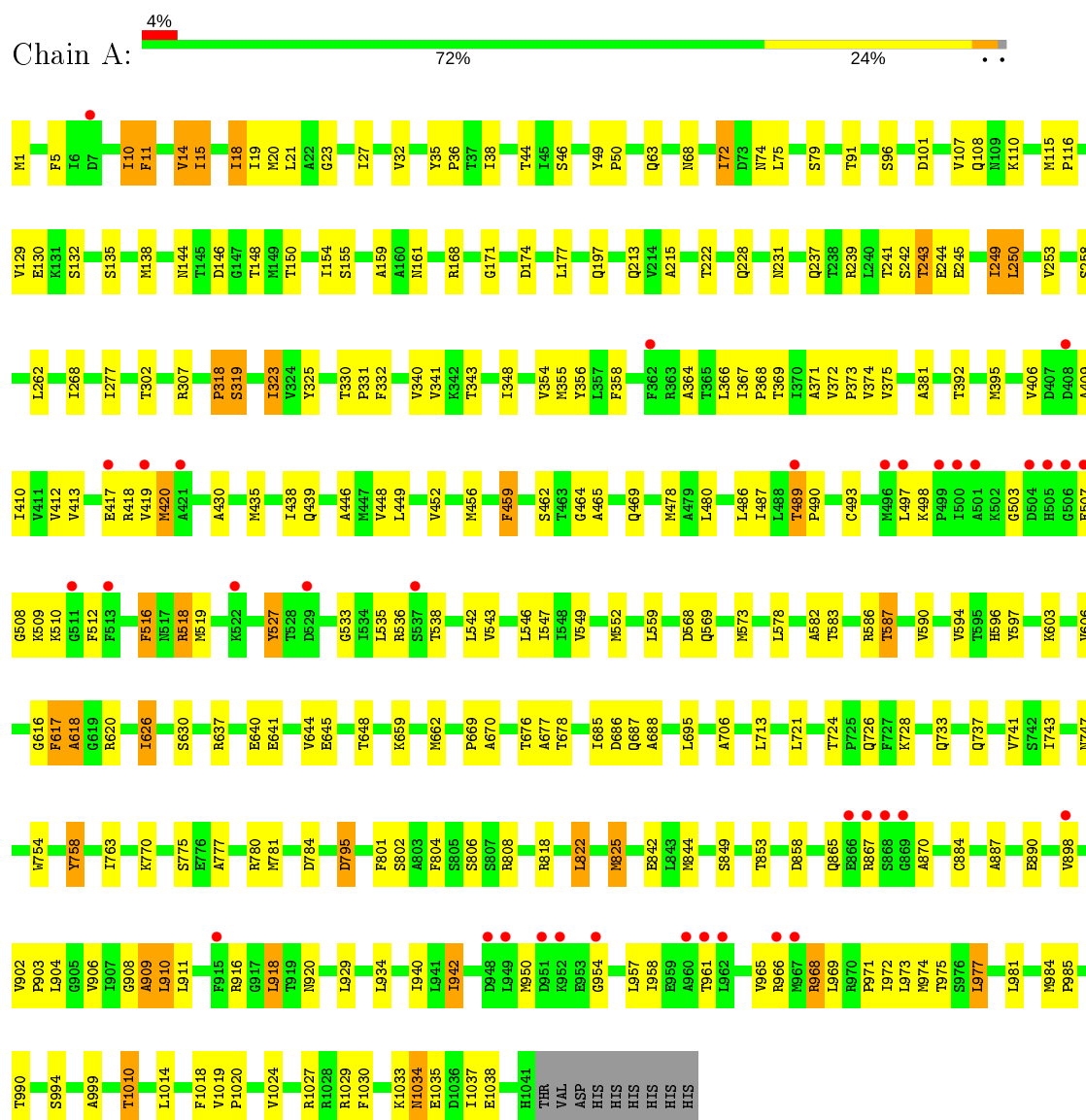
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P31224
A	1048	HIS	-	expression tag	UNP P31224
A	1049	HIS	-	expression tag	UNP P31224
A	1050	HIS	-	expression tag	UNP P31224
B	1047	HIS	-	expression tag	UNP P31224
B	1048	HIS	-	expression tag	UNP P31224
B	1049	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
C	1047	HIS	-	expression tag	UNP P31224
C	1048	HIS	-	expression tag	UNP P31224
C	1049	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224

### 3 Residue-property plots

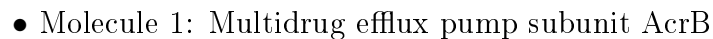
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB





I166	D73	M1
D174	L75	F5
L177	M76	I6
I181	M78	D7
Y182	S79	R6
R185	S80	P9
M194	N81	I10
K195	S82	F11
F196	D83	A12
Q197	S84	I13
D202		A16
I207	T91	I17
K208	L92	I18
A209	T93	I19
V214	F94	X20
L219	E95	L21
Q228	I102	A22
I234	A103	G23
I235	Q104	A26
A236	V105	I27
Q237	Q106	L28
T238		K29
R239	N109	P31
L240	K110	V32
S242	L111	A33
K252	E121	Q34
P253	V122	I35
N254	Q123	P36
G271	Q124	T37
I277	G126	I38
Q284	V127	A39
P285	I128	P40
I291	V129	A42
K292	K131	P41
G296	S134	V43
A297	I143	Y49
N298	T144	P50
A299	T145	G51
L300	D146	A52
D301	G147	D53
	T148	A54
	M149	X55
		T56
		V57
		Q58
		D59
		T60
		V61
		T62
		I65
		P69
		T72



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.98Å 139.81Å 285.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.00 98.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (100.00-3.00) 94.5 (98.45-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.224 , 0.273 0.226 , 0.272	Depositor DCC
$R_{free}$ test set	5112 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 74.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.69	0/8070	0.86	0/10957
1	B	0.64	0/7974	0.83	0/10829
1	C	0.69	0/7974	0.89	2/10829 (0.0%)
All	All	0.67	0/24018	0.86	2/32615 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	SER	CB-CA-C	-6.51	97.73	110.10
1	C	131	LYS	N-CA-C	-5.49	96.18	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	A	7918	0	8059	127	0
1	B	7824	0	7976	221	0
1	C	7824	0	7976	283	0
All	All	23566	0	24011	608	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 13.

All (608) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HD23	1:B:402:ILE:CD1	1.46	1.45
1:B:449:LEU:HB3	1:B:478:MET:CE	1.52	1.37
1:B:344:LEU:CD2	1:B:402:ILE:CD1	2.18	1.20
1:B:344:LEU:CD2	1:B:402:ILE:HD11	1.79	1.12
1:B:449:LEU:HB3	1:B:478:MET:HE2	1.23	1.10
1:B:449:LEU:CB	1:B:478:MET:HE1	1.82	1.09
1:C:568:ASP:OD1	1:C:644:VAL:HG23	1.52	1.07
1:B:449:LEU:CB	1:B:478:MET:CE	2.33	1.04
1:B:404:LEU:H	1:B:404:LEU:HD12	1.22	1.02
1:B:344:LEU:HD23	1:B:402:ILE:HD13	0.98	0.97
1:B:449:LEU:HB3	1:B:478:MET:HE1	1.37	0.96
1:B:445:ILE:HG23	1:B:449:LEU:HG	1.47	0.94
1:B:731:ILE:HD13	1:B:731:ILE:H	1.30	0.93
1:B:180:SER:O	1:B:181:GLN:O	1.87	0.92
1:B:344:LEU:HD21	1:B:402:ILE:HD11	1.51	0.92
1:C:130:GLU:OE1	1:C:174:ASP:OD2	1.89	0.90
1:C:446:ALA:HB2	1:C:482:VAL:HG11	1.52	0.88
1:C:940:ILE:O	1:C:944:GLU:HB2	1.76	0.86
1:C:885:LEU:HD12	1:C:886:ALA:N	1.89	0.86
1:B:344:LEU:CD2	1:B:402:ILE:HD13	1.93	0.82
1:B:375:VAL:O	1:B:379:THR:HG23	1.80	0.80
1:B:445:ILE:O	1:B:449:LEU:HB2	1.80	0.80
1:A:410:ILE:HD11	1:A:975:THR:HG23	1.61	0.80
1:A:38:ILE:HD13	1:A:465:ALA:HB3	1.62	0.80
1:B:445:ILE:CG2	1:B:449:LEU:HG	2.13	0.78
1:B:449:LEU:CD1	1:B:478:MET:CE	2.63	0.77
1:B:449:LEU:HB2	1:B:478:MET:HE1	1.66	0.76
1:C:881:VAL:HA	1:C:884:CYS:SG	2.27	0.75
1:C:951:ASP:HB3	1:C:952:LYS:HZ2	1.52	0.75
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.22	0.75
1:C:872:SER:O	1:C:876:ILE:HG12	1.87	0.75
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.69	0.74
1:B:449:LEU:CB	1:B:478:MET:HE2	2.11	0.74
1:B:445:ILE:O	1:B:449:LEU:N	2.19	0.73
1:C:422:GLU:OE2	1:C:423:GLU:N	2.21	0.73
1:C:30:LEU:HD22	1:C:390:ILE:HG13	1.71	0.73
1:C:641:GLU:O	1:C:650:ARG:NH2	2.22	0.73
1:C:952:LYS:HA	1:C:952:LYS:HE3	1.69	0.73
1:C:104:GLN:NE2	1:C:129:VAL:O	2.22	0.72
1:C:952:LYS:O	1:C:954:GLY:N	2.23	0.72
1:B:454:VAL:O	1:B:456:MET:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:ILE:O	1:C:944:GLU:CB	2.37	0.71
1:B:174:ASP:C	1:B:175:VAL:HG13	2.11	0.71
1:B:401:ALA:HA	1:B:404:LEU:CD1	2.21	0.71
1:B:454:VAL:HB	1:B:455:PRO:HD3	1.71	0.71
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.26	0.71
1:B:404:LEU:N	1:B:404:LEU:HD12	2.03	0.70
1:B:889:TYR:O	1:B:891:SER:N	2.24	0.70
1:B:641:GLU:O	1:B:650:ARG:NH1	2.25	0.70
1:C:36:PRO:O	1:C:38:ILE:N	2.25	0.69
1:C:425:LEU:HB2	1:C:426:PRO:HD2	1.74	0.69
1:C:61:VAL:O	1:C:62:THR:OG1	2.08	0.69
1:C:885:LEU:HD11	1:C:895:PRO:HG3	1.73	0.69
1:B:180:SER:O	1:B:181:GLN:C	2.30	0.69
1:B:449:LEU:HD13	1:B:478:MET:HE2	1.74	0.69
1:B:449:LEU:HD13	1:B:478:MET:CE	2.23	0.68
1:C:427:PRO:O	1:C:430:ALA:N	2.27	0.67
1:A:348:ILE:HD11	1:A:372:VAL:HG11	1.75	0.67
1:A:44:THR:HG22	1:A:91:THR:HG23	1.76	0.67
1:C:36:PRO:O	1:C:38:ILE:HG23	1.93	0.67
1:C:298:ASN:O	1:C:301:ASP:N	2.28	0.67
1:C:901:VAL:HG21	1:C:939:ALA:HB2	1.76	0.67
1:A:249:ILE:O	1:A:250:LEU:HB3	1.95	0.67
1:B:174:ASP:C	1:B:175:VAL:CG1	2.64	0.66
1:A:695:LEU:HD23	1:A:825:MET:SD	2.36	0.66
1:B:174:ASP:O	1:B:175:VAL:CG1	2.43	0.66
1:B:234:ILE:HD11	1:C:729:ILE:HG21	1.78	0.66
1:C:976:SER:HB3	1:C:1012:THR:HG21	1.77	0.66
1:C:692:HIS:O	1:C:694:LYS:N	2.29	0.65
1:C:882:PHE:CE2	1:C:883:LEU:HD21	2.32	0.65
1:A:412:VAL:HG12	1:A:438:ILE:HD12	1.77	0.65
1:B:444:GLY:O	1:B:448:VAL:N	2.25	0.65
1:B:898:VAL:HG11	1:B:940:ILE:HG13	1.79	0.65
1:B:990:THR:HG23	1:B:998:ASN:HD21	1.62	0.65
1:C:940:ILE:O	1:C:944:GLU:N	2.30	0.65
1:B:379:THR:OG1	1:B:398:MET:HE3	1.97	0.64
1:B:372:VAL:HG12	1:B:373:PRO:HD3	1.80	0.64
1:C:376:LEU:HD22	1:C:398:MET:HG2	1.80	0.64
1:B:174:ASP:O	1:B:175:VAL:HG12	1.98	0.64
1:B:478:MET:O	1:B:481:SER:N	2.30	0.64
1:B:379:THR:HG21	1:B:477:ALA:HA	1.78	0.63
1:C:134:SER:O	1:C:292:LYS:HE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:HB2	1:C:729:ILE:HG23	1.81	0.63
1:B:401:ALA:C	1:B:403:GLY:H	2.02	0.63
1:C:129:VAL:O	1:C:129:VAL:HG12	1.97	0.63
1:C:36:PRO:HG2	1:C:469:GLN:NE2	2.14	0.63
1:B:478:MET:SD	1:B:479:ALA:N	2.72	0.62
1:C:415:ASN:OD1	1:C:968:ARG:NH2	2.32	0.62
1:C:54:ALA:CB	1:C:816:LEU:HD12	2.29	0.62
1:C:425:LEU:HB2	1:C:426:PRO:CD	2.29	0.62
1:A:228:GLN:O	1:B:583:THR:HG21	1.99	0.61
1:C:843:LEU:HD23	1:C:847:LEU:HD13	1.82	0.61
1:A:72:ILE:HD12	1:A:72:ILE:N	2.15	0.61
1:B:38:ILE:HG22	1:B:462:SER:OG	2.01	0.61
1:C:877:SER:O	1:C:881:VAL:HG22	2.00	0.61
1:B:444:GLY:O	1:B:448:VAL:HB	1.99	0.61
1:B:583:THR:HG22	1:B:586:ARG:HG3	1.81	0.61
1:C:885:LEU:HD11	1:C:895:PRO:CB	2.29	0.61
1:C:613:ASN:HD22	1:C:614:GLY:N	1.99	0.61
1:B:548:ILE:HD12	1:B:904:LEU:HD22	1.82	0.60
1:B:443:VAL:HG12	1:B:443:VAL:O	2.01	0.60
1:B:449:LEU:CD1	1:B:478:MET:SD	2.90	0.60
1:B:643:LYS:O	1:B:645:GLU:N	2.34	0.60
1:C:655:PHE:O	1:C:658:ILE:HG13	2.02	0.60
1:C:969:LEU:HA	1:C:972:ILE:HG22	1.83	0.60
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.84	0.60
1:A:277:ILE:HD11	1:A:620:ARG:HD2	1.84	0.60
1:C:143:ILE:HD12	1:C:284:GLN:HE22	1.67	0.60
1:B:77:TYR:HA	1:B:820:ASN:HD21	1.66	0.60
1:C:423:GLU:O	1:C:425:LEU:HD12	2.02	0.60
1:C:425:LEU:HD22	1:C:426:PRO:HD2	1.82	0.60
1:B:158:VAL:CG1	1:B:289:LEU:HD13	2.32	0.59
1:C:885:LEU:HD11	1:C:895:PRO:CG	2.31	0.59
1:B:139:VAL:HG13	1:B:178:PHE:HE2	1.67	0.59
1:B:599:LEU:O	1:B:599:LEU:HD12	2.03	0.59
1:C:431:THR:O	1:C:433:LYS:N	2.35	0.59
1:C:722:GLU:O	1:C:723:ASP:O	2.19	0.59
1:B:350:LEU:HD23	1:B:981:LEU:HB3	1.85	0.59
1:C:957:LEU:HD23	1:C:958:ILE:HG13	1.83	0.59
1:C:54:ALA:HB3	1:C:816:LEU:HD12	1.85	0.59
1:C:35:TYR:CE2	1:C:671:ILE:HG22	2.37	0.59
1:C:641:GLU:O	1:C:646:ALA:HB3	2.02	0.59
1:C:613:ASN:C	1:C:613:ASN:HD22	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HA	1:B:377:LEU:HD21	1.86	0.58
1:C:724:THR:HG22	1:C:814:PRO:HD3	1.86	0.58
1:C:901:VAL:HG22	1:C:1019:VAL:HG22	1.85	0.58
1:B:452:VAL:HG13	1:B:453:PHE:N	2.19	0.58
1:B:963:ASP:HA	1:B:966:ARG:HB3	1.86	0.58
1:B:380:PHE:CE1	1:B:398:MET:HE2	2.39	0.57
1:B:403:GLY:O	1:B:406:VAL:N	2.37	0.57
1:B:379:THR:CG2	1:B:477:ALA:HA	2.34	0.57
1:C:149:MET:CE	1:C:321:LEU:HD13	2.33	0.57
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.85	0.57
1:C:121:GLU:O	1:C:125:GLN:NE2	2.38	0.57
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.37	0.57
1:B:402:ILE:O	1:B:402:ILE:HG22	2.05	0.57
1:B:403:GLY:O	1:B:406:VAL:HG12	2.04	0.57
1:B:449:LEU:HD13	1:B:478:MET:SD	2.45	0.56
1:C:425:LEU:HD13	1:C:426:PRO:O	2.05	0.56
1:C:641:GLU:HG2	1:C:642:ASN:N	2.20	0.56
1:B:730:ASP:N	1:B:730:ASP:OD1	2.38	0.56
1:C:542:LEU:HD21	1:C:1025:VAL:HG11	1.86	0.56
1:C:111:LEU:HD21	1:C:127:VAL:HG21	1.86	0.56
1:C:875:ALA:O	1:C:878:LEU:N	2.35	0.56
1:C:390:ILE:O	1:C:390:ILE:HG22	2.06	0.56
1:B:399:VAL:HA	1:B:402:ILE:HG13	1.86	0.56
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.86	0.56
1:C:641:GLU:O	1:C:646:ALA:CB	2.54	0.56
1:C:876:ILE:O	1:C:880:VAL:HG12	2.05	0.56
1:C:699:ARG:CG	1:C:827:ILE:HD11	2.36	0.56
1:B:354:VAL:HG12	1:B:974:MET:HB2	1.87	0.56
1:C:38:ILE:HD12	1:C:38:ILE:C	2.26	0.56
1:C:885:LEU:C	1:C:885:LEU:HD12	2.26	0.56
1:B:383:LEU:HD11	1:B:473:THR:HG22	1.87	0.56
1:C:76:MET:CG	1:C:95:GLU:HG3	2.36	0.56
1:A:527:TYR:CD2	1:A:969:LEU:HD22	2.41	0.56
1:C:61:VAL:HG11	1:C:122:VAL:HG21	1.88	0.56
1:A:1010:THR:HG23	1:A:1014:LEU:HD13	1.86	0.55
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.88	0.55
1:A:583:THR:HG22	1:A:586:ARG:HG3	1.87	0.55
1:C:880:VAL:O	1:C:884:CYS:HB3	2.06	0.55
1:B:5:PHE:CD2	1:B:487:ILE:HG23	2.40	0.55
1:C:424:GLY:O	1:C:425:LEU:HB3	2.06	0.55
1:B:403:GLY:O	1:B:404:LEU:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:988:ILE:O	1:B:990:THR:N	2.38	0.55
1:B:447:MET:HB3	1:B:884:CYS:SG	2.47	0.55
1:C:76:MET:HG2	1:C:95:GLU:HG3	1.89	0.55
1:B:178:PHE:CZ	1:B:290:GLY:N	2.75	0.55
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.88	0.55
1:B:702:LEU:HD13	1:B:851:LEU:HD11	1.89	0.55
1:B:177:LEU:O	1:B:179:GLY:N	2.38	0.55
1:C:424:GLY:C	1:C:425:LEU:HD12	2.27	0.55
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.38	0.54
1:C:9:PRO:HB2	1:C:10:ILE:HD12	1.88	0.54
1:A:159:ALA:HB2	1:A:177:LEU:HD21	1.88	0.54
1:B:818:ARG:NH1	1:B:821:GLY:O	2.38	0.54
1:C:686:ASP:HB2	1:C:823:PRO:O	2.07	0.54
1:A:904:LEU:O	1:A:1010:THR:O	2.25	0.54
1:C:38:ILE:HD13	1:C:462:SER:HB3	1.88	0.54
1:C:104:GLN:CG	1:C:129:VAL:HG12	2.36	0.54
1:C:412:VAL:HG22	1:C:442:LEU:HD11	1.88	0.54
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.90	0.54
1:B:987:VAL:HG21	1:B:1005:MET:CG	2.37	0.54
1:C:752:ALA:O	1:C:774:MET:HA	2.08	0.54
1:B:454:VAL:HB	1:B:455:PRO:CD	2.38	0.54
1:B:444:GLY:O	1:B:448:VAL:CB	2.55	0.54
1:C:146:ASP:OD1	1:C:148:THR:HG23	2.08	0.54
1:C:425:LEU:CD2	1:C:426:PRO:HD2	2.37	0.54
1:B:150:THR:OG1	1:B:151:GLN:N	2.40	0.54
1:B:449:LEU:HD12	1:B:478:MET:SD	2.48	0.54
1:A:733:GLN:HE22	1:A:743:ILE:HD13	1.73	0.54
1:C:127:VAL:O	1:C:127:VAL:HG23	2.08	0.54
1:C:38:ILE:O	1:C:38:ILE:HD12	2.08	0.54
1:C:427:PRO:O	1:C:428:LYS:C	2.45	0.54
1:C:38:ILE:CD1	1:C:462:SER:HB3	2.38	0.54
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.38	0.53
1:B:398:MET:O	1:B:402:ILE:HG13	2.08	0.53
1:C:878:LEU:HA	1:C:881:VAL:HG23	1.90	0.53
1:B:449:LEU:CD1	1:B:478:MET:HE2	2.33	0.53
1:B:980:ILE:O	1:B:984:MET:HG2	2.08	0.53
1:C:30:LEU:HD21	1:C:388:PHE:O	2.07	0.53
1:C:348:ILE:HG22	1:C:402:ILE:HG21	1.90	0.53
1:C:376:LEU:HD22	1:C:398:MET:CG	2.38	0.53
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.90	0.53
1:B:731:ILE:CD1	1:B:731:ILE:H	2.02	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:PHE:O	1:C:1027:ARG:HB2	2.09	0.53
1:C:124:GLN:O	1:C:125:GLN:C	2.48	0.52
1:C:57:VAL:HG13	1:C:61:VAL:HG23	1.91	0.52
1:C:692:HIS:O	1:C:693:GLU:C	2.47	0.52
1:A:20:MET:SD	1:A:374:VAL:HG12	2.50	0.52
1:A:63:GLN:HE22	1:C:767:ARG:HA	1.75	0.52
1:C:57:VAL:O	1:C:61:VAL:O	2.27	0.52
1:A:5:PHE:CD2	1:A:487:ILE:HG22	2.45	0.52
1:B:520:PHE:O	1:B:524:THR:HG22	2.10	0.52
1:C:885:LEU:CD1	1:C:895:PRO:HB3	2.40	0.52
1:A:961:THR:HG21	1:A:1024:VAL:HG13	1.91	0.52
1:B:210:GLN:HB2	1:B:249:ILE:HD12	1.92	0.52
1:C:699:ARG:CD	1:C:827:ILE:HD11	2.40	0.52
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.91	0.52
1:C:858:ASP:O	1:C:860:THR:N	2.43	0.52
1:C:877:SER:C	1:C:880:VAL:HG12	2.30	0.52
1:A:583:THR:HG22	1:A:586:ARG:CG	2.39	0.51
1:B:441:ALA:C	1:B:443:VAL:H	2.14	0.51
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.91	0.51
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.92	0.51
1:C:298:ASN:ND2	1:C:301:ASP:HB2	2.25	0.51
1:B:986:LEU:HD22	1:B:997:GLN:HE21	1.75	0.51
1:B:379:THR:OG1	1:B:398:MET:CE	2.57	0.51
1:C:946:ALA:HB1	1:C:1023:PHE:CE2	2.44	0.51
1:C:425:LEU:HD22	1:C:426:PRO:CD	2.41	0.51
1:C:470:PHE:O	1:C:471:SER:C	2.49	0.51
1:A:243:THR:HG22	1:A:268:ILE:HG22	1.91	0.51
1:A:590:VAL:O	1:A:594:VAL:HG23	2.11	0.51
1:A:743:ILE:HD12	1:C:209:ALA:HB1	1.92	0.51
1:C:641:GLU:HG2	1:C:642:ASN:H	1.75	0.51
1:C:644:VAL:O	1:C:648:THR:HG23	2.10	0.51
1:C:40:PRO:CD	1:C:674:LEU:HD11	2.41	0.51
1:A:583:THR:HG22	1:A:586:ARG:HD3	1.93	0.51
1:C:453:PHE:CD2	1:C:474:ILE:HG21	2.45	0.51
1:C:42:ALA:HB2	1:C:93:THR:HG23	1.93	0.51
1:A:942:ILE:HD11	1:A:965:VAL:HG22	1.92	0.50
1:A:687:GLN:O	1:A:688:ALA:HB2	2.12	0.50
1:A:72:ILE:HD13	1:A:75:LEU:HD22	1.93	0.50
1:B:371:ALA:HB1	1:B:488:LEU:HD23	1.93	0.50
1:B:762:PHE:CZ	1:B:764:ASP:HB2	2.47	0.50
1:C:480:LEU:O	1:C:484:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:VAL:HG23	1:B:903:PRO:HD3	1.93	0.50
1:B:180:SER:C	1:B:181:GLN:O	2.49	0.50
1:B:246:PHE:O	1:B:249:ILE:HG12	2.10	0.50
1:B:649:MET:O	1:B:652:THR:HG22	2.10	0.50
1:B:211:ASN:ND2	1:B:761:ASP:O	2.43	0.50
1:B:375:VAL:HG22	1:B:484:VAL:HG11	1.94	0.50
1:B:696:THR:O	1:B:699:ARG:HB3	2.10	0.50
1:A:413:VAL:HG12	1:A:493:CYS:SG	2.51	0.50
1:B:83:ASP:OD1	1:B:83:ASP:C	2.50	0.50
1:C:352:PHE:CG	1:C:352:PHE:O	2.65	0.50
1:C:422:GLU:O	1:C:424:GLY:N	2.44	0.50
1:A:573:MET:CE	1:A:626:ILE:HD11	2.41	0.50
1:B:406:VAL:HG22	1:B:410:ILE:HD12	1.93	0.49
1:A:818:ARG:NH1	1:A:822:LEU:HA	2.27	0.49
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.94	0.49
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.41	0.49
1:C:874:TYR:O	1:C:878:LEU:N	2.46	0.49
1:B:441:ALA:O	1:B:443:VAL:N	2.44	0.49
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.47	0.49
1:A:908:GLY:O	1:A:909:ALA:HB2	2.12	0.49
1:C:937:LYS:HD3	1:C:938:ASN:HD22	1.77	0.49
1:B:120:GLN:O	1:B:123:GLN:HB3	2.11	0.49
1:B:401:ALA:O	1:B:405:LEU:HB2	2.12	0.49
1:C:519:MET:O	1:C:523:SER:OG	2.27	0.49
1:C:885:LEU:CD1	1:C:895:PRO:CB	2.91	0.49
1:C:411:VAL:HG21	1:C:941:LEU:HD23	1.95	0.49
1:A:241:THR:HG22	1:A:245:GLU:OE1	2.13	0.49
1:A:518:ARG:HE	1:A:518:ARG:HA	1.78	0.49
1:B:454:VAL:CB	1:B:455:PRO:HD3	2.38	0.49
1:B:898:VAL:HG13	1:B:939:ALA:HB3	1.93	0.49
1:C:425:LEU:HD22	1:C:426:PRO:O	2.12	0.49
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.43	0.49
1:C:688:ALA:O	1:C:689:GLY:C	2.51	0.49
1:C:882:PHE:O	1:C:885:LEU:HG	2.13	0.49
1:A:237:GLN:HG3	1:B:731:ILE:HD11	1.95	0.49
1:C:885:LEU:HD13	1:C:895:PRO:HB3	1.95	0.48
1:B:158:VAL:HG11	1:B:289:LEU:HD13	1.96	0.48
1:B:375:VAL:HG21	1:B:481:SER:HA	1.95	0.48
1:B:448:VAL:O	1:B:452:VAL:HG12	2.12	0.48
1:B:874:TYR:CE2	1:B:878:LEU:HD13	2.48	0.48
1:C:20:MET:SD	1:C:373:PRO:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:943:VAL:HA	1:C:946:ALA:HB3	1.93	0.48
1:B:20:MET:HA	1:B:377:LEU:CD2	2.43	0.48
1:C:23:GLY:CA	1:C:381:ALA:HB2	2.42	0.48
1:C:578:LEU:HD13	1:C:587:THR:HB	1.94	0.48
1:A:354:VAL:O	1:A:354:VAL:HG12	2.13	0.48
1:A:685:ILE:CG2	1:A:822:LEU:HD13	2.43	0.48
1:B:143:ILE:HG22	1:B:286:ALA:HB1	1.94	0.48
1:C:424:GLY:O	1:C:425:LEU:CB	2.61	0.48
1:C:104:GLN:CG	1:C:129:VAL:CG1	2.91	0.48
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.96	0.48
1:B:142:VAL:HG12	1:B:154:ILE:CG2	2.43	0.48
1:C:13:TRP:HA	1:C:13:TRP:CE3	2.49	0.48
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.95	0.48
1:C:343:THR:HG23	1:C:985:PRO:HB2	1.96	0.48
1:A:410:ILE:HA	1:A:413:VAL:HG22	1.96	0.48
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.47	0.48
1:A:984:MET:N	1:A:985:PRO:HD2	2.29	0.48
1:C:421:ALA:O	1:C:422:GLU:O	2.30	0.48
1:A:168:ARG:HG2	1:B:69:MET:O	2.14	0.47
1:C:298:ASN:O	1:C:300:LEU:N	2.48	0.47
1:B:1022:PHE:O	1:B:1026:VAL:HG22	2.14	0.47
1:C:27:ILE:HG23	1:C:390:ILE:CD1	2.44	0.47
1:C:382:VAL:HG11	1:C:476:SER:OG	2.15	0.47
1:A:902:VAL:HB	1:A:903:PRO:HD3	1.97	0.47
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.49	0.47
1:A:957:LEU:HD23	1:A:958:ILE:HD13	1.96	0.47
1:B:53:ASP:O	1:B:54:ALA:C	2.53	0.47
1:A:11:PHE:CE1	1:B:887:ALA:HB1	2.49	0.47
1:C:214:VAL:HG23	1:C:236:ALA:HB3	1.95	0.47
1:A:596:HIS:O	1:A:597:TYR:C	2.52	0.47
1:B:396:PHE:O	1:B:400:LEU:HG	2.14	0.47
1:C:721:LEU:O	1:C:722:GLU:C	2.52	0.47
1:A:410:ILE:HD13	1:A:974:MET:CB	2.44	0.47
1:A:686:ASP:HB2	1:A:695:LEU:HD13	1.95	0.47
1:A:918:LEU:HD21	1:A:999:ALA:HB2	1.97	0.47
1:B:115:MET:N	1:B:116:PRO:CD	2.78	0.47
1:B:382:VAL:HG21	1:B:480:LEU:HD13	1.96	0.47
1:C:181:GLN:NE2	1:C:767:ARG:NH2	2.63	0.47
1:A:968:ARG:CZ	1:A:968:ARG:HB3	2.44	0.47
1:B:965:VAL:HG12	1:B:969:LEU:HD12	1.95	0.47
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:HG23	1:C:162:MET:SD	2.54	0.47
1:A:249:ILE:O	1:A:250:LEU:CB	2.59	0.47
1:B:1009:VAL:O	1:B:1013:VAL:HG22	2.15	0.47
1:B:590:VAL:O	1:B:594:VAL:HG23	2.15	0.47
1:C:1020:PRO:O	1:C:1024:VAL:HG22	2.15	0.47
1:C:360:GLN:OE1	1:C:509:LYS:NZ	2.42	0.47
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.96	0.47
1:A:758:TYR:CZ	1:A:770:LYS:HD3	2.50	0.47
1:C:639:GLY:O	1:C:642:ASN:N	2.45	0.47
1:C:375:VAL:O	1:C:379:THR:HG22	2.14	0.46
1:C:719:ASN:HD22	1:C:826:GLU:HB3	1.80	0.46
1:B:198:LEU:HD23	1:B:251:LEU:HD13	1.96	0.46
1:C:965:VAL:HG21	1:C:1020:PRO:HG3	1.97	0.46
1:C:149:MET:HE1	1:C:321:LEU:HD13	1.97	0.46
1:C:578:LEU:HD11	1:C:590:VAL:HG21	1.98	0.46
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.46
1:A:516:PHE:HA	1:A:519:MET:HB2	1.98	0.46
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.80	0.46
1:B:418:ARG:NH1	1:B:967:MET:SD	2.88	0.46
1:C:104:GLN:HG3	1:C:129:VAL:CG1	2.44	0.46
1:B:119:PRO:O	1:B:122:VAL:HG12	2.15	0.46
1:C:951:ASP:HB3	1:C:952:LYS:NZ	2.28	0.46
1:C:532:GLY:CA	1:C:962:LEU:HD21	2.45	0.46
1:B:563:PHE:HD2	1:B:677:ALA:HB2	1.80	0.46
1:C:556:PHE:HB2	1:C:910:LEU:HD11	1.97	0.46
1:A:364:ALA:HA	1:A:367:ILE:HD12	1.98	0.46
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.98	0.46
1:B:412:VAL:HG12	1:B:438:ILE:CD1	2.46	0.46
1:A:890:GLU:C	1:C:10:ILE:HD13	2.36	0.46
1:A:977:LEU:HD23	1:A:981:LEU:HD23	1.98	0.46
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.46	0.46
1:C:390:ILE:CG2	1:C:390:ILE:O	2.64	0.46
1:A:549:VAL:HG12	1:A:549:VAL:O	2.15	0.46
1:B:393:LEU:CD2	1:B:466:ILE:HG23	2.45	0.46
1:B:65:ILE:O	1:B:66:GLU:C	2.53	0.46
1:A:10:ILE:HG12	1:B:890:GLU:O	2.15	0.46
1:A:754:TRP:CE3	1:C:234:ILE:CD1	2.99	0.46
1:C:13:TRP:CZ3	1:C:488:LEU:HD11	2.50	0.46
1:B:344:LEU:CD2	1:B:402:ILE:CG1	2.91	0.46
1:C:182:TYR:HA	1:C:271:GLY:O	2.15	0.46
1:C:880:VAL:HG22	1:C:880:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ILE:HG22	1:A:20:MET:N	2.31	0.45
1:A:1:MET:CE	1:A:486:LEU:HD23	2.47	0.45
1:A:72:ILE:HD12	1:A:72:ILE:H	1.79	0.45
1:A:695:LEU:CD2	1:A:825:MET:SD	3.03	0.45
1:C:777:ALA:O	1:C:781:MET:HG2	2.16	0.45
1:A:38:ILE:CG1	1:A:462:SER:O	2.64	0.45
1:B:379:THR:C	1:B:381:ALA:N	2.69	0.45
1:B:684:LEU:HD22	1:B:699:ARG:HA	1.97	0.45
1:C:453:PHE:CE2	1:C:474:ILE:HD13	2.52	0.45
1:C:527:TYR:OH	1:C:1016:ILE:HB	2.16	0.45
1:B:449:LEU:HD12	1:B:478:MET:CE	2.46	0.45
1:C:517:ASN:HD22	1:C:518:ARG:N	2.14	0.45
1:C:791:VAL:HG12	1:C:791:VAL:O	2.17	0.45
1:A:568:ASP:OD1	1:A:644:VAL:HG23	2.16	0.45
1:B:582:ALA:HB3	1:B:623:ASN:CB	2.46	0.45
1:C:445:ILE:HB	1:C:449:LEU:HD12	1.98	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.17	0.45
1:C:20:MET:SD	1:C:373:PRO:CB	3.05	0.45
1:C:467:TYR:OH	1:C:925:GLN:OE1	2.30	0.45
1:A:578:LEU:HD13	1:A:587:THR:HB	1.98	0.45
1:A:446:ALA:HA	1:A:478:MET:HE2	1.99	0.45
1:A:972:ILE:HG22	1:A:973:LEU:HD12	1.98	0.45
1:A:171:GLY:O	1:A:302:THR:HG21	2.17	0.45
1:A:222:THR:HG21	1:B:276:ASP:CG	2.37	0.45
1:C:400:LEU:O	1:C:401:ALA:CB	2.63	0.45
1:A:318:PRO:O	1:A:319:SER:O	2.35	0.45
1:B:137:LEU:HD12	1:B:329:THR:CG2	2.46	0.45
1:C:453:PHE:HA	1:C:456:MET:HG2	1.99	0.45
1:C:207:ILE:HG22	1:C:759:VAL:HG11	1.99	0.45
1:C:875:ALA:O	1:C:878:LEU:HB2	2.17	0.45
1:A:706:ALA:HB1	1:A:713:LEU:HD13	1.98	0.44
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.99	0.44
1:A:559:LEU:HD23	1:A:920:ASN:HB2	2.00	0.44
1:B:1013:VAL:HG23	1:B:1014:LEU:HD12	1.99	0.44
1:B:634:TRP:CE3	1:B:992:ALA:HB2	2.52	0.44
1:C:207:ILE:CG2	1:C:759:VAL:HG11	2.47	0.44
1:A:777:ALA:O	1:A:781:MET:HG2	2.17	0.44
1:B:375:VAL:HG22	1:B:484:VAL:CG1	2.47	0.44
1:B:401:ALA:C	1:B:403:GLY:N	2.68	0.44
1:C:688:ALA:HB3	1:C:854:GLY:HA3	1.99	0.44
1:B:399:VAL:HA	1:B:402:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.82	0.44
1:C:545:TYR:O	1:C:548:ILE:HG13	2.17	0.44
1:C:651:ALA:O	1:C:654:ALA:N	2.50	0.44
1:A:146:ASP:OD1	1:A:148:THR:HG23	2.18	0.44
1:A:11:PHE:HA	1:A:14:VAL:HG22	1.99	0.44
1:A:409:ALA:HA	1:A:489:THR:HG21	2.00	0.44
1:C:181:GLN:NE2	1:C:767:ARG:HH22	2.15	0.44
1:C:343:THR:O	1:C:344:LEU:C	2.56	0.44
1:B:30:LEU:HD11	1:B:380:PHE:O	2.18	0.44
1:C:124:GLN:O	1:C:126:GLY:N	2.51	0.44
1:C:372:VAL:CG2	1:C:373:PRO:HD3	2.46	0.44
1:C:478:MET:O	1:C:479:ALA:C	2.56	0.44
1:C:498:LYS:HB2	1:C:499:PRO:CD	2.48	0.44
1:A:1019:VAL:N	1:A:1020:PRO:CD	2.81	0.44
1:A:323:ILE:HG23	1:A:325:TYR:CE2	2.52	0.44
1:A:330:THR:O	1:A:331:PRO:C	2.55	0.44
1:B:185:ARG:HG3	1:B:187:TRP:CE2	2.53	0.44
1:C:472:ILE:O	1:C:476:SER:OG	2.30	0.44
1:A:542:LEU:CD2	1:A:546:LEU:HD21	2.48	0.44
1:B:184:MET:HB3	1:B:771:VAL:HG22	2.00	0.44
1:C:65:ILE:HG13	1:C:118:LEU:HD21	1.99	0.44
1:C:26:ALA:O	1:C:30:LEU:HB2	2.18	0.44
1:C:181:GLN:HE21	1:C:767:ARG:NH2	2.16	0.44
1:C:885:LEU:HD21	1:C:895:PRO:HB2	1.99	0.44
1:A:318:PRO:O	1:A:319:SER:C	2.56	0.44
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.00	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.99	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.80	0.44
1:A:332:PHE:C	1:A:332:PHE:CD2	2.90	0.44
1:A:449:LEU:HD12	1:A:478:MET:HE1	1.99	0.44
1:A:72:ILE:HD13	1:A:75:LEU:CD2	2.47	0.44
1:B:151:GLN:NE2	1:B:278:ILE:HA	2.33	0.44
1:B:366:LEU:HD13	1:B:369:THR:HG22	1.99	0.44
1:B:478:MET:C	1:B:478:MET:SD	2.96	0.44
1:B:655:PHE:O	1:B:656:SER:C	2.56	0.44
1:C:34:GLN:O	1:C:35:TYR:HD1	2.01	0.44
1:B:444:GLY:O	1:B:448:VAL:HG23	2.18	0.43
1:B:876:ILE:HA	1:B:879:ILE:HG22	2.00	0.43
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.98	0.43
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.43
1:C:845:GLU:O	1:C:849:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LYS:C	1:C:954:GLY:H	2.19	0.43
1:B:182:TYR:CD2	1:B:270:LEU:HD23	2.54	0.43
1:B:344:LEU:HD23	1:B:402:ILE:CG1	2.36	0.43
1:B:5:PHE:CE2	1:B:487:ILE:HG23	2.53	0.43
1:C:26:ALA:HB1	1:C:384:ALA:HB3	2.00	0.43
1:B:997:GLN:O	1:B:1000:VAL:HG22	2.19	0.43
1:B:1013:VAL:HG23	1:B:1014:LEU:CD1	2.48	0.43
1:C:399:VAL:O	1:C:401:ALA:N	2.52	0.43
1:C:639:GLY:O	1:C:641:GLU:N	2.51	0.43
1:C:873:LEU:O	1:C:877:SER:N	2.33	0.43
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.52	0.43
1:B:166:ILE:HD13	1:B:289:LEU:CD2	2.49	0.43
1:C:194:ASN:ND2	1:C:790:TYR:CG	2.86	0.43
1:C:277:ILE:N	1:C:277:ILE:CD1	2.82	0.43
1:C:166:ILE:HD11	1:C:310:LEU:CD1	2.48	0.43
1:A:23:GLY:CA	1:A:381:ALA:HB2	2.44	0.43
1:A:420:MET:SD	1:A:430:ALA:HB3	2.59	0.43
1:B:994:SER:O	1:B:998:ASN:ND2	2.52	0.43
1:C:425:LEU:HD13	1:C:425:LEU:C	2.39	0.43
1:A:906:VAL:HG12	1:A:910:LEU:CD2	2.49	0.43
1:B:399:VAL:CA	1:B:402:ILE:HG13	2.49	0.43
1:B:866:GLU:O	1:B:867:ARG:HB2	2.18	0.43
1:C:30:LEU:HD22	1:C:390:ILE:CG1	2.46	0.43
1:B:403:GLY:HA2	1:B:406:VAL:HG12	2.01	0.43
1:B:449:LEU:O	1:B:453:PHE:HB2	2.19	0.43
1:B:108:GLN:HE21	1:C:109:ASN:HD22	1.67	0.43
1:C:952:LYS:HA	1:C:952:LYS:CE	2.42	0.43
1:B:731:ILE:HA	1:B:804:PHE:O	2.19	0.43
1:B:878:LEU:HA	1:B:881:VAL:HG22	2.00	0.43
1:C:30:LEU:HD12	1:C:384:ALA:HB2	1.99	0.43
1:A:1:MET:HE2	1:A:486:LEU:HD23	2.01	0.42
1:A:448:VAL:HG12	1:A:884:CYS:CB	2.49	0.42
1:A:676:THR:O	1:A:678:THR:N	2.52	0.42
1:A:961:THR:HG21	1:A:1024:VAL:CG1	2.48	0.42
1:B:102:ILE:O	1:B:105:VAL:HG12	2.19	0.42
1:C:399:VAL:HA	1:C:402:ILE:HD11	2.01	0.42
1:C:916:ARG:O	1:C:918:LEU:N	2.52	0.42
1:A:107:VAL:HG12	1:A:108:GLN:N	2.34	0.42
1:A:332:PHE:CD1	1:A:569:GLN:HA	2.54	0.42
1:A:743:ILE:HG22	1:A:747:ASN:ND2	2.35	0.42
1:B:452:VAL:CG1	1:B:453:PHE:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:THR:HG21	1:C:228:GLN:O	2.19	0.42
1:C:350:LEU:HD13	1:C:981:LEU:HD22	2.00	0.42
1:C:478:MET:O	1:C:481:SER:N	2.52	0.42
1:B:374:VAL:O	1:B:378:GLY:N	2.51	0.42
1:B:382:VAL:O	1:B:385:ALA:HB3	2.19	0.42
1:C:327:TYR:O	1:C:327:TYR:CD2	2.72	0.42
1:A:215:ALA:HB1	1:B:51:GLY:C	2.40	0.42
1:B:11:PHE:CD1	1:B:15:ILE:HD11	2.54	0.42
1:B:185:ARG:NH1	1:B:272:GLY:O	2.43	0.42
1:B:333:VAL:O	1:B:337:ILE:HD12	2.19	0.42
1:B:692:HIS:O	1:B:693:GLU:C	2.57	0.42
1:C:895:PRO:C	1:C:897:SER:N	2.73	0.42
1:A:887:ALA:HB1	1:C:11:PHE:HD2	1.84	0.42
1:B:578:LEU:HD13	1:B:587:THR:HG23	2.01	0.42
1:B:731:ILE:O	1:B:731:ILE:HG12	2.18	0.42
1:C:904:LEU:O	1:C:1010:THR:O	2.36	0.42
1:C:36:PRO:HD3	1:C:391:ASN:ND2	2.34	0.42
1:B:903:PRO:HA	1:B:906:VAL:HG22	2.01	0.42
1:C:357:LEU:HD21	1:C:516:PHE:CZ	2.55	0.42
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.50	0.42
1:C:572:PHE:CZ	1:C:629:VAL:HG11	2.54	0.42
1:C:878:LEU:HA	1:C:881:VAL:CG2	2.49	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.20	0.42
1:A:583:THR:HG22	1:A:586:ARG:CD	2.49	0.42
1:B:454:VAL:CB	1:B:455:PRO:CD	2.97	0.42
1:C:422:GLU:O	1:C:502:LYS:O	2.38	0.42
1:C:160:ALA:HA	1:C:767:ARG:NH2	2.35	0.42
1:C:885:LEU:CD1	1:C:885:LEU:C	2.88	0.42
1:A:130:GLU:OE2	1:A:174:ASP:OD2	2.37	0.42
1:C:453:PHE:O	1:C:454:VAL:HG23	2.20	0.42
1:B:903:PRO:O	1:B:905:GLY:N	2.53	0.42
1:B:906:VAL:O	1:B:910:LEU:HD13	2.20	0.42
1:C:194:ASN:O	1:C:195:LYS:C	2.58	0.42
1:A:213:GLN:HB2	1:A:239:ARG:HG2	2.01	0.42
1:A:410:ILE:HD13	1:A:974:MET:HB2	2.01	0.42
1:B:216:ALA:HB1	1:B:234:ILE:O	2.19	0.42
1:B:27:ILE:CG2	1:B:380:PHE:HD2	2.33	0.42
1:B:45:ILE:HG12	1:B:129:VAL:HG22	2.02	0.42
1:C:409:ALA:HA	1:C:489:THR:HG21	2.02	0.42
1:C:928:LEU:O	1:C:931:THR:N	2.53	0.42
1:A:641:GLU:N	1:A:641:GLU:OE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:CD1	1:C:333:VAL:HG11	2.50	0.41
1:C:655:PHE:C	1:C:657:GLN:N	2.73	0.41
1:A:372:VAL:HB	1:A:373:PRO:CD	2.49	0.41
1:B:367:ILE:HB	1:B:368:PRO:CD	2.50	0.41
1:B:445:ILE:CG2	1:B:449:LEU:CG	2.91	0.41
1:C:36:PRO:HG2	1:C:469:GLN:HE22	1.84	0.41
1:C:474:ILE:O	1:C:477:ALA:N	2.53	0.41
1:C:882:PHE:C	1:C:882:PHE:CD1	2.92	0.41
1:C:940:ILE:O	1:C:944:GLU:CA	2.68	0.41
1:B:595:THR:HG22	1:B:609:VAL:CG2	2.50	0.41
1:B:882:PHE:HB2	1:B:899:MET:HE1	2.01	0.41
1:C:34:GLN:OE1	1:C:35:TYR:CE1	2.73	0.41
1:C:425:LEU:CB	1:C:426:PRO:CD	2.97	0.41
1:A:144:ASN:HB2	1:A:154:ILE:HD11	2.03	0.41
1:B:976:SER:OG	1:B:1012:THR:HG21	2.21	0.41
1:A:410:ILE:HD13	1:A:974:MET:HB3	2.03	0.41
1:A:578:LEU:HD11	1:A:590:VAL:HG21	2.03	0.41
1:B:236:ALA:O	1:B:237:GLN:C	2.58	0.41
1:C:425:LEU:CD1	1:C:426:PRO:O	2.67	0.41
1:C:877:SER:O	1:C:880:VAL:HG12	2.21	0.41
1:B:572:PHE:CD2	1:B:644:VAL:HG23	2.56	0.41
1:C:576:VAL:HG22	1:C:663:VAL:HG22	2.02	0.41
1:A:918:LEU:HD21	1:A:999:ALA:CB	2.51	0.41
1:B:102:ILE:O	1:B:103:ALA:C	2.59	0.41
1:C:74:ASN:O	1:C:95:GLU:N	2.52	0.41
1:C:819:TYR:N	1:C:821:GLY:O	2.53	0.41
1:C:902:VAL:HB	1:C:903:PRO:HD3	2.02	0.41
1:C:949:LEU:HD23	1:C:953:GLU:HB3	2.02	0.41
1:A:371:ALA:O	1:A:374:VAL:HG22	2.21	0.41
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.55	0.41
1:B:20:MET:CA	1:B:377:LEU:HD21	2.51	0.41
1:C:129:VAL:CG1	1:C:129:VAL:O	2.68	0.41
1:C:298:ASN:C	1:C:300:LEU:N	2.73	0.41
1:A:15:ILE:HA	1:A:18:ILE:HG22	2.03	0.41
1:A:916:ARG:O	1:A:916:ARG:HG3	2.19	0.41
1:B:317:PHE:CG	1:B:321:LEU:HD23	2.56	0.41
1:B:987:VAL:HG11	1:B:1005:MET:HG3	2.02	0.41
1:C:13:TRP:HA	1:C:13:TRP:HE3	1.83	0.41
1:C:406:VAL:O	1:C:407:ASP:C	2.58	0.41
1:C:412:VAL:HG12	1:C:412:VAL:O	2.21	0.41
1:C:409:ALA:O	1:C:413:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:THR:OG1	1:C:725:PRO:N	2.53	0.41
1:C:749:THR:O	1:C:750:LEU:C	2.59	0.41
1:C:937:LYS:CD	1:C:938:ASN:HD22	2.33	0.41
1:A:726:GLN:NE2	1:C:235:ILE:CD1	2.84	0.41
1:B:164:ASP:O	1:B:165:ALA:HB2	2.21	0.41
1:B:5:PHE:CE2	1:B:487:ILE:HD12	2.55	0.41
1:B:609:VAL:HG13	1:B:609:VAL:O	2.21	0.41
1:B:868:SER:HA	1:B:869:GLY:HA3	1.88	0.41
1:B:964:ALA:HA	1:B:967:MET:HE3	2.02	0.41
1:C:464:GLY:O	1:C:468:ARG:HG3	2.20	0.41
1:B:445:ILE:O	1:B:449:LEU:CB	2.61	0.40
1:C:40:PRO:HD2	1:C:674:LEU:HD11	2.03	0.40
1:C:882:PHE:O	1:C:885:LEU:CD1	2.69	0.40
1:B:240:LEU:CD2	1:B:249:ILE:HD11	2.52	0.40
1:C:284:GLN:HE21	1:C:284:GLN:HB3	1.61	0.40
1:C:952:LYS:CA	1:C:952:LYS:HE3	2.47	0.40
1:A:456:MET:HA	1:A:459:PHE:CD2	2.57	0.40
1:A:617:PHE:O	1:A:618:ALA:HB2	2.21	0.40
1:A:968:ARG:HG2	1:A:971:PRO:HG3	2.04	0.40
1:B:324:VAL:HG12	1:B:325:TYR:H	1.87	0.40
1:C:72:ILE:O	1:C:73:ASP:C	2.60	0.40
1:C:878:LEU:O	1:C:881:VAL:N	2.46	0.40
1:C:882:PHE:HA	1:C:899:MET:HE1	2.02	0.40
1:C:76:MET:SD	1:C:95:GLU:HA	2.61	0.40
1:A:898:VAL:HG11	1:A:940:ILE:HA	2.04	0.40
1:B:388:PHE:CE2	1:B:472:ILE:HG21	2.55	0.40
1:A:728:LYS:HA	1:C:235:ILE:O	2.22	0.40
1:C:555:LEU:O	1:C:559:LEU:N	2.55	0.40
1:C:677:ALA:HB1	1:C:717:ARG:HH21	1.87	0.40
1:C:382:VAL:HG12	1:C:472:ILE:HD11	2.03	0.40
1:C:470:PHE:HA	1:C:473:THR:HG22	2.02	0.40
1:C:69:MET:HE2	1:C:92:LEU:HD21	2.04	0.40
1:C:901:VAL:HG12	1:C:935:SER:HB3	2.03	0.40
1:C:983:VAL:O	1:C:983:VAL:HG12	2.22	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	A	1039/1050 (99%)	877 (84%)	116 (11%)	46 (4%)	2	15
1	B	1028/1050 (98%)	825 (80%)	148 (14%)	55 (5%)	2	11
1	C	1028/1050 (98%)	791 (77%)	155 (15%)	82 (8%)	1	4
All	All	3095/3150 (98%)	2493 (80%)	419 (14%)	183 (6%)	1	9

All (183) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	SER
1	A	366	LEU
1	A	464	GLY
1	A	543	VAL
1	A	582	ALA
1	A	677	ALA
1	A	865	GLN
1	A	909	ALA
1	A	1033	LYS
1	B	68	ASN
1	B	165	ALA
1	B	181	GLN
1	B	215	ALA
1	B	337	ILE
1	B	362	PHE
1	B	633	ASP
1	B	636	ASP
1	B	644	VAL
1	B	659	LYS
1	B	861	GLY
1	B	863	SER
1	B	890	GLU
1	B	988	ILE
1	B	989	SER

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Mol	Chain	Res	Type
1	C	7	ASP
1	C	9	PRO
1	C	10	ILE
1	C	62	THR
1	C	82	SER
1	C	83	ASP
1	C	124	GLN
1	C	125	GLN
1	C	401	ALA
1	C	422	GLU
1	C	425	LEU
1	C	431	THR
1	C	432	ARG
1	C	644	VAL
1	C	689	GLY
1	C	693	GLU
1	C	723	ASP
1	C	853	THR
1	C	859	TRP
1	C	870	ALA
1	C	917	GLY
1	C	922	VAL
1	C	936	ALA
1	C	953	GLU
1	A	161	ASN
1	A	318	PRO
1	A	420	MET
1	A	435	MET
1	A	439	GLN
1	A	503	GLY
1	A	508	GLY
1	A	616	GLY
1	A	618	ALA
1	A	670	ALA
1	A	994	SER
1	A	1018	PHE
1	A	1034	ASN
1	A	1035	GLU
1	B	34	GLN
1	B	209	ALA
1	B	237	GLN
1	B	319	SER

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Mol	Chain	Res	Type
1	B	359	LEU
1	B	364	ALA
1	B	388	PHE
1	B	432	ARG
1	B	440	GLY
1	B	455	PRO
1	B	456	MET
1	B	778	LYS
1	B	802	SER
1	B	867	ARG
1	C	51	GLY
1	C	61	VAL
1	C	296	GLY
1	C	298	ASN
1	C	299	ALA
1	C	356	TYR
1	C	362	PHE
1	C	400	LEU
1	C	409	ALA
1	C	428	LYS
1	C	437	GLN
1	C	471	SER
1	C	510	LYS
1	C	511	GLY
1	C	640	GLU
1	C	656	SER
1	C	687	GLN
1	C	701	GLN
1	C	722	GLU
1	C	778	LYS
1	C	855	VAL
1	C	861	GLY
1	C	887	ALA
1	C	952	LYS
1	C	957	LEU
1	C	1029	ARG
1	A	21	LEU
1	A	250	LEU
1	A	490	PRO
1	A	533	GLY
1	A	645	GLU
1	A	669	PRO

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Mol	Chain	Res	Type
1	A	795	ASP
1	A	867	ARG
1	A	950	MET
1	B	135	SER
1	B	243	THR
1	B	320	GLY
1	B	367	ILE
1	B	657	GLN
1	B	661	ALA
1	B	678	THR
1	B	795	ASP
1	B	814	PRO
1	B	866	GLU
1	B	959	GLU
1	C	53	ASP
1	C	81	ASN
1	C	106	GLN
1	C	423	GLU
1	C	427	PRO
1	C	454	VAL
1	C	618	ALA
1	C	896	PHE
1	A	35	TYR
1	A	459	PHE
1	A	507	GLU
1	A	538	THR
1	B	36	PRO
1	B	380	PHE
1	B	439	GLN
1	B	800	PRO
1	B	820	ASN
1	C	73	ASP
1	C	390	ILE
1	C	501	ALA
1	C	871	PRO
1	C	875	ALA
1	C	913	ALA
1	C	915	PHE
1	C	955	LYS
1	A	358	PHE
1	A	418	ARG
1	A	509	LYS

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Mol	Chain	Res	Type
1	B	54	ALA
1	B	431	THR
1	B	510	LYS
1	B	895	PRO
1	C	22	ALA
1	C	683	GLU
1	C	692	HIS
1	C	852	PRO
1	C	939	ALA
1	A	929	LEU
1	A	1037	ILE
1	B	402	ILE
1	B	442	LEU
1	B	454	VAL
1	B	539	GLY
1	B	676	THR
1	B	949	LEU
1	C	76	MET
1	C	285	PRO
1	C	387	GLY
1	C	825	MET
1	C	929	LEU
1	C	942	ILE
1	A	368	PRO
1	A	954	GLY
1	C	685	ILE
1	C	823	PRO
1	A	419	VAL
1	C	129	VAL
1	C	822	LEU
1	A	870	ALA
1	C	932	ILE
1	A	14	VAL

### 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	A	847/856 (99%)	748 (88%)	99 (12%)	5	22
1	B	836/856 (98%)	737 (88%)	99 (12%)	5	22
1	C	836/856 (98%)	719 (86%)	117 (14%)	3	16
All	All	2519/2568 (98%)	2204 (88%)	315 (12%)	4	20

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	PHE
1	A	15	ILE
1	A	18	ILE
1	A	27	ILE
1	A	32	VAL
1	A	46	SER
1	A	49	TYR
1	A	50	PRO
1	A	72	ILE
1	A	74	ASN
1	A	79	SER
1	A	96	SER
1	A	101	ASP
1	A	129	VAL
1	A	132	SER
1	A	135	SER
1	A	138	MET
1	A	150	THR
1	A	155	SER
1	A	197	GLN
1	A	231	ASN
1	A	242	SER
1	A	243	THR
1	A	244	GLU
1	A	249	ILE
1	A	253	VAL
1	A	258	SER
1	A	262	LEU
1	A	307	ARG
1	A	323	ILE
1	A	341	VAL
1	A	343	THR
1	A	355	MET

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Mol	Chain	Res	Type
1	A	356	TYR
1	A	369	THR
1	A	375	VAL
1	A	392	THR
1	A	406	VAL
1	A	417	GLU
1	A	452	VAL
1	A	480	LEU
1	A	489	THR
1	A	497	LEU
1	A	498	LYS
1	A	510	LYS
1	A	512	PHE
1	A	516	PHE
1	A	518	ARG
1	A	527	TYR
1	A	535	LEU
1	A	536	ARG
1	A	547	ILE
1	A	552	MET
1	A	587	THR
1	A	603	LYS
1	A	606	VAL
1	A	617	PHE
1	A	626	ILE
1	A	630	SER
1	A	637	ARG
1	A	640	GLU
1	A	648	THR
1	A	659	LYS
1	A	662	MET
1	A	721	LEU
1	A	724	THR
1	A	737	GLN
1	A	741	VAL
1	A	758	TYR
1	A	784	ASP
1	A	795	ASP
1	A	801	PHE
1	A	802	SER
1	A	804	PHE
1	A	806	SER

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Mol	Chain	Res	Type
1	A	808	ARG
1	A	822	LEU
1	A	825	MET
1	A	842	GLU
1	A	844	MET
1	A	849	SER
1	A	853	THR
1	A	858	ASP
1	A	910	LEU
1	A	911	LEU
1	A	918	LEU
1	A	934	LEU
1	A	942	ILE
1	A	966	ARG
1	A	968	ARG
1	A	977	LEU
1	A	990	THR
1	A	1010	THR
1	A	1027	ARG
1	A	1029	ARG
1	A	1030	PHE
1	A	1034	ASN
1	A	1038	GLU
1	B	1	MET
1	B	4	PHE
1	B	11	PHE
1	B	25	LEU
1	B	34	GLN
1	B	49	TYR
1	B	57	VAL
1	B	68	ASN
1	B	70	ASN
1	B	75	LEU
1	B	78	MET
1	B	82	SER
1	B	83	ASP
1	B	91	THR
1	B	117	LEU
1	B	130	GLU
1	B	134	SER
1	B	151	GLN
1	B	185	ARG

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Mol	Chain	Res	Type
1	B	193	LEU
1	B	214	VAL
1	B	219	LEU
1	B	233	SER
1	B	234	ILE
1	B	237	GLN
1	B	241	THR
1	B	267	LYS
1	B	284	GLN
1	B	293	LEU
1	B	330	THR
1	B	345	VAL
1	B	349	ILE
1	B	356	TYR
1	B	361	ASN
1	B	362	PHE
1	B	369	THR
1	B	370	ILE
1	B	372	VAL
1	B	377	LEU
1	B	393	LEU
1	B	404	LEU
1	B	418	ARG
1	B	423	GLU
1	B	478	MET
1	B	481	SER
1	B	484	VAL
1	B	486	LEU
1	B	495	THR
1	B	500	ILE
1	B	519	MET
1	B	524	THR
1	B	526	HIS
1	B	529	ASP
1	B	535	LEU
1	B	556	PHE
1	B	577	GLN
1	B	586	ARG
1	B	599	LEU
1	B	604	ASN
1	B	608	SER
1	B	626	ILE

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Mol	Chain	Res	Type
1	B	630	SER
1	B	652	THR
1	B	666	PHE
1	B	674	LEU
1	B	693	GLU
1	B	708	LYS
1	B	713	LEU
1	B	714	THR
1	B	717	ARG
1	B	726	GLN
1	B	729	ILE
1	B	730	ASP
1	B	731	ILE
1	B	791	VAL
1	B	797	GLN
1	B	825	MET
1	B	828	LEU
1	B	843	LEU
1	B	846	GLN
1	B	858	ASP
1	B	862	MET
1	B	865	GLN
1	B	867	ARG
1	B	874	TYR
1	B	877	SER
1	B	879	ILE
1	B	883	LEU
1	B	891	SER
1	B	893	SER
1	B	900	LEU
1	B	914	THR
1	B	915	PHE
1	B	918	LEU
1	B	919	THR
1	B	959	GLU
1	B	963	ASP
1	B	969	LEU
1	B	1027	ARG
1	C	13	TRP
1	C	18	ILE
1	C	29	LYS
1	C	30	LEU

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	38	ILE
1	C	43	VAL
1	C	49	TYR
1	C	58	GLN
1	C	61	VAL
1	C	77	TYR
1	C	78	MET
1	C	79	SER
1	C	80	SER
1	C	84	SER
1	C	91	THR
1	C	93	THR
1	C	102	ILE
1	C	125	GLN
1	C	145	THR
1	C	158	VAL
1	C	177	LEU
1	C	185	ARG
1	C	197	GLN
1	C	202	ASP
1	C	237	GLN
1	C	239	ARG
1	C	241	THR
1	C	242	SER
1	C	252	LYS
1	C	254	ASN
1	C	285	PRO
1	C	300	LEU
1	C	301	ASP
1	C	310	LEU
1	C	314	GLU
1	C	329	THR
1	C	337	ILE
1	C	348	ILE
1	C	357	LEU
1	C	389	SER
1	C	394	THR
1	C	404	LEU
1	C	408	ASP
1	C	413	VAL
1	C	414	GLU

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Mol	Chain	Res	Type
1	C	417	GLU
1	C	422	GLU
1	C	423	GLU
1	C	425	LEU
1	C	435	MET
1	C	447	MET
1	C	456	MET
1	C	463	THR
1	C	469	GLN
1	C	471	SER
1	C	483	LEU
1	C	495	THR
1	C	504	ASP
1	C	517	ASN
1	C	550	VAL
1	C	552	MET
1	C	583	THR
1	C	587	THR
1	C	591	LEU
1	C	604	ASN
1	C	613	ASN
1	C	620	ARG
1	C	622	GLN
1	C	624	THR
1	C	626	ILE
1	C	641	GLU
1	C	656	SER
1	C	690	LEU
1	C	699	ARG
1	C	701	GLN
1	C	729	ILE
1	C	730	ASP
1	C	733	GLN
1	C	737	GLN
1	C	758	TYR
1	C	763	ILE
1	C	767	ARG
1	C	768	VAL
1	C	784	ASP
1	C	786	ILE
1	C	801	PHE
1	C	815	ARG

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Mol	Chain	Res	Type
1	C	825	MET
1	C	828	LEU
1	C	841	MET
1	C	845	GLU
1	C	849	SER
1	C	853	THR
1	C	863	SER
1	C	881	VAL
1	C	882	PHE
1	C	884	CYS
1	C	885	LEU
1	C	889	TYR
1	C	891	SER
1	C	896	PHE
1	C	918	LEU
1	C	930	THR
1	C	937	LYS
1	C	938	ASN
1	C	941	LEU
1	C	952	LYS
1	C	953	GLU
1	C	963	ASP
1	C	967	MET
1	C	981	LEU
1	C	987	VAL
1	C	1014	LEU
1	C	1016	ILE
1	C	1026	VAL
1	C	1029	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	GLN
1	A	68	ASN
1	A	231	ASN
1	A	596	HIS
1	A	726	GLN
1	A	737	GLN
1	A	925	GLN
1	A	998	ASN

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	108	GLN
1	B	151	GLN
1	B	191	ASN
1	B	197	GLN
1	B	237	GLN
1	B	284	GLN
1	B	469	GLN
1	B	569	GLN
1	B	604	ASN
1	B	605	ASN
1	B	642	ASN
1	B	797	GLN
1	B	820	ASN
1	B	865	GLN
1	B	997	GLN
1	B	998	ASN
1	C	70	ASN
1	C	104	GLN
1	C	109	ASN
1	C	181	GLN
1	C	228	GLN
1	C	284	GLN
1	C	298	ASN
1	C	469	GLN
1	C	525	HIS
1	C	613	ASN
1	C	657	GLN
1	C	719	ASN
1	C	733	GLN
1	C	744	ASN
1	C	820	ASN
1	C	938	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1041/1050 (99%)	0.07	37 (3%)	42	17	21, 70, 147, 190	0
1	B	1030/1050 (98%)	0.26	66 (6%)	19	6	27, 98, 147, 173	0
1	C	1030/1050 (98%)	0.24	58 (5%)	24	8	24, 87, 142, 207	0
All	All	3101/3150 (98%)	0.19	161 (5%)	27	10	21, 86, 147, 207	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	ILE	9.7
1	C	6	ILE	5.8
1	C	497	LEU	5.5
1	C	707	ALA	5.4
1	B	497	LEU	5.2
1	B	986	LEU	5.0
1	B	527	TYR	4.8
1	C	511	GLY	4.6
1	C	1030	PHE	4.5
1	C	512	PHE	4.5
1	C	426	PRO	4.4
1	A	501	ALA	4.2
1	B	408	ASP	4.2
1	B	421	ALA	4.1
1	A	954	GLY	4.0
1	C	516	PHE	3.9
1	C	5	PHE	3.9
1	B	606	VAL	3.9
1	B	604	ASN	3.9
1	B	1028	ARG	3.8
1	B	526	HIS	3.8
1	B	507	GLU	3.7
1	A	419	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	3.7
1	B	419	VAL	3.6
1	B	634	TRP	3.6
1	C	496	MET	3.6
1	A	868	SER	3.6
1	B	516	PHE	3.5
1	A	506	GLY	3.4
1	A	511	GLY	3.4
1	C	513	PHE	3.3
1	B	509	LYS	3.3
1	C	408	ASP	3.3
1	C	507	GLU	3.3
1	C	55	LYS	3.3
1	A	505	HIS	3.2
1	C	935	SER	3.2
1	C	504	ASP	3.2
1	B	501	ALA	3.2
1	A	961	THR	3.1
1	A	869	GLY	3.1
1	C	500	ILE	3.1
1	C	503	GLY	3.1
1	B	511	GLY	3.1
1	C	494	ALA	3.1
1	C	438	ILE	3.1
1	C	938	ASN	3.1
1	B	412	VAL	3.1
1	B	522	LYS	3.1
1	C	509	LYS	3.0
1	B	510	LYS	3.0
1	A	513	PHE	3.0
1	C	833	PRO	3.0
1	B	1029	ARG	3.0
1	B	520	PHE	3.0
1	C	681	ASP	3.0
1	A	417	GLU	2.9
1	B	535	LEU	2.9
1	A	866	GLU	2.9
1	C	441	ALA	2.9
1	B	523	SER	2.9
1	B	505	HIS	2.9
1	C	836	SER	2.9
1	A	967	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	499	PRO	2.8
1	B	605	ASN	2.8
1	B	500	ILE	2.8
1	B	361	ASN	2.7
1	C	966	ARG	2.7
1	B	931	THR	2.7
1	C	506	GLY	2.7
1	A	867	ARG	2.7
1	A	898	VAL	2.6
1	B	962	LEU	2.6
1	B	513	PHE	2.6
1	B	968	ARG	2.6
1	B	498	LYS	2.6
1	B	506	GLY	2.6
1	B	437	GLN	2.5
1	A	504	ASP	2.5
1	A	421	ALA	2.5
1	B	961	THR	2.5
1	B	959	GLU	2.5
1	C	364	ALA	2.5
1	C	675	GLY	2.5
1	B	360	GLN	2.5
1	C	1002	THR	2.5
1	A	949	LEU	2.5
1	C	691	GLY	2.5
1	C	834	GLY	2.5
1	B	874	TYR	2.4
1	A	537	SER	2.4
1	B	635	ALA	2.4
1	C	536	ARG	2.4
1	B	935	SER	2.4
1	C	493	CYS	2.4
1	B	599	LEU	2.4
1	B	362	PHE	2.4
1	B	994	SER	2.4
1	C	435	MET	2.4
1	C	510	LYS	2.4
1	A	496	MET	2.4
1	C	945	PHE	2.4
1	B	946	ALA	2.4
1	B	966	ARG	2.4
1	B	991	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	952	LYS	2.4
1	B	427	PRO	2.3
1	C	519	MET	2.3
1	B	402	ILE	2.3
1	B	947	LYS	2.3
1	A	962	LEU	2.3
1	B	904	LEU	2.3
1	C	855	VAL	2.3
1	C	837	THR	2.3
1	C	403	GLY	2.3
1	B	897	SER	2.3
1	B	499	PRO	2.3
1	B	409	ALA	2.3
1	A	489	THR	2.2
1	C	680	PHE	2.2
1	C	415	ASN	2.2
1	A	408	ASP	2.2
1	B	367	ILE	2.2
1	C	831	ALA	2.2
1	A	522	LYS	2.2
1	B	958	ILE	2.2
1	C	359	LEU	2.2
1	B	1008	MET	2.2
1	A	7	ASP	2.2
1	B	420	MET	2.2
1	B	519	MET	2.2
1	A	948	ASP	2.2
1	C	499	PRO	2.2
1	A	507	GLU	2.2
1	C	9	PRO	2.1
1	A	966	ARG	2.1
1	C	978	ALA	2.1
1	A	362	PHE	2.1
1	B	508	GLY	2.1
1	A	915	PHE	2.1
1	C	870	ALA	2.1
1	C	957	LEU	2.1
1	A	960	ALA	2.1
1	B	493	CYS	2.1
1	A	529	ASP	2.1
1	B	540	ARG	2.1
1	B	436	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	418	ARG	2.1
1	C	1026	VAL	2.1
1	C	713	LEU	2.0
1	A	951	ASP	2.0
1	A	497	LEU	2.0
1	B	969	LEU	2.0
1	C	854	GLY	2.0
1	B	641	GLU	2.0
1	C	59	ASP	2.0
1	B	952	LYS	2.0
1	C	416	VAL	2.0
1	C	485	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.