



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:11 am BST

PDB ID : 6IIA  
Title : MexB in complex with LMNG  
Authors : Nakashima, R.; Sakurai, K.; Nakao, K.  
Deposited on : 2018-10-04  
Resolution : 2.91 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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

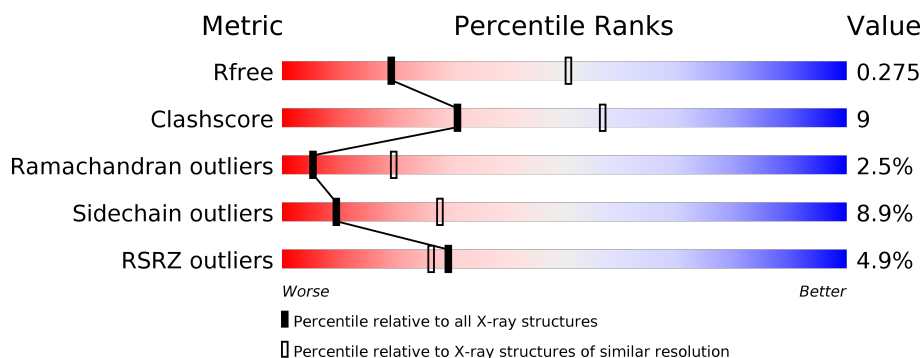
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	1052	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	1052	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	1052	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>• •</div> </div> </div>
1	D	1052	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	E	1052	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
1	F	1052	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46876 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 resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1017	Total	C	N	O	S	0	0	0
			7718	4972	1279	1427	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	D	1020	Total	C	N	O	S	0	0	0
			7744	4990	1283	1431	40			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	F	1033	Total	C	N	O	S	0	0	0
			7840	5046	1302	1452	40			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression tag	UNP P52002
B	1048	HIS	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002
B	1052	HIS	-	expression tag	UNP P52002
C	1047	HIS	-	expression tag	UNP P52002
C	1048	HIS	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	expression tag	UNP P52002
D	1047	HIS	-	expression tag	UNP P52002
D	1048	HIS	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression tag	UNP P52002
E	1047	HIS	-	expression tag	UNP P52002
E	1048	HIS	-	expression tag	UNP P52002
E	1049	HIS	-	expression tag	UNP P52002
E	1050	HIS	-	expression tag	UNP P52002
E	1051	HIS	-	expression tag	UNP P52002
E	1052	HIS	-	expression tag	UNP P52002
F	1047	HIS	-	expression tag	UNP P52002
F	1048	HIS	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002

- # AVO



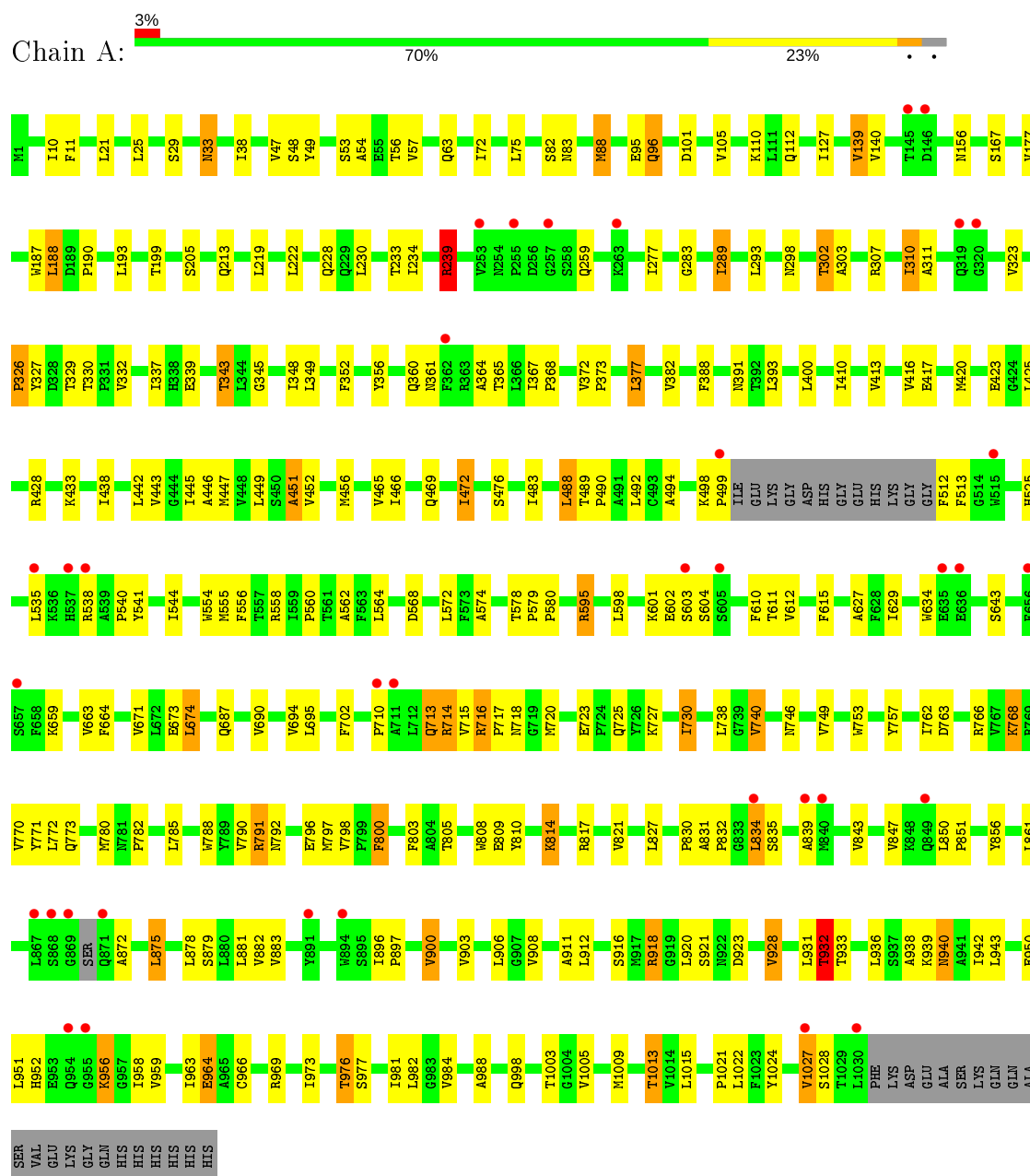
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			69	47	22		

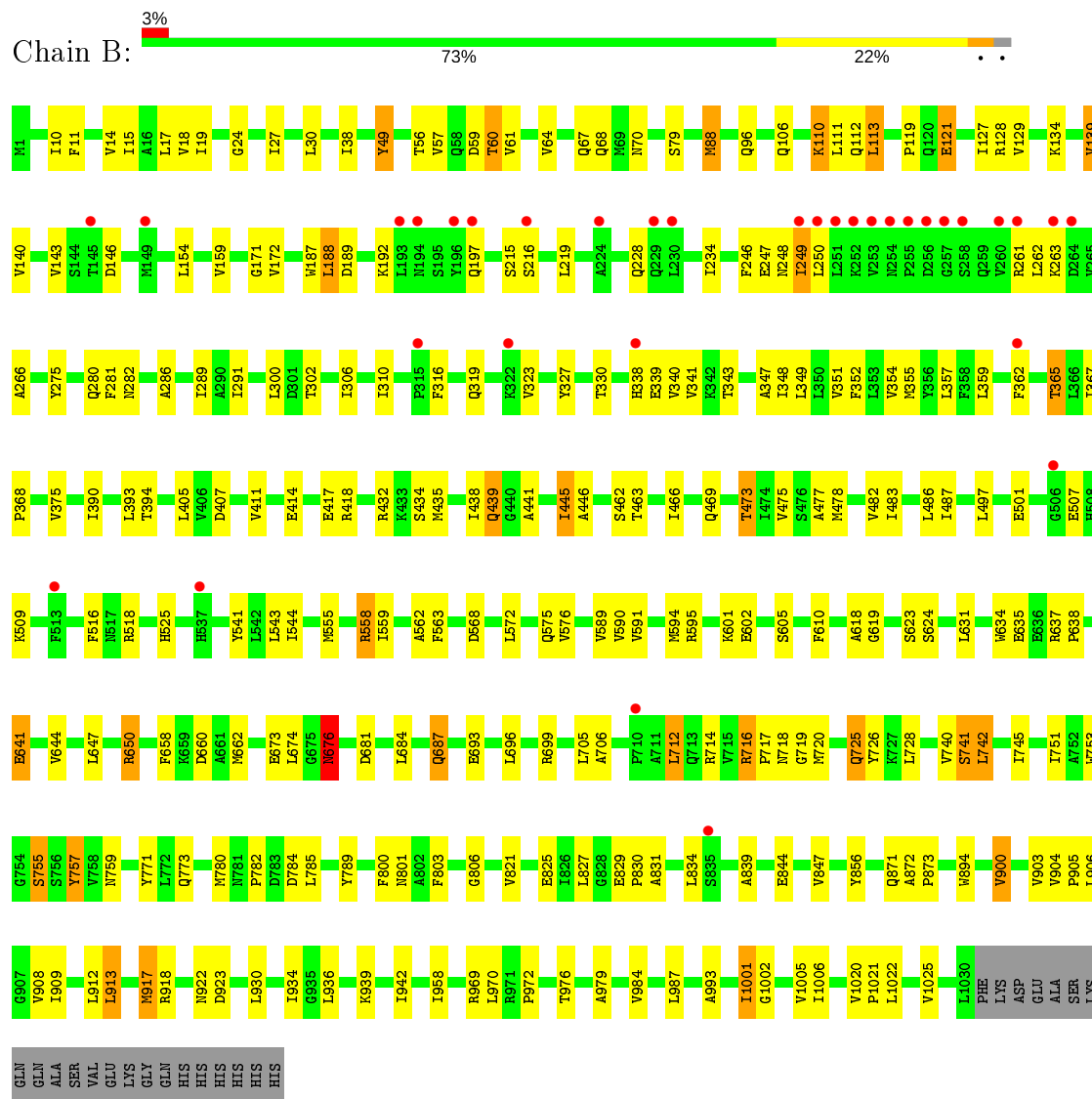
### 3 Residue-property plots [i](#)

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.

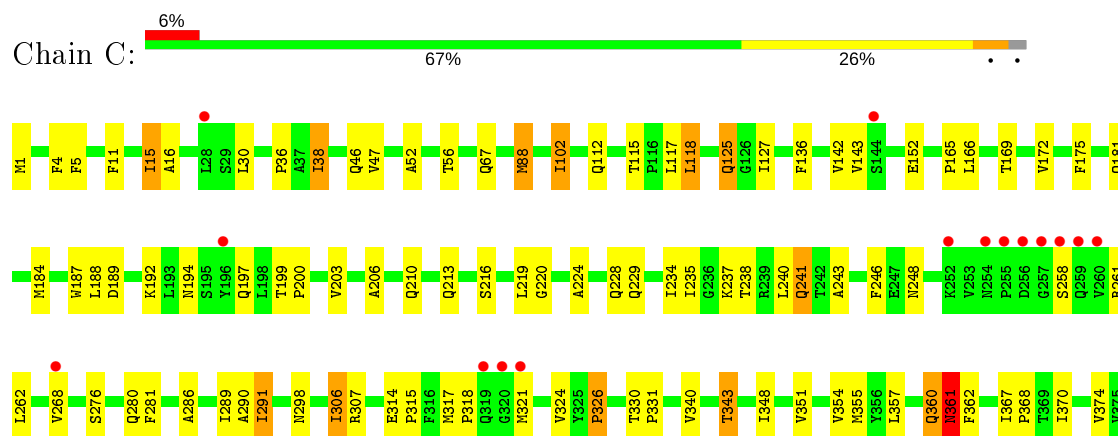
- Molecule 1: Multidrug resistance protein MexB

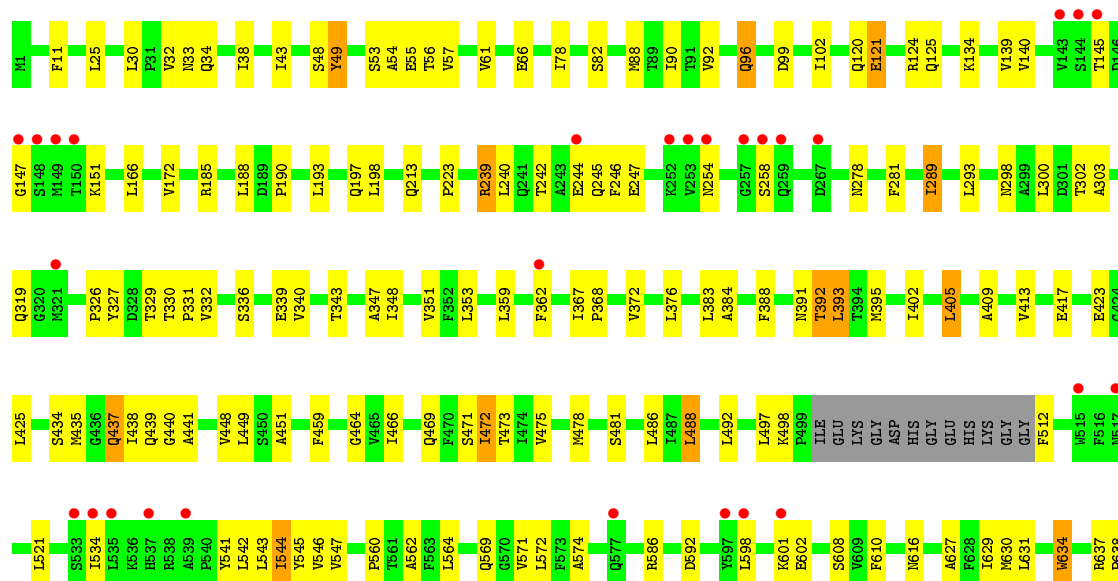
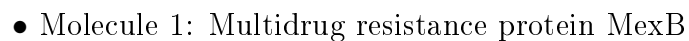


• Molecule 1: Multidrug resistance protein MexB

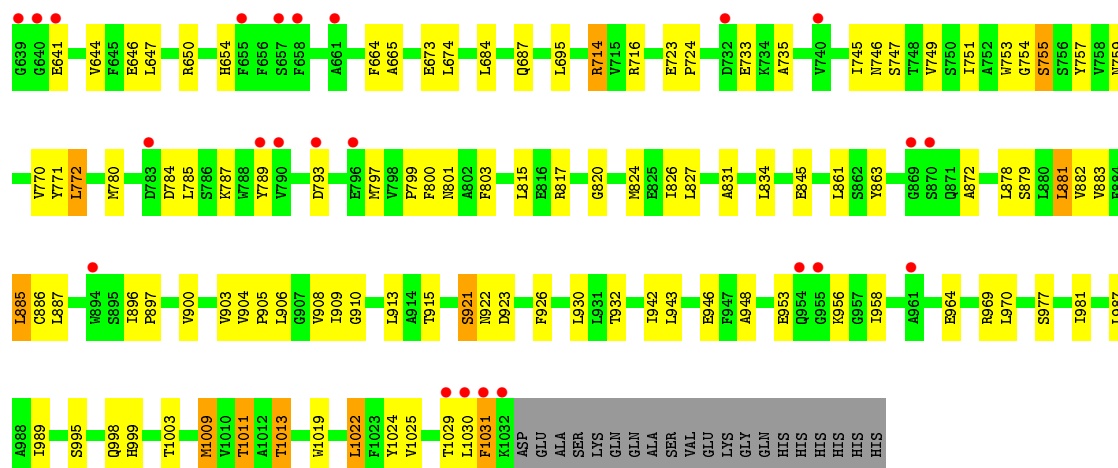


• Molecule 1: Multidrug resistance protein MexB

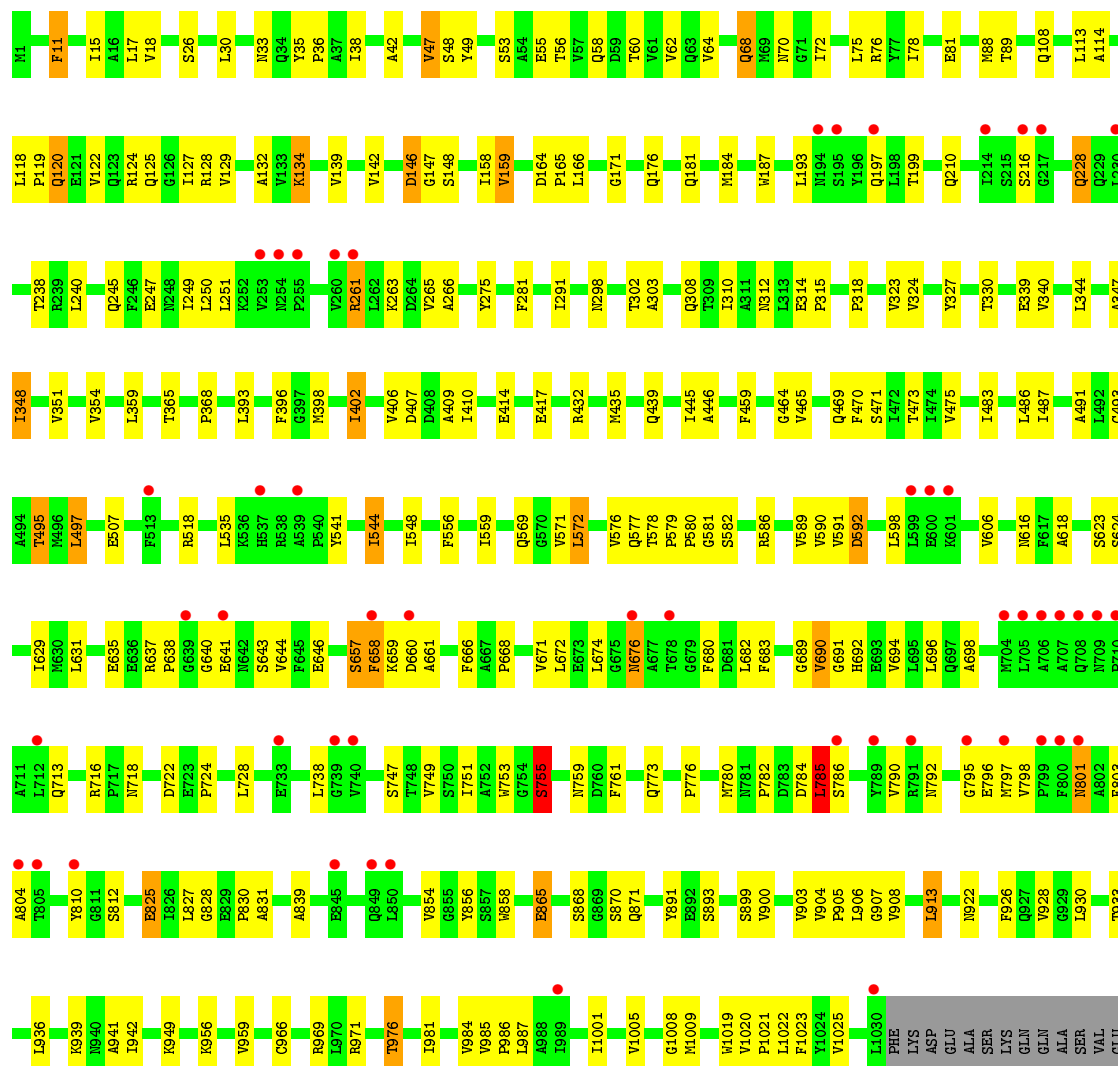








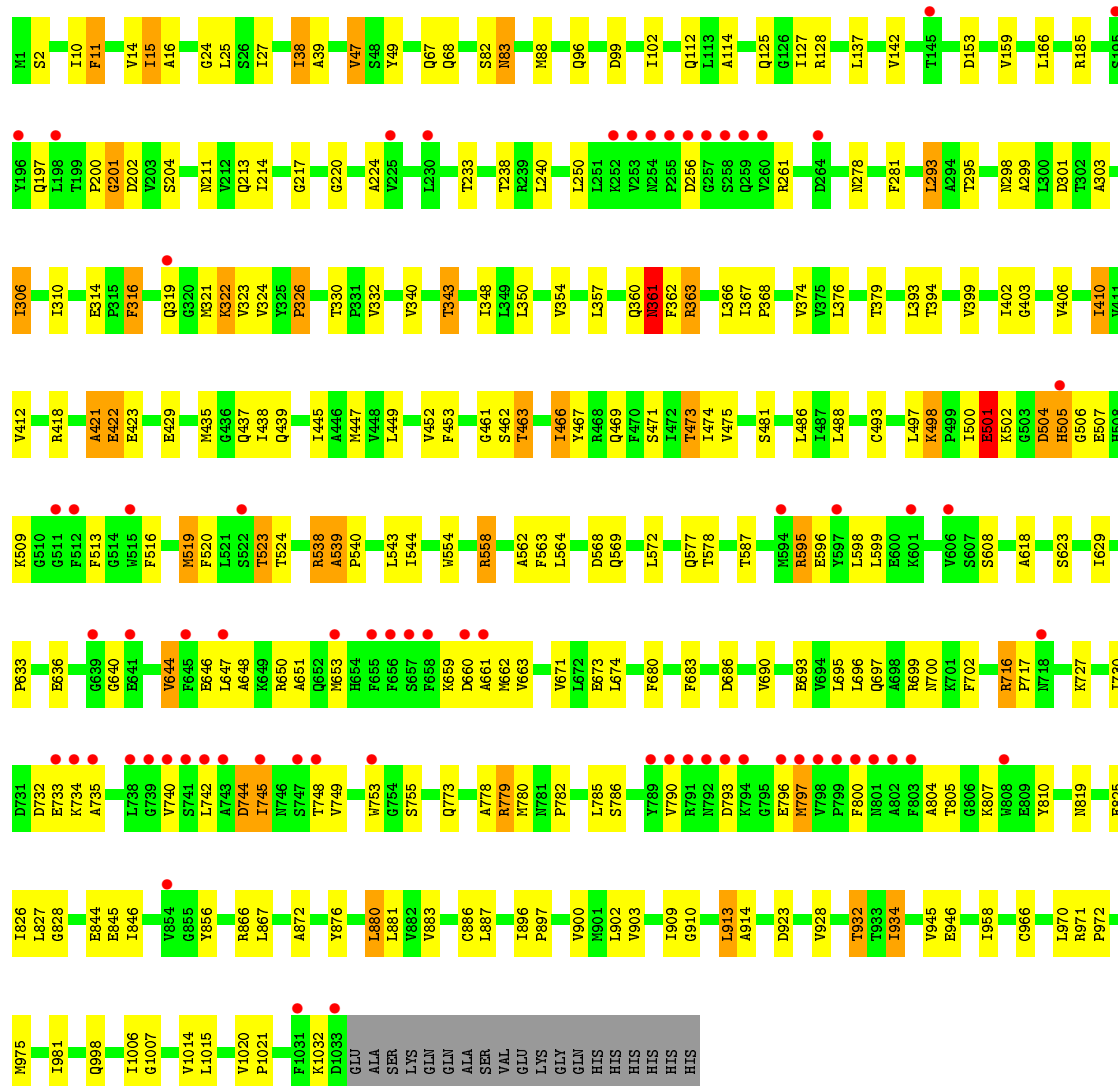
• Molecule 1: Multidrug resistance protein MexB



LYS  
GLY  
GLN  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

● Molecule 1: Multidrug resistance protein MexB

Chain F:  7% 73% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.95Å 134.34Å 149.69Å 87.53° 70.20° 89.02°	Depositor
Resolution (Å)	140.73 – 2.91 50.05 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.7 (140.73-2.91) 92.8 (50.05-2.91)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.234 , 0.278 0.234 , 0.275	Depositor DCC
$R_{free}$ test set	9196 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	46876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AV0

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	0.66	1/7873 (0.0%)	0.84	3/10701 (0.0%)
1	B	0.68	0/7971	0.86	0/10833
1	C	0.61	0/7971	0.81	0/10833
1	D	0.62	0/7901	0.80	0/10739
1	E	0.61	0/7971	0.79	1/10833 (0.0%)
1	F	0.61	0/8000	0.80	1/10871 (0.0%)
All	All	0.63	1/47687 (0.0%)	0.82	5/64810 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	TRP	CB-CG	-5.43	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	791	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	E	971	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	F	293	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	674	LEU	CA-CB-CG	5.01	126.83	115.30

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	7718	0	7858	167	0
1	B	7812	0	7944	131	0
1	C	7812	0	7944	183	0
1	D	7744	0	7886	129	0
1	E	7812	0	7944	147	0
1	F	7840	0	7970	136	0
2	B	69	0	0	1	0
2	E	69	0	0	0	0
All	All	46876	0	47546	858	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 9.

All (858) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HG	1:C:234:ILE:HD11	1.52	0.92
1:E:782:PRO:O	1:E:785:LEU:HG	1.75	0.86
1:E:142:VAL:HG21	1:E:158:ILE:HD11	1.57	0.84
1:B:56:THR:O	1:B:60:THR:HB	1.81	0.81
1:F:524:THR:HG22	1:F:970:LEU:HD12	1.61	0.81
1:C:354:VAL:HG21	1:C:982:LEU:HD23	1.63	0.80
1:D:34:GLN:O	1:D:392:THR:HG22	1.82	0.80
1:E:905:PRO:HA	1:E:908:VAL:HG12	1.64	0.79
1:D:471:SER:O	1:D:475:VAL:HG12	1.84	0.77
1:D:999:HIS:O	1:D:1003:THR:HG23	1.88	0.74
1:D:780:MET:HE1	1:F:224:ALA:HB1	1.69	0.74
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.68	0.74
1:D:541:TYR:HA	1:D:544:ILE:HG22	1.70	0.73
1:B:469:GLN:O	1:B:473:THR:HG22	1.88	0.73
1:C:447:MET:SD	1:C:886:CYS:HB3	2.29	0.72
1:D:780:MET:HE3	1:F:220:GLY:HA2	1.69	0.72
1:E:589:VAL:HA	1:E:592:ASP:HB2	1.72	0.72
1:D:293:LEU:CD1	1:D:302:THR:HG21	2.20	0.71
1:E:908:VAL:HG23	1:E:930:LEU:HD11	1.71	0.71
1:B:359:LEU:HD22	1:B:417:GLU:HG2	1.72	0.71
1:C:563:PHE:HB2	1:C:865:GLU:HG2	1.70	0.71
1:E:668:PRO:HB2	1:E:672:LEU:HD21	1.71	0.71
1:E:541:TYR:HA	1:E:544:ILE:HG22	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG11	1:B:405:LEU:HD11	1.72	0.71
1:E:146:ASP:O	1:E:148:SER:N	2.25	0.70
1:D:139:VAL:HG22	1:D:327:TYR:HB3	1.74	0.69
1:F:137:LEU:HD22	1:F:293:LEU:HD13	1.74	0.69
1:A:400:LEU:HD23	1:A:932:THR:HG21	1.75	0.68
1:A:875:LEU:HD21	1:A:931:LEU:HD11	1.74	0.68
1:B:650:ARG:HG2	1:B:650:ARG:HH11	1.58	0.68
1:A:310:ILE:HD13	1:A:323:VAL:HG11	1.75	0.68
1:B:541:TYR:HA	1:B:544:ILE:HG22	1.76	0.68
1:A:213:GLN:OE1	1:B:56:THR:HG22	1.95	0.67
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.75	0.67
1:C:717:PRO:HA	1:C:826:ILE:HG22	1.76	0.67
1:E:435:MET:O	1:E:439:GLN:HB2	1.95	0.67
1:F:38:ILE:HD12	1:F:671:VAL:HG11	1.77	0.67
1:E:193:LEU:HD13	1:E:265:VAL:HG13	1.77	0.66
1:F:340:VAL:HA	1:F:343:THR:HG23	1.78	0.66
1:A:918:ARG:HD2	1:A:920:LEU:HD11	1.78	0.66
1:E:187:TRP:O	1:E:266:ALA:HB1	1.96	0.66
1:A:38:ILE:O	1:A:96:GLN:NE2	2.29	0.66
1:D:1025:VAL:O	1:D:1029:THR:HG23	1.95	0.66
1:D:213:GLN:HB2	1:D:239:ARG:HG3	1.78	0.66
1:D:293:LEU:HD11	1:D:302:THR:HG21	1.77	0.65
1:C:46:GLN:HA	1:C:88:MET:HE3	1.76	0.65
1:C:910:GLY:O	1:C:1007:GLY:HA3	1.96	0.65
1:C:912:LEU:HD23	1:C:926:PHE:HZ	1.61	0.65
1:D:747:SER:O	1:D:751:ILE:HG12	1.96	0.65
1:E:159:VAL:HG21	1:E:181:GLN:HG3	1.78	0.65
1:D:343:THR:HG21	1:D:998:GLN:OE1	1.97	0.65
1:C:367:ILE:HD11	1:C:496:MET:HB2	1.78	0.65
1:E:359:LEU:HD22	1:E:417:GLU:HG2	1.80	0.64
1:C:306:ILE:HD13	1:C:307:ARG:N	2.12	0.64
1:C:471:SER:O	1:C:475:VAL:HG13	1.96	0.64
1:A:343:THR:HG21	1:A:998:GLN:OE1	1.97	0.64
1:F:928:VAL:O	1:F:932:THR:HG22	1.97	0.64
1:B:831:ALA:HB3	1:B:834:LEU:HD12	1.79	0.64
1:E:900:VAL:HG21	1:E:942:ILE:HG13	1.80	0.64
1:A:167:SER:HB3	1:B:70:ASN:CB	2.28	0.63
1:E:616:ASN:HD22	1:E:624:SER:HB3	1.64	0.63
1:D:120:GLN:O	1:D:124:ARG:HG3	1.99	0.63
1:E:491:ALA:O	1:E:495:THR:HB	1.97	0.63
1:A:780:MET:HE2	1:C:224:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ILE:HD11	1:E:75:LEU:HD12	1.81	0.62
1:B:900:VAL:O	1:B:903:VAL:HG22	1.99	0.62
1:D:684:LEU:HD11	1:D:826:ILE:HD12	1.80	0.62
1:B:681:ASP:OD2	1:B:825:GLU:OE2	2.17	0.62
1:A:574:ALA:HB3	1:A:627:ALA:HB3	1.82	0.61
1:F:82:SER:C	1:F:83:ASN:HD22	2.04	0.61
1:D:213:GLN:HG3	1:E:56:THR:HG22	1.81	0.61
1:E:108:GLN:HB3	1:E:129:VAL:HG11	1.83	0.61
1:C:966:CYS:SG	1:C:1021:PRO:HG3	2.39	0.61
1:E:247:GLU:HB3	1:E:263:LYS:HB3	1.83	0.61
1:C:187:TRP:HA	1:C:773:GLN:O	2.00	0.61
1:C:563:PHE:CD2	1:C:564:LEU:HD23	2.36	0.61
1:B:351:VAL:O	1:B:355:MET:HB2	2.01	0.60
1:F:38:ILE:HD11	1:F:674:LEU:HD11	1.83	0.60
1:B:362:PHE:O	1:B:365:THR:HG22	2.01	0.60
1:C:541:TYR:HA	1:C:544:ILE:HG22	1.84	0.60
1:C:966:CYS:SG	1:C:1021:PRO:CG	2.90	0.60
1:B:282:ASN:C	1:B:595:ARG:HD2	2.22	0.60
1:D:534:ILE:HG22	1:D:1022:LEU:HD23	1.84	0.60
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.84	0.60
1:C:115:THR:HA	1:C:118:LEU:HD22	1.82	0.59
1:E:683:PHE:CZ	1:E:825:GLU:HG2	2.37	0.59
1:A:710:PRO:O	1:A:831:ALA:HB2	2.01	0.59
1:A:918:ARG:NH2	1:A:988:ALA:O	2.35	0.59
1:C:665:ALA:O	1:C:714:ARG:NH1	2.35	0.59
1:A:928:VAL:O	1:A:932:THR:HG22	2.02	0.59
1:D:562:ALA:O	1:D:923:ASP:HA	2.01	0.59
1:E:11:PHE:CE1	1:E:15:ILE:HD11	2.36	0.59
1:F:732:ASP:HA	1:F:735:ALA:HB3	1.84	0.59
1:A:791:ARG:HG3	1:A:797:MET:HE2	1.83	0.59
1:A:713:GLN:O	1:A:714:ARG:CB	2.50	0.59
1:A:906:LEU:HD22	1:A:1015:LEU:HD23	1.84	0.59
1:C:197:GLN:HA	1:C:797:MET:SD	2.43	0.59
2:B:1101:AV0:OAQ	2:B:1101:AV0:OAI	2.19	0.59
1:C:340:VAL:HA	1:C:343:THR:HG23	1.85	0.59
1:E:64:VAL:CG2	1:E:118:LEU:HD23	2.33	0.59
1:E:900:VAL:HG23	1:E:941:ALA:HB3	1.85	0.59
1:F:539:ALA:HB3	1:F:540:PRO:CD	2.32	0.58
1:B:139:VAL:CG1	1:B:327:TYR:HB3	2.33	0.58
1:C:402:ILE:HD12	1:C:403:GLY:H	1.69	0.58
1:C:181:GLN:OE1	1:C:766:ARG:NH1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:LEU:O	1:C:357:LEU:HD23	2.04	0.58
1:F:572:LEU:HB3	1:F:629:ILE:HB	1.86	0.58
1:A:918:ARG:NE	1:A:1003:THR:HG21	2.19	0.57
1:D:57:VAL:HG13	1:D:82:SER:HB3	1.85	0.57
1:F:500:ILE:O	1:F:501:GLU:O	2.23	0.57
1:B:913:LEU:O	1:B:917:MET:HB2	2.04	0.57
1:C:887:LEU:CD1	1:C:900:VAL:HG21	2.34	0.57
1:F:782:PRO:O	1:F:785:LEU:HG	2.05	0.57
1:A:791:ARG:HD3	1:A:797:MET:HE1	1.85	0.57
1:C:206:ALA:O	1:C:210:GLN:HG3	2.04	0.57
1:F:696:LEU:O	1:F:700:ASN:ND2	2.37	0.57
1:C:47:VAL:HG22	1:C:127:ILE:HG13	1.87	0.57
1:E:471:SER:O	1:E:475:VAL:HG12	2.05	0.57
1:E:785:LEU:HD22	1:E:804:ALA:HB1	1.87	0.57
1:F:461:GLY:HA3	1:F:867:LEU:HD21	1.87	0.57
1:A:293:LEU:HD11	1:A:302:THR:HG21	1.85	0.57
1:B:441:ALA:O	1:B:445:ILE:HG23	2.05	0.57
1:C:415:ASN:HB3	1:C:434:SER:OG	2.05	0.57
1:E:680:PHE:HB2	1:E:858:TRP:CZ3	2.40	0.57
1:D:637:ARG:N	1:D:638:PRO:HD3	2.20	0.56
1:D:977:SER:HB3	1:D:1013:THR:HG21	1.86	0.56
1:C:241:GLN:HG3	1:C:762:ILE:O	2.06	0.56
1:D:38:ILE:O	1:D:96:GLN:NE2	2.38	0.56
1:E:251:LEU:HD22	1:E:265:VAL:HG21	1.87	0.56
1:C:246:PHE:O	1:C:262:LEU:HD23	2.05	0.56
1:C:501:GLU:O	1:C:504:ASP:HB2	2.05	0.56
1:D:906:LEU:O	1:D:1011:THR:HB	2.05	0.56
1:E:689:GLY:O	1:E:691:GLY:N	2.38	0.56
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.86	0.56
1:D:745:ILE:O	1:D:749:VAL:HG23	2.05	0.56
1:E:303:ALA:HB2	1:E:330:THR:HG21	1.86	0.56
1:A:554:TRP:CH2	1:A:558:ARG:HD2	2.40	0.56
1:F:412:VAL:HG13	1:F:435:MET:HE1	1.86	0.56
1:D:78:ILE:HD13	1:D:92:VAL:HG22	1.87	0.56
1:A:428:ARG:HG3	1:A:494:ALA:HB1	1.88	0.56
1:C:172:VAL:HG22	1:C:291:ILE:HD12	1.88	0.56
1:C:598:LEU:HD23	1:C:606:VAL:HG21	1.88	0.56
1:F:568:ASP:OD1	1:F:644:VAL:HG22	2.05	0.56
1:F:844:GLU:OE2	1:F:866:ARG:NH2	2.39	0.56
1:B:740:VAL:HG21	1:B:745:ILE:HD11	1.87	0.56
1:D:197:GLN:HA	1:D:797:MET:SD	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ALA:O	1:D:351:VAL:HG23	2.06	0.55
1:D:124:ARG:NH2	1:D:757:TYR:CD2	2.74	0.55
1:F:896:ILE:HG13	1:F:945:VAL:CG1	2.36	0.55
1:A:456:MET:CE	1:A:931:LEU:HD12	2.36	0.55
1:D:240:LEU:HD22	1:D:245:GLN:HG2	1.88	0.55
1:F:1014:VAL:HG23	1:F:1015:LEU:HD22	1.88	0.55
1:A:303:ALA:CB	1:A:330:THR:HG21	2.37	0.55
1:A:780:MET:SD	1:C:220:GLY:HA2	2.47	0.55
1:E:75:LEU:HD23	1:E:76:ARG:N	2.20	0.55
1:F:159:VAL:O	1:F:159:VAL:HG12	2.06	0.55
1:B:407:ASP:OD1	1:B:976:THR:HG21	2.06	0.55
1:E:598:LEU:HD12	1:E:606:VAL:HG21	1.87	0.55
1:C:706:ALA:HB1	1:C:715:VAL:HG21	1.87	0.55
1:E:900:VAL:O	1:E:903:VAL:HG22	2.07	0.55
1:F:2:SER:HB3	1:F:435:MET:HG3	1.88	0.55
1:C:370:ILE:O	1:C:374:VAL:HG12	2.07	0.55
1:D:574:ALA:HB3	1:D:627:ALA:HB3	1.87	0.55
1:C:543:LEU:O	1:C:547:VAL:HG23	2.07	0.55
1:D:242:THR:OG1	1:D:245:GLN:HB2	2.06	0.55
1:A:940:ASN:HD21	1:A:976:THR:HG21	1.72	0.54
1:C:910:GLY:O	1:C:1007:GLY:CA	2.55	0.54
1:E:469:GLN:O	1:E:473:THR:HG22	2.06	0.54
1:E:690:VAL:CG1	1:E:694:VAL:HB	2.37	0.54
1:F:27:ILE:O	1:F:27:ILE:HG22	2.06	0.54
1:B:375:VAL:CG1	1:B:405:LEU:HD11	2.35	0.54
1:F:745:ILE:HG22	1:F:790:VAL:HG11	1.89	0.54
1:A:382:VAL:HG21	1:A:476:SER:OG	2.08	0.54
1:A:713:GLN:O	1:A:714:ARG:HB2	2.07	0.54
1:A:112:GLN:HG3	1:B:112:GLN:OE1	2.08	0.54
1:C:376:LEU:HA	1:C:379:THR:HG22	1.90	0.54
1:D:376:LEU:HD11	1:D:402:ILE:CD1	2.38	0.54
1:F:538:ARG:CG	1:F:538:ARG:HH11	2.20	0.54
1:C:520:PHE:HA	1:C:523:THR:HG22	1.88	0.54
1:F:504:ASP:O	1:F:506:GLY:O	2.26	0.54
1:B:463:THR:HG22	1:B:563:PHE:HE1	1.73	0.54
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.90	0.54
1:C:686:ASP:HA	1:C:854:VAL:HA	1.90	0.54
1:D:448:VAL:HG22	1:D:886:CYS:HB3	1.90	0.54
1:F:572:LEU:HD11	1:F:648:ALA:HB2	1.90	0.54
1:A:277:ILE:HD12	1:A:615:PHE:HB2	1.89	0.54
1:B:958:ILE:HG22	1:B:1025:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:LEU:HD21	1:C:516:PHE:CZ	2.43	0.54
1:C:727:LYS:HG2	1:C:729:GLU:HG2	1.90	0.54
1:A:410:ILE:HA	1:A:413:VAL:HG12	1.89	0.53
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.91	0.53
1:F:683:PHE:CE1	1:F:825:GLU:HB2	2.43	0.53
1:C:280:GLN:HB2	1:C:611:THR:HG22	1.91	0.53
1:E:576:VAL:HG21	1:E:591:VAL:HG12	1.91	0.53
1:D:298:ASN:O	1:D:302:THR:HG22	2.07	0.53
1:D:684:LEU:CD1	1:D:826:ILE:HD12	2.37	0.53
1:F:520:PHE:O	1:F:524:THR:HG23	2.08	0.53
1:F:362:PHE:O	1:F:363:ARG:HB2	2.09	0.53
1:B:631:LEU:CD1	1:B:644:VAL:HG22	2.39	0.53
1:E:171:GLY:HA3	1:E:302:THR:HG22	1.91	0.53
1:F:410:ILE:C	1:F:410:ILE:HD12	2.27	0.53
1:A:57:VAL:HG21	1:A:88:MET:HB3	1.91	0.53
1:C:357:LEU:C	1:C:357:LEU:HD23	2.29	0.53
1:C:788:TRP:O	1:C:800:PHE:HB2	2.09	0.53
1:E:747:SER:O	1:E:751:ILE:HG12	2.09	0.53
1:B:745:ILE:HD12	1:B:803:PHE:CZ	2.44	0.53
1:D:193:LEU:HG	1:D:198:LEU:O	2.08	0.53
1:F:452:VAL:HG22	1:F:883:VAL:HG21	1.91	0.53
1:B:139:VAL:HG13	1:B:327:TYR:HB3	1.90	0.53
1:A:791:ARG:HG3	1:A:797:MET:CE	2.40	0.52
1:B:70:ASN:O	1:B:110:LYS:HD2	2.09	0.52
1:C:984:VAL:HG12	1:C:987:LEU:HD12	1.91	0.52
1:E:310:ILE:CG2	1:E:323:VAL:HG21	2.39	0.52
1:E:905:PRO:HA	1:E:908:VAL:CG1	2.38	0.52
1:A:167:SER:HB3	1:B:70:ASN:HB2	1.92	0.52
1:A:1024:TYR:O	1:A:1028:SER:HB2	2.09	0.52
1:A:763:ASP:HB3	1:A:768:LYS:HD3	1.91	0.52
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.90	0.52
1:C:189:ASP:HB3	1:C:192:LYS:HB2	1.90	0.52
1:A:780:MET:CE	1:C:224:ALA:HB1	2.39	0.52
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.92	0.52
1:B:987:LEU:HD13	1:B:1001:ILE:HD12	1.91	0.52
1:A:562:ALA:O	1:A:923:ASP:HA	2.10	0.52
1:C:713:GLN:HG2	1:C:714:ARG:HG3	1.92	0.52
1:C:142:VAL:O	1:C:286:ALA:HB1	2.10	0.52
1:F:749:VAL:HA	1:F:753:TRP:CE3	2.45	0.52
1:D:753:TRP:CZ2	1:D:785:LEU:HG	2.45	0.52
1:F:702:PHE:CE2	1:F:826:ILE:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:CG	1:A:239:ARG:HH11	2.23	0.52
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.92	0.52
1:A:690:VAL:HG21	1:A:694:VAL:HB	1.91	0.52
1:C:5:PHE:CD2	1:C:487:ILE:HG23	2.45	0.52
1:D:240:LEU:HB2	1:D:246:PHE:CZ	2.45	0.52
1:D:449:LEU:HD12	1:D:478:MET:HG3	1.92	0.52
1:A:339:GLU:O	1:A:343:THR:HG23	2.10	0.52
1:C:469:GLN:O	1:C:473:THR:HG23	2.10	0.52
1:C:189:ASP:HA	1:C:775:ARG:HD3	1.91	0.52
1:C:816:GLU:OE1	1:C:824:MET:HA	2.10	0.52
1:A:348:ILE:HD12	1:A:372:VAL:HG11	1.91	0.51
1:D:754:GLY:O	1:D:755:SER:CB	2.58	0.51
1:D:78:ILE:HD11	1:D:90:ILE:CG2	2.40	0.51
1:A:959:VAL:O	1:A:963:ILE:HG12	2.11	0.51
1:C:36:PRO:O	1:C:38:ILE:HG23	2.11	0.51
1:C:451:ALA:HB1	1:C:882:VAL:HG12	1.92	0.51
1:C:934:ILE:C	1:C:934:ILE:HD13	2.29	0.51
1:D:48:SER:O	1:D:125:GLN:HG2	2.11	0.51
1:E:108:GLN:CB	1:E:129:VAL:HG11	2.40	0.51
1:F:516:PHE:O	1:F:519:MET:HG3	2.09	0.51
1:B:740:VAL:CG2	1:B:745:ILE:HD11	2.39	0.51
1:E:713:GLN:HE21	1:E:831:ALA:HA	1.75	0.51
1:E:535:LEU:HD22	1:E:1025:VAL:HG21	1.92	0.51
1:B:631:LEU:HD12	1:B:644:VAL:HG22	1.93	0.51
1:C:544:ILE:O	1:C:547:VAL:HB	2.11	0.51
1:C:169:THR:HB	1:C:172:VAL:CG2	2.41	0.51
1:C:565:PRO:HG3	1:C:997:SER:HA	1.91	0.51
1:D:749:VAL:HG22	1:D:753:TRP:HZ3	1.76	0.51
1:F:578:THR:HG21	1:F:587:THR:HA	1.91	0.51
1:B:1002:GLY:O	1:B:1006:ILE:HG12	2.11	0.51
1:B:753:TRP:CZ2	1:B:785:LEU:HB3	2.46	0.51
1:C:964:GLU:O	1:C:968:MET:HG3	2.11	0.51
1:D:1009:MET:O	1:D:1013:THR:HG22	2.10	0.51
1:D:831:ALA:HB3	1:D:834:LEU:HD12	1.92	0.51
1:F:717:PRO:HA	1:F:826:ILE:HG22	1.93	0.51
1:A:1009:MET:O	1:A:1013:THR:HG23	2.11	0.51
1:A:101:ASP:O	1:A:105:VAL:HG23	2.11	0.51
1:C:928:VAL:O	1:C:932:THR:HG22	2.10	0.51
1:B:930:LEU:O	1:B:934:ILE:HG23	2.11	0.51
1:F:211:ASN:HA	1:F:240:LEU:HD13	1.91	0.51
1:C:592:ASP:O	1:C:595:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:943:LEU:HD13	1:D:969:ARG:HH21	1.76	0.51
1:F:498:LYS:H	1:F:498:LYS:HE3	1.76	0.51
1:A:969:ARG:O	1:A:973:ILE:HG12	2.11	0.50
1:C:933:THR:HA	1:C:936:LEU:HD12	1.92	0.50
1:D:735:ALA:HB2	1:D:803:PHE:HB2	1.91	0.50
1:F:966:CYS:SG	1:F:1021:PRO:HG3	2.51	0.50
1:A:140:VAL:HB	1:A:289:ILE:CD1	2.41	0.50
1:B:751:ILE:HG22	1:B:751:ILE:O	2.11	0.50
1:C:572:LEU:HD12	1:C:666:PHE:O	2.11	0.50
1:D:213:GLN:HE21	1:E:56:THR:HG22	1.75	0.50
1:F:469:GLN:O	1:F:473:THR:CG2	2.60	0.50
1:A:233:THR:HB	1:B:725:GLN:HB3	1.94	0.50
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.76	0.50
1:A:702:PHE:HZ	1:A:843:VAL:HG13	1.77	0.50
1:B:741:SER:O	1:B:742:LEU:HB2	2.11	0.50
1:C:1020:VAL:HB	1:C:1021:PRO:HD3	1.93	0.50
1:C:682:LEU:HD21	1:C:826:ILE:HG13	1.93	0.50
1:F:554:TRP:CZ2	1:F:558:ARG:HD3	2.46	0.50
1:F:99:ASP:HB3	1:F:102:ILE:HG12	1.94	0.50
1:E:483:ILE:HG22	1:E:487:ILE:HD12	1.91	0.50
1:F:733:GLU:HG3	1:F:734:LYS:HG2	1.94	0.50
1:C:922:ASN:OD1	1:C:926:PHE:HD2	1.94	0.50
1:A:598:LEU:O	1:A:602:GLU:HB2	2.12	0.50
1:A:664:PHE:CE1	1:A:714:ARG:HD3	2.46	0.50
1:A:931:LEU:C	1:A:933:THR:H	2.14	0.50
1:A:725:GLN:OE1	1:C:235:ILE:HD11	2.12	0.50
1:D:140:VAL:HB	1:D:289:ILE:HG13	1.93	0.50
1:D:910:GLY:HA3	1:D:1011:THR:OG1	2.12	0.50
1:E:240:LEU:HD22	1:E:245:GLN:HB3	1.93	0.50
1:F:99:ASP:O	1:F:102:ILE:HG12	2.11	0.50
1:F:303:ALA:HA	1:F:306:ILE:HG22	1.92	0.50
1:C:219:LEU:CG	1:C:234:ILE:HD11	2.35	0.50
1:C:782:PRO:O	1:C:785:LEU:HG	2.11	0.50
1:D:244:GLU:HA	1:D:247:GLU:HG2	1.93	0.50
1:E:680:PHE:CZ	1:E:828:GLY:HA3	2.46	0.50
1:F:910:GLY:O	1:F:1007:GLY:HA3	2.11	0.50
1:A:234:ILE:HG23	1:B:728:LEU:HD23	1.93	0.50
1:E:435:MET:O	1:E:439:GLN:CB	2.59	0.50
1:E:755:SER:HA	1:E:773:GLN:HB3	1.93	0.50
1:E:407:ASP:OD1	1:E:976:THR:HG21	2.11	0.50
1:A:310:ILE:HG13	1:A:311:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:GLU:HA	1:C:317:MET:SD	2.52	0.49
1:E:692:HIS:CE1	1:E:812:SER:OG	2.65	0.49
1:A:451:ALA:HB1	1:A:882:VAL:HG12	1.95	0.49
1:B:872:ALA:HB3	1:B:873:PRO:HD3	1.94	0.49
1:D:488:LEU:HD22	1:D:492:LEU:HG	1.93	0.49
1:E:298:ASN:O	1:E:302:THR:HG23	2.12	0.49
1:E:507:GLU:O	1:E:518:ARG:NH1	2.45	0.49
1:F:393:LEU:HD13	1:F:466:ILE:HB	1.94	0.49
1:A:456:MET:HE3	1:A:931:LEU:HD12	1.94	0.49
1:F:367:ILE:HB	1:F:368:PRO:CD	2.41	0.49
1:F:773:GLN:HG2	1:F:779:ARG:HH12	1.78	0.49
1:A:345:GLY:HA2	1:A:348:ILE:HG22	1.94	0.49
1:D:185:ARG:HH11	1:D:771:TYR:HB2	1.78	0.49
1:E:303:ALA:CB	1:E:330:THR:HG21	2.42	0.49
1:E:586:ARG:O	1:E:590:VAL:HG23	2.13	0.49
1:E:62:VAL:HG22	1:E:88:MET:CE	2.43	0.49
1:F:903:VAL:CG2	1:F:1020:VAL:HG22	2.43	0.49
1:E:493:CYS:HA	1:E:497:LEU:HD22	1.95	0.49
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.93	0.49
1:B:637:ARG:N	1:B:638:PRO:HD3	2.26	0.49
1:C:702:PHE:CD2	1:C:826:ILE:HD12	2.47	0.49
1:C:248:ASN:HA	1:C:261:ARG:HD3	1.93	0.49
1:C:448:VAL:O	1:C:452:VAL:HG23	2.13	0.49
1:D:746:ASN:OD1	1:F:214:ILE:HD13	2.13	0.49
1:A:555:MET:HB2	1:A:912:LEU:HD13	1.94	0.49
1:A:57:VAL:HG13	1:A:82:SER:HB3	1.95	0.49
1:A:791:ARG:CG	1:A:797:MET:CE	2.91	0.49
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.43	0.49
1:C:745:ILE:HG22	1:C:790:VAL:HG21	1.94	0.49
1:C:929:GLY:HA2	1:C:932:THR:HG23	1.95	0.49
1:E:966:CYS:SG	1:E:1021:PRO:HG3	2.53	0.49
1:F:47:VAL:HG22	1:F:127:ILE:HG23	1.95	0.49
1:C:314:GLU:N	1:C:315:PRO:HD2	2.27	0.49
1:F:716:ARG:NH1	1:F:827:LEU:HB2	2.27	0.49
1:A:746:ASN:HD21	1:C:237:LYS:HD2	1.78	0.48
1:A:718:ASN:HB2	1:A:827:LEU:HD22	1.95	0.48
1:C:410:ILE:C	1:C:410:ILE:HD12	2.33	0.48
1:C:598:LEU:CD2	1:C:606:VAL:HG21	2.43	0.48
1:E:164:ASP:HB3	1:E:165:PRO:HD3	1.95	0.48
1:B:631:LEU:HD21	1:B:647:LEU:CD2	2.43	0.48
1:C:420:MET:HG3	1:C:425:LEU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:LEU:O	1:F:453:PHE:HD2	1.96	0.48
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.48	0.48
1:A:727:LYS:HD3	1:A:809:GLU:OE1	2.12	0.48
1:B:568:ASP:OD1	1:B:644:VAL:HG23	2.13	0.48
1:C:453:PHE:HZ	1:C:932:THR:HB	1.78	0.48
1:E:984:VAL:HG11	1:E:1005:VAL:HG21	1.95	0.48
1:D:754:GLY:HA2	1:F:217:GLY:HA2	1.94	0.48
1:F:343:THR:HG21	1:F:998:GLN:OE1	2.13	0.48
1:A:782:PRO:HA	1:A:785:LEU:HD13	1.95	0.48
1:B:1020:VAL:N	1:B:1021:PRO:HD2	2.27	0.48
1:C:393:LEU:HD13	1:C:466:ILE:HB	1.95	0.48
1:E:801:ASN:HA	1:E:804:ALA:HB2	1.96	0.48
1:C:910:GLY:O	1:C:1007:GLY:C	2.51	0.48
1:D:329:THR:O	1:D:332:VAL:HG12	2.13	0.48
1:B:171:GLY:HA3	1:B:302:THR:HG22	1.95	0.48
1:C:399:VAL:O	1:C:402:ILE:HG13	2.14	0.48
1:D:376:LEU:HD11	1:D:402:ILE:HD11	1.95	0.48
1:D:409:ALA:O	1:D:413:VAL:HG12	2.14	0.48
1:D:896:ILE:N	1:D:897:PRO:HD2	2.29	0.48
1:F:453:PHE:CE2	1:F:474:ILE:HG21	2.49	0.48
1:A:611:THR:HG22	1:A:627:ALA:HB2	1.95	0.48
1:C:801:ASN:HA	1:C:804:ALA:HB2	1.96	0.48
1:C:862:SER:O	1:C:865:GLU:HB2	2.14	0.48
1:D:188:LEU:HD13	1:D:772:LEU:HD21	1.96	0.48
1:E:347:ALA:O	1:E:351:VAL:HG23	2.14	0.48
1:A:984:VAL:HG11	1:A:1005:VAL:CG2	2.44	0.48
1:C:563:PHE:O	1:C:923:ASP:HB2	2.13	0.48
1:D:49:TYR:CE2	1:D:121:GLU:HG3	2.49	0.48
1:D:326:PRO:HB3	1:D:610:PHE:HB2	1.95	0.48
1:F:577:GLN:HB3	1:F:662:MET:HB2	1.94	0.48
1:A:228:GLN:NE2	1:B:780:MET:HB3	2.29	0.48
1:A:663:VAL:O	1:A:663:VAL:HG12	2.14	0.48
1:A:792:ASN:HD21	1:A:796:GLU:HB2	1.79	0.48
1:B:618:ALA:HB1	1:B:718:ASN:O	2.13	0.48
1:C:453:PHE:CE2	1:C:474:ILE:HG21	2.49	0.48
1:C:884:PHE:CD1	1:C:897:PRO:HB2	2.49	0.48
1:D:124:ARG:NH2	1:D:757:TYR:O	2.47	0.48
1:F:406:VAL:O	1:F:410:ILE:HG23	2.14	0.48
1:F:539:ALA:HB3	1:F:540:PRO:HD3	1.95	0.48
1:A:900:VAL:O	1:A:903:VAL:HG22	2.14	0.48
1:B:905:PRO:HA	1:B:908:VAL:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LEU:HD13	1:C:200:PRO:HB3	1.95	0.48
1:F:702:PHE:CE2	1:F:826:ILE:CD1	2.97	0.48
1:C:393:LEU:CD1	1:C:466:ILE:HB	2.44	0.47
1:C:942:ILE:HD12	1:C:942:ILE:C	2.34	0.47
1:E:36:PRO:HG2	1:E:38:ILE:HD13	1.97	0.47
1:E:445:ILE:HG13	1:E:446:ALA:N	2.29	0.47
1:E:749:VAL:O	1:E:753:TRP:HB2	2.14	0.47
1:F:39:ALA:HB2	1:F:673:GLU:HB3	1.94	0.47
1:F:520:PHE:HA	1:F:523:THR:HG22	1.96	0.47
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.96	0.47
1:A:738:LEU:HD23	1:A:798:VAL:HG11	1.94	0.47
1:D:336:SER:O	1:D:340:VAL:HG23	2.12	0.47
1:C:199:THR:HB	1:C:200:PRO:HD2	1.96	0.47
1:D:915:THR:HG21	1:D:926:PHE:CD1	2.49	0.47
1:E:127:ILE:HD12	1:E:127:ILE:N	2.30	0.47
1:E:579:PRO:HD3	1:E:660:ASP:O	2.13	0.47
1:E:792:ASN:HD21	1:E:796:GLU:HB2	1.79	0.47
1:B:478:MET:O	1:B:482:VAL:HG23	2.14	0.47
1:E:578:THR:HG22	1:E:661:ALA:HB2	1.96	0.47
1:E:904:VAL:HB	1:E:905:PRO:HD3	1.96	0.47
1:E:984:VAL:HG13	1:E:987:LEU:HD12	1.96	0.47
1:C:648:ALA:HA	1:C:651:ALA:HB3	1.96	0.47
1:E:396:PHE:CD1	1:E:1001:ILE:HD11	2.50	0.47
1:C:15:ILE:HG13	1:C:16:ALA:N	2.28	0.47
1:C:896:ILE:HG13	1:C:945:VAL:CG1	2.44	0.47
1:E:132:ALA:O	1:E:134:LYS:HE3	2.15	0.47
1:A:47:VAL:HG22	1:A:48:SER:H	1.80	0.47
1:B:188:LEU:HA	1:B:266:ALA:HB2	1.96	0.47
1:B:829:GLU:HB2	1:B:830:PRO:HD2	1.96	0.47
1:C:330:THR:N	1:C:331:PRO:HD2	2.30	0.47
1:D:383:LEU:HD21	1:D:473:THR:HG22	1.96	0.47
1:E:199:THR:HG23	1:E:797:MET:HE3	1.96	0.47
1:B:972:PRO:O	1:B:976:THR:HG22	2.15	0.47
1:A:53:SER:O	1:A:56:THR:N	2.48	0.47
1:A:938:ALA:O	1:A:942:ILE:HG12	2.15	0.47
1:F:298:ASN:O	1:F:299:ALA:C	2.51	0.47
1:F:680:PHE:CZ	1:F:828:GLY:HA3	2.50	0.47
1:A:298:ASN:O	1:A:302:THR:HG23	2.15	0.47
1:A:488:LEU:HD22	1:A:492:LEU:HG	1.97	0.47
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.97	0.47
1:F:10:ILE:O	1:F:14:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:VAL:HG13	1:A:753:TRP:CE3	2.50	0.47
1:A:800:PHE:HA	1:A:803:PHE:CZ	2.50	0.47
1:C:596:GLU:O	1:C:598:LEU:N	2.48	0.47
1:C:757:TYR:OH	1:C:760:ASP:OD1	2.33	0.47
1:D:543:LEU:O	1:D:547:VAL:HG23	2.15	0.47
1:F:197:GLN:HA	1:F:797:MET:SD	2.55	0.47
1:A:535:LEU:HD12	1:A:963:ILE:HD11	1.96	0.46
1:C:693:GLU:HA	1:C:696:LEU:HD12	1.96	0.46
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.97	0.46
1:F:519:MET:O	1:F:523:THR:HB	2.15	0.46
1:F:733:GLU:HG3	1:F:734:LYS:N	2.30	0.46
1:B:463:THR:HG22	1:B:563:PHE:CE1	2.49	0.46
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.51	0.46
1:B:10:ILE:O	1:B:14:VAL:HG23	2.15	0.46
1:B:234:ILE:HG22	1:C:726:TYR:HB3	1.96	0.46
1:B:634:TRP:CE3	1:B:993:ALA:HB2	2.50	0.46
1:B:782:PRO:O	1:B:785:LEU:HG	2.16	0.46
1:B:908:VAL:HB	1:B:930:LEU:HD11	1.97	0.46
1:E:35:TYR:CE2	1:E:671:VAL:HG12	2.51	0.46
1:D:598:LEU:O	1:D:602:GLU:HB2	2.15	0.46
1:E:668:PRO:CB	1:E:672:LEU:HD21	2.44	0.46
1:A:112:GLN:HG3	1:B:112:GLN:CD	2.36	0.46
1:E:985:VAL:HB	1:E:986:PRO:HD3	1.97	0.46
1:F:321:MET:O	1:F:322:LYS:C	2.54	0.46
1:D:32:VAL:HG13	1:D:300:LEU:HD12	1.97	0.46
1:D:723:GLU:HB2	1:D:724:PRO:HD2	1.96	0.46
1:B:847:VAL:HG11	1:B:856:TYR:CE2	2.50	0.46
1:C:318:PRO:HD2	1:C:321:MET:SD	2.56	0.46
1:A:72:ILE:HD11	1:A:110:LYS:HG3	1.97	0.46
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.51	0.46
1:C:169:THR:HB	1:C:172:VAL:HG21	1.98	0.46
1:D:909:ILE:HG13	1:D:1011:THR:HG21	1.97	0.46
1:A:188:LEU:HD13	1:A:772:LEU:HD11	1.96	0.46
1:A:75:LEU:HD23	1:A:75:LEU:C	2.35	0.46
1:B:507:GLU:O	1:B:518:ARG:NH1	2.48	0.46
1:C:430:ALA:O	1:C:434:SER:HB2	2.16	0.46
1:E:577:GLN:NE2	1:E:624:SER:OG	2.49	0.46
1:A:738:LEU:HD23	1:A:798:VAL:CG1	2.46	0.46
1:C:1009:MET:HA	1:C:1009:MET:HE3	1.98	0.46
1:D:641:GLU:HA	1:D:646:GLU:HG2	1.98	0.46
1:D:757:TYR:HB2	1:D:771:TYR:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLU:CB	1:A:425:LEU:HD13	2.46	0.45
1:C:752:ALA:HB3	1:C:753:TRP:CE3	2.52	0.45
1:E:171:GLY:HA3	1:E:302:THR:CG2	2.46	0.45
1:E:535:LEU:HD13	1:E:959:VAL:HG23	1.98	0.45
1:E:631:LEU:CD1	1:E:644:VAL:HG22	2.46	0.45
1:F:539:ALA:CB	1:F:540:PRO:CD	2.94	0.45
1:A:791:ARG:HD3	1:A:797:MET:CE	2.45	0.45
1:B:984:VAL:HG21	1:B:1005:VAL:HG21	1.99	0.45
1:B:830:PRO:HB3	1:B:839:ALA:HB2	1.99	0.45
1:D:569:GLN:N	1:D:634:TRP:HH2	2.14	0.45
1:E:166:LEU:HD21	1:E:291:ILE:HD11	1.98	0.45
1:E:631:LEU:HD11	1:E:644:VAL:HG22	1.98	0.45
1:F:447:MET:HE3	1:F:886:CYS:HB3	1.99	0.45
1:F:453:PHE:HZ	1:F:932:THR:HB	1.81	0.45
1:F:693:GLU:O	1:F:697:GLN:HG2	2.17	0.45
1:A:918:ARG:HE	1:A:1003:THR:HG21	1.82	0.45
1:A:445:ILE:HD12	1:A:446:ALA:N	2.31	0.45
1:B:247:GLU:HB3	1:B:263:LYS:HB3	1.98	0.45
1:C:524:THR:HG22	1:C:970:LEU:HD12	1.98	0.45
1:D:881:LEU:HD22	1:D:885:LEU:HD22	1.98	0.45
1:E:643:SER:HB3	1:E:646:GLU:HG2	1.98	0.45
1:E:657:SER:O	1:E:658:PHE:C	2.55	0.45
1:F:421:ALA:O	1:F:423:GLU:N	2.50	0.45
1:A:465:VAL:O	1:A:469:GLN:HG2	2.16	0.45
1:A:554:TRP:CZ2	1:A:558:ARG:HD2	2.52	0.45
1:A:847:VAL:HG23	1:A:850:LEU:HD12	1.97	0.45
1:C:188:LEU:HD21	1:C:203:VAL:HG11	1.97	0.45
1:F:201:GLY:O	1:F:204:SER:N	2.48	0.45
1:F:402:ILE:HD12	1:F:403:GLY:H	1.81	0.45
1:F:872:ALA:HB1	1:F:876:TYR:CE2	2.51	0.45
1:A:538:ARG:HG3	1:A:1022:LEU:HD21	1.98	0.45
1:A:156:ASN:OD1	1:A:768:LYS:NZ	2.48	0.45
1:C:584:ALA:O	1:C:588:GLN:HB2	2.16	0.45
1:D:244:GLU:HA	1:D:247:GLU:CG	2.46	0.45
1:D:534:ILE:HG23	1:D:541:TYR:CG	2.51	0.45
1:E:569:GLN:O	1:E:571:VAL:N	2.46	0.45
1:E:922:ASN:HD22	1:E:926:PHE:HD2	1.64	0.45
1:F:68:GLN:HG3	1:F:114:ALA:HB2	1.97	0.45
1:F:785:LEU:HD12	1:F:786:SER:N	2.31	0.45
1:B:984:VAL:HG11	1:B:1005:VAL:CG2	2.46	0.45
1:B:676:ASN:HD22	1:B:676:ASN:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:HG2	1:B:780:MET:CE	2.46	0.45
1:E:62:VAL:HG22	1:E:88:MET:HE2	1.97	0.45
1:E:830:PRO:HB3	1:E:839:ALA:HB2	1.99	0.45
1:E:981:ILE:O	1:E:985:VAL:HG23	2.17	0.45
1:F:504:ASP:O	1:F:505:HIS:C	2.55	0.45
1:A:329:THR:O	1:A:332:VAL:HG12	2.16	0.45
1:A:33:ASN:O	1:A:391:ASN:HA	2.17	0.45
1:D:904:VAL:HB	1:D:905:PRO:HD3	1.97	0.45
1:E:470:PHE:CD1	1:E:928:VAL:HG11	2.51	0.45
1:F:880:LEU:CD1	1:F:934:ILE:HD13	2.47	0.45
1:A:193:LEU:HD21	1:A:199:THR:HA	1.99	0.45
1:A:702:PHE:HB2	1:A:850:LEU:HD21	1.99	0.45
1:A:730:ILE:HD11	1:C:237:LYS:HE2	1.99	0.45
1:B:143:VAL:HG11	1:B:281:PHE:CD2	2.50	0.45
1:D:66:GLU:OE1	1:D:820:GLY:HA2	2.17	0.45
1:E:718:ASN:HB3	1:E:825:GLU:HB3	1.99	0.45
1:A:190:PRO:HB3	1:A:788:TRP:CE3	2.52	0.45
1:A:449:LEU:C	1:A:449:LEU:HD13	2.37	0.45
1:A:918:ARG:HD2	1:A:920:LEU:CD1	2.44	0.45
1:C:175:PHE:HB2	1:C:289:ILE:HD11	1.99	0.45
1:C:357:LEU:O	1:C:360:GLN:NE2	2.48	0.45
1:C:595:ARG:O	1:C:599:LEU:HB2	2.16	0.45
1:D:339:GLU:O	1:D:343:THR:HG23	2.17	0.45
1:D:900:VAL:O	1:D:903:VAL:HG22	2.17	0.45
1:E:47:VAL:HG11	1:E:122:VAL:HG13	1.99	0.45
1:E:60:THR:HG22	1:E:119:PRO:HD3	1.98	0.45
1:F:650:ARG:O	1:F:653:MET:N	2.50	0.45
1:A:757:TYR:HB2	1:A:771:TYR:CE1	2.52	0.45
1:B:900:VAL:HG21	1:B:942:ILE:HG13	1.98	0.45
1:E:368:PRO:HB3	1:E:409:ALA:HB1	1.99	0.45
1:E:776:PRO:O	1:E:780:MET:SD	2.75	0.45
1:F:500:ILE:O	1:F:500:ILE:HG22	2.16	0.45
1:A:977:SER:HB3	1:A:1013:THR:HG21	1.98	0.44
1:A:966:CYS:SG	1:A:1021:PRO:HB3	2.57	0.44
1:B:30:LEU:HD23	1:B:390:ILE:HD11	1.98	0.44
1:D:190:PRO:HB2	1:D:787:LYS:O	2.17	0.44
1:D:405:LEU:HD12	1:D:405:LEU:C	2.37	0.44
1:D:879:SER:O	1:D:883:VAL:HG23	2.18	0.44
1:D:908:VAL:HG22	1:D:930:LEU:HD11	1.98	0.44
1:E:53:SER:OG	1:E:56:THR:HG23	2.17	0.44
1:E:410:ILE:HG13	1:E:976:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:PRO:HG3	1:F:748:THR:HG23	1.99	0.44
1:A:749:VAL:CG1	1:C:216:SER:HB3	2.46	0.44
1:E:690:VAL:HG12	1:E:694:VAL:HB	1.98	0.44
1:F:686:ASP:O	1:F:686:ASP:OD2	2.36	0.44
1:A:560:PRO:O	1:A:921:SER:HB2	2.17	0.44
1:B:405:LEU:HD21	1:B:477:ALA:HB1	2.00	0.44
1:C:632:LYS:O	1:C:633:PRO:O	2.35	0.44
1:C:887:LEU:HD11	1:C:900:VAL:HG21	1.98	0.44
1:D:54:ALA:HB1	1:D:815:LEU:HD23	1.99	0.44
1:D:572:LEU:HB3	1:D:629:ILE:HB	1.99	0.44
1:B:1001:ILE:C	1:B:1001:ILE:HD13	2.38	0.44
1:B:555:MET:HG2	1:B:912:LEU:HB3	1.99	0.44
1:E:718:ASN:HB2	1:E:827:LEU:HD13	1.99	0.44
1:A:443:VAL:O	1:A:447:MET:HG3	2.18	0.44
1:C:946:GLU:O	1:C:950:GLU:HG3	2.18	0.44
1:D:981:ILE:HD11	1:D:1009:MET:HB3	2.00	0.44
1:F:540:PRO:O	1:F:543:LEU:N	2.50	0.44
1:F:683:PHE:CZ	1:F:825:GLU:HB2	2.52	0.44
1:F:887:LEU:CD1	1:F:900:VAL:HG21	2.47	0.44
1:A:352:PHE:CD1	1:A:365:THR:HG22	2.53	0.44
1:B:435:MET:O	1:B:439:GLN:HB2	2.17	0.44
1:B:590:VAL:O	1:B:594:MET:HG3	2.18	0.44
1:B:602:GLU:OE1	1:B:650:ARG:NH1	2.51	0.44
1:B:60:THR:HG22	1:B:61:VAL:HG23	1.99	0.44
1:C:281:PHE:CE1	1:C:608:SER:HB2	2.53	0.44
1:C:402:ILE:HD12	1:C:403:GLY:N	2.31	0.44
1:C:655:PHE:HA	1:C:658:PHE:CB	2.48	0.44
1:C:818:TYR:HE2	1:C:857:SER:HG	1.64	0.44
1:D:451:ALA:HB1	1:D:882:VAL:HG12	1.99	0.44
1:A:239:ARG:HG2	1:A:239:ARG:HH11	1.83	0.44
1:D:887:LEU:HD21	1:D:942:ILE:HD11	2.00	0.44
1:F:360:GLN:HB3	1:F:513:PHE:CD2	2.52	0.44
1:A:580:PRO:HB3	1:A:723:GLU:HB3	2.00	0.44
1:B:338:HIS:C	1:B:340:VAL:H	2.20	0.44
1:C:395:MET:O	1:C:398:MET:HB2	2.17	0.44
1:C:563:PHE:CE2	1:C:564:LEU:HD23	2.53	0.44
1:D:151:LYS:HD3	1:D:278:ASN:HB3	1.99	0.44
1:D:388:PHE:HE2	1:D:472:ILE:HG13	1.83	0.44
1:E:72:ILE:CD1	1:E:75:LEU:HD12	2.46	0.44
1:F:981:ILE:HG23	1:F:1006:ILE:CD1	2.48	0.44
1:A:498:LYS:N	1:A:499:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:CE1	1:B:121:GLU:HG3	2.53	0.44
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.47	0.44
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.38	0.44
1:C:361:ASN:O	1:C:362:PHE:C	2.56	0.44
1:E:310:ILE:HG21	1:E:323:VAL:HG21	2.00	0.44
1:E:868:SER:O	1:E:871:GLN:HG2	2.18	0.44
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.52	0.44
1:F:897:PRO:HA	1:F:900:VAL:HG22	1.99	0.44
1:F:903:VAL:HG21	1:F:1020:VAL:HG22	1.99	0.44
1:B:15:ILE:O	1:B:19:ILE:HG12	2.17	0.43
1:B:469:GLN:O	1:B:473:THR:CG2	2.62	0.43
1:C:377:LEU:O	1:C:380:PHE:HB2	2.18	0.43
1:C:701:LYS:HE2	1:C:705:LEU:HD11	2.00	0.43
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.99	0.43
1:E:637:ARG:O	1:E:637:ARG:HG3	2.18	0.43
1:E:933:THR:HG23	1:E:1009:MET:HE2	2.00	0.43
1:B:189:ASP:HB3	1:B:192:LYS:HB2	2.00	0.43
1:B:714:ARG:O	1:B:716:ARG:HD3	2.18	0.43
1:B:726:TYR:CZ	1:B:806:GLY:HA3	2.54	0.43
1:B:755:SER:HA	1:B:773:GLN:HB3	2.01	0.43
1:C:774:GLY:O	1:C:779:ARG:NH1	2.51	0.43
1:E:281:PHE:CE2	1:E:324:VAL:HG11	2.54	0.43
1:E:544:ILE:O	1:E:548:ILE:HG13	2.18	0.43
1:A:966:CYS:SG	1:A:1021:PRO:HG3	2.58	0.43
1:B:483:ILE:HG22	1:B:487:ILE:HD12	2.00	0.43
1:D:646:GLU:HG3	1:D:650:ARG:HH12	1.83	0.43
1:F:303:ALA:HA	1:F:306:ILE:CG2	2.48	0.43
1:F:740:VAL:HG21	1:F:744:ASP:HB3	2.00	0.43
1:F:913:LEU:O	1:F:914:ALA:C	2.56	0.43
1:A:936:LEU:HD12	1:A:1009:MET:SD	2.59	0.43
1:B:847:VAL:HG11	1:B:856:TYR:CD2	2.53	0.43
1:C:165:PRO:O	1:C:169:THR:OG1	2.36	0.43
1:C:542:LEU:O	1:C:546:VAL:HG23	2.18	0.43
1:C:729:GLU:O	1:C:805:THR:HB	2.19	0.43
1:D:185:ARG:HH11	1:D:771:TYR:CB	2.30	0.43
1:D:569:GLN:H	1:D:634:TRP:HH2	1.64	0.43
1:B:641:GLU:O	1:B:650:ARG:NH2	2.51	0.43
1:C:790:VAL:HG12	1:C:791:ARG:N	2.33	0.43
1:D:909:ILE:HG13	1:D:910:GLY:N	2.33	0.43
1:C:399:VAL:O	1:C:402:ILE:CD1	2.66	0.43
1:A:63:GLN:OE1	1:C:767:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:465:VAL:O	1:E:469:GLN:HG2	2.19	0.43
1:E:903:VAL:HG11	1:E:1020:VAL:HG22	2.01	0.43
1:E:906:LEU:HD21	1:E:1019:TRP:HB2	2.01	0.43
1:A:283:GLY:HA2	1:A:595:ARG:NH1	2.34	0.43
1:B:282:ASN:HA	1:B:595:ARG:HD2	2.00	0.43
1:C:354:VAL:HG21	1:C:982:LEU:CD2	2.39	0.43
1:C:420:MET:HG2	1:C:500:ILE:HG22	2.01	0.43
1:C:785:LEU:HD12	1:C:786:SER:N	2.33	0.43
1:D:423:GLU:HG3	1:D:425:LEU:HD13	1.99	0.43
1:E:120:GLN:O	1:E:124:ARG:HG3	2.19	0.43
1:E:640:GLY:O	1:E:646:GLU:HG3	2.19	0.43
1:E:724:PRO:HA	1:E:810:TYR:HA	1.99	0.43
1:E:891:TYR:HA	1:E:949:LYS:HE2	2.01	0.43
1:F:493:CYS:O	1:F:497:LEU:HB2	2.19	0.43
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.47	0.43
1:B:300:LEU:HD23	1:B:330:THR:HG23	2.00	0.43
1:C:52:ALA:HB1	1:C:56:THR:HB	2.00	0.43
1:C:730:ILE:HD13	1:C:730:ILE:H	1.84	0.43
1:D:254:ASN:ND2	1:D:258:SER:O	2.52	0.43
1:D:30:LEU:HD21	1:D:384:ALA:HA	2.01	0.43
1:F:281:PHE:CE2	1:F:324:VAL:HG11	2.54	0.43
1:B:706:ALA:HB1	1:B:712:LEU:HD12	2.01	0.43
1:B:354:VAL:HG21	1:B:979:ALA:HB2	2.00	0.43
1:C:980:PHE:O	1:C:984:VAL:HG22	2.19	0.43
1:D:99:ASP:HB3	1:D:102:ILE:HD12	2.00	0.43
1:E:312:ASN:N	1:E:312:ASN:HD22	2.17	0.43
1:E:683:PHE:CE1	1:E:825:GLU:HG2	2.53	0.43
1:F:650:ARG:O	1:F:651:ALA:C	2.56	0.43
1:A:908:VAL:O	1:A:911:ALA:HB3	2.19	0.42
1:C:136:PHE:CD1	1:C:290:ALA:HB1	2.54	0.42
1:C:406:VAL:O	1:C:407:ASP:C	2.57	0.42
1:E:68:GLN:HG2	1:E:114:ALA:HB2	2.01	0.42
1:E:26:SER:O	1:E:30:LEU:HB2	2.19	0.42
1:A:187:TRP:HA	1:A:773:GLN:O	2.19	0.42
1:A:766:ARG:CZ	1:B:67:GLN:HE21	2.33	0.42
1:B:576:VAL:HG21	1:B:591:VAL:HG12	2.00	0.42
1:C:548:ILE:HG23	1:C:909:ILE:HD13	2.00	0.42
1:D:223:PRO:HD3	1:E:275:TYR:CD2	2.54	0.42
1:D:53:SER:O	1:D:57:VAL:HG12	2.19	0.42
1:E:250:LEU:HD23	1:E:261:ARG:HG3	2.01	0.42
1:A:47:VAL:HG22	1:A:48:SER:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLY:O	1:B:27:ILE:HG13	2.19	0.42
1:C:569:GLN:NE2	1:C:669:PRO:O	2.52	0.42
1:E:637:ARG:N	1:E:638:PRO:HD3	2.34	0.42
1:F:587:THR:OG1	1:F:623:SER:HA	2.20	0.42
1:B:249:ILE:HD11	1:B:262:LEU:HD12	2.02	0.42
1:B:918:ARG:HG2	1:B:918:ARG:O	2.20	0.42
1:C:1:MET:O	1:C:4:PHE:HB3	2.19	0.42
1:C:351:VAL:HG12	1:C:355:MET:HE2	2.00	0.42
1:C:583:SER:HA	1:C:622:GLN:HB3	2.00	0.42
1:C:702:PHE:HZ	1:C:843:VAL:HG13	1.84	0.42
1:D:393:LEU:CD1	1:D:466:ILE:HG23	2.48	0.42
1:D:948:ALA:HB1	1:D:1024:TYR:CE2	2.54	0.42
1:E:671:VAL:HG23	1:E:674:LEU:CB	2.49	0.42
1:F:24:GLY:O	1:F:25:LEU:C	2.58	0.42
1:F:250:LEU:HG	1:F:261:ARG:NH1	2.34	0.42
1:F:800:PHE:O	1:F:804:ALA:HB2	2.19	0.42
1:A:749:VAL:HG12	1:C:216:SER:HB3	2.00	0.42
1:B:246:PHE:O	1:B:249:ILE:HG12	2.19	0.42
1:B:445:ILE:HD13	1:B:939:LYS:HG3	2.02	0.42
1:B:699:ARG:HD2	1:B:717:PRO:HB3	2.02	0.42
1:C:47:VAL:HG23	1:C:127:ILE:HG23	2.01	0.42
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.49	0.42
1:D:545:TYR:HB2	1:D:1019:TRP:NE1	2.34	0.42
1:E:680:PHE:HB2	1:E:858:TRP:HZ3	1.84	0.42
1:F:96:GLN:CD	1:F:461:GLY:O	2.57	0.42
1:C:1011:THR:O	1:C:1015:LEU:HB2	2.19	0.42
1:D:571:VAL:HG12	1:D:630:MET:HE3	2.00	0.42
1:D:759:ASN:O	1:D:770:VAL:HG12	2.19	0.42
1:F:562:ALA:O	1:F:923:ASP:HA	2.19	0.42
1:A:541:TYR:HA	1:A:544:ILE:HG12	2.01	0.42
1:B:349:LEU:O	1:B:352:PHE:HB3	2.20	0.42
1:B:441:ALA:O	1:B:445:ILE:CG2	2.66	0.42
1:B:619:GLY:HA3	1:B:720:MET:SD	2.60	0.42
1:C:422:GLU:HG2	1:C:505:HIS:NE2	2.35	0.42
1:C:454:LEU:HB2	1:C:455:PRO:HD3	2.02	0.42
1:D:449:LEU:CD1	1:D:478:MET:HG3	2.49	0.42
1:D:665:ALA:O	1:D:714:ARG:NH2	2.53	0.42
1:F:332:VAL:HG11	1:F:569:GLN:HB3	2.00	0.42
1:F:563:PHE:O	1:F:923:ASP:HB2	2.20	0.42
1:A:831:ALA:HB3	1:A:834:LEU:CD1	2.50	0.42
1:A:951:LEU:O	1:A:956:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD12	1:B:275:TYR:O	2.19	0.42
1:B:38:ILE:HD12	1:B:466:ILE:HD13	2.01	0.42
1:C:243:ALA:HB1	1:C:268:VAL:O	2.20	0.42
1:D:435:MET:O	1:D:437:GLN:O	2.37	0.42
1:F:15:ILE:HD13	1:F:16:ALA:H	1.85	0.42
1:F:466:ILE:HG13	1:F:467:TYR:N	2.35	0.42
1:A:326:PRO:HB3	1:A:610:PHE:HB2	2.02	0.42
1:A:879:SER:O	1:A:883:VAL:HG23	2.20	0.42
1:C:102:ILE:HD12	1:C:102:ILE:C	2.40	0.42
1:C:281:PHE:CD2	1:C:324:VAL:HG21	2.54	0.42
1:E:64:VAL:HG21	1:E:118:LEU:HD23	2.02	0.42
1:E:344:LEU:O	1:E:348:ILE:HG23	2.19	0.42
1:F:595:ARG:HG3	1:F:596:GLU:N	2.35	0.42
1:A:293:LEU:HA	1:A:293:LEU:HD12	1.84	0.42
1:C:391:ASN:H	1:C:394:THR:HG22	1.85	0.42
1:F:399:VAL:O	1:F:402:ILE:HG13	2.19	0.42
1:A:578:THR:HB	1:A:579:PRO:HD2	2.02	0.41
1:A:951:LEU:CD1	1:A:964:GLU:HB3	2.49	0.41
1:C:184:MET:HB3	1:C:770:VAL:HG22	2.02	0.41
1:C:194:ASN:OD1	1:C:797:MET:HG2	2.20	0.41
1:A:56:THR:HG23	1:C:213:GLN:HG2	2.01	0.41
1:C:547:VAL:O	1:C:550:ALA:HB3	2.20	0.41
1:D:391:ASN:ND2	1:D:469:GLN:OE1	2.50	0.41
1:D:56:THR:HG23	1:F:213:GLN:HG2	2.02	0.41
1:E:784:ASP:C	1:E:786:SER:H	2.23	0.41
1:F:438:ILE:O	1:F:439:GLN:C	2.59	0.41
1:F:471:SER:O	1:F:475:VAL:HG22	2.20	0.41
1:A:416:VAL:O	1:A:420:MET:HB2	2.19	0.41
1:A:127:ILE:O	1:B:113:LEU:HG	2.20	0.41
1:A:88:MET:C	1:A:88:MET:SD	2.98	0.41
1:A:943:LEU:HD13	1:A:969:ARG:NH2	2.35	0.41
1:B:302:THR:O	1:B:306:ILE:HG12	2.20	0.41
1:C:592:ASP:HA	1:C:595:ARG:HG2	2.01	0.41
1:C:914:ALA:HA	1:C:917:MET:HG2	2.01	0.41
1:D:459:PHE:O	1:D:464:GLY:HA3	2.20	0.41
1:E:698:ALA:HB2	1:E:854:VAL:HG21	2.01	0.41
1:F:298:ASN:HB3	1:F:301:ASP:HB2	2.02	0.41
1:F:361:ASN:C	1:F:361:ASN:HD22	2.23	0.41
1:B:187:TRP:HA	1:B:773:GLN:O	2.21	0.41
1:D:303:ALA:CB	1:D:330:THR:HG21	2.49	0.41
1:D:542:LEU:O	1:D:546:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:VAL:HG22	1:E:127:ILE:HG23	2.03	0.41
1:F:15:ILE:HD13	1:F:16:ALA:N	2.36	0.41
1:A:981:ILE:HD11	1:A:1009:MET:HB3	2.03	0.41
1:A:791:ARG:CG	1:A:797:MET:HE2	2.49	0.41
1:A:452:VAL:HG22	1:A:883:VAL:HG21	2.02	0.41
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.56	0.41
1:C:655:PHE:HA	1:C:658:PHE:HB2	2.01	0.41
1:C:884:PHE:CE1	1:C:897:PRO:HB2	2.55	0.41
1:D:1030:LEU:HB3	1:D:1031:PHE:CE2	2.56	0.41
1:D:434:SER:O	1:D:437:GLN:HG2	2.21	0.41
1:E:572:LEU:HB3	1:E:629:ILE:HB	2.02	0.41
1:A:602:GLU:O	1:A:604:SER:N	2.53	0.41
1:A:714:ARG:O	1:A:716:ARG:N	2.53	0.41
1:B:154:LEU:HD13	1:B:286:ALA:HA	2.01	0.41
1:B:310:ILE:CG2	1:B:323:VAL:HG21	2.51	0.41
1:C:480:LEU:O	1:C:484:VAL:HG13	2.20	0.41
1:D:560:PRO:HG2	1:D:921:SER:HB3	2.02	0.41
1:E:738:LEU:HD13	1:E:798:VAL:HG11	2.03	0.41
1:F:316:PHE:CD1	1:F:316:PHE:N	2.89	0.41
1:E:228:GLN:OE1	1:F:780:MET:HB3	2.21	0.41
1:D:749:VAL:HG22	1:D:753:TRP:CZ3	2.54	0.41
1:E:210:GLN:HE22	1:E:249:ILE:HD13	1.85	0.41
1:E:690:VAL:HG13	1:E:694:VAL:HB	2.00	0.41
1:D:780:MET:CE	1:F:220:GLY:HA2	2.43	0.41
1:A:780:MET:HE3	1:C:228:GLN:OE1	2.21	0.41
1:D:438:ILE:HG13	1:D:439:GLN:N	2.35	0.41
1:F:303:ALA:C	1:F:306:ILE:HG22	2.41	0.41
1:F:749:VAL:HA	1:F:753:TRP:CZ3	2.56	0.41
1:A:740:VAL:HG13	1:A:790:VAL:HG11	2.01	0.41
1:A:702:PHE:CZ	1:A:843:VAL:HG13	2.54	0.41
1:A:896:ILE:N	1:A:897:PRO:HD2	2.35	0.41
1:B:219:LEU:HB2	1:B:234:ILE:CG2	2.51	0.41
1:B:757:TYR:HB2	1:B:771:TYR:CE1	2.56	0.41
1:C:545:TYR:CE1	1:C:1023:PHE:HZ	2.39	0.41
1:E:344:LEU:HD23	1:E:402:ILE:HG13	2.02	0.41
1:E:792:ASN:ND2	1:E:796:GLU:HB2	2.36	0.41
1:F:966:CYS:SG	1:F:1021:PRO:CG	3.09	0.41
1:F:410:ILE:HD13	1:F:975:MET:CE	2.51	0.41
1:A:289:ILE:HD12	1:A:289:ILE:H	1.85	0.41
1:A:540:PRO:O	1:A:544:ILE:HG12	2.21	0.41
1:A:572:LEU:HB3	1:A:629:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ALA:O	1:B:351:VAL:HG23	2.20	0.41
1:B:57:VAL:HG11	1:B:88:MET:HB3	2.03	0.41
1:B:562:ALA:O	1:B:923:ASP:HA	2.21	0.41
1:C:908:VAL:O	1:C:912:LEU:HG	2.20	0.41
1:D:330:THR:N	1:D:331:PRO:CD	2.84	0.41
1:E:406:VAL:O	1:E:410:ILE:HG12	2.21	0.41
1:E:184:MET:HB2	1:E:761:PHE:CZ	2.56	0.41
1:E:865:GLU:HA	1:E:868:SER:HB2	2.02	0.41
1:F:350:LEU:O	1:F:354:VAL:HG23	2.20	0.41
1:A:10:ILE:HG23	1:B:894:TRP:CZ2	2.56	0.41
1:A:388:PHE:CE2	1:A:472:ILE:HG13	2.56	0.41
1:C:228:GLN:HG3	1:C:229:GLN:N	2.36	0.41
1:E:314:GLU:N	1:E:315:PRO:HD2	2.36	0.41
1:E:459:PHE:O	1:E:464:GLY:HA3	2.20	0.41
1:F:418:ARG:NH2	1:F:437:GLN:OE1	2.53	0.41
1:F:971:ARG:HB3	1:F:972:PRO:CD	2.52	0.41
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.03	0.40
1:A:489:THR:HB	1:A:490:PRO:HD3	2.02	0.40
1:B:687:GLN:OE1	1:B:821:VAL:HG21	2.20	0.40
1:B:904:VAL:HB	1:B:905:PRO:HD3	2.02	0.40
1:C:326:PRO:HB3	1:C:610:PHE:HB2	2.02	0.40
1:C:418:ARG:HD2	1:C:968:MET:HE2	2.02	0.40
1:D:637:ARG:N	1:D:638:PRO:CD	2.84	0.40
1:D:789:TYR:CZ	1:D:799:PRO:HB3	2.56	0.40
1:E:899:SER:HA	1:E:1023:PHE:HB3	2.03	0.40
1:E:42:ALA:HB3	1:E:132:ALA:HB3	2.03	0.40
1:F:421:ALA:O	1:F:422:GLU:C	2.59	0.40
1:B:650:ARG:CG	1:B:650:ARG:HH11	2.30	0.40
1:C:5:PHE:CE2	1:C:487:ILE:HG23	2.57	0.40
1:E:445:ILE:CD1	1:E:939:LYS:HE3	2.52	0.40
1:E:579:PRO:O	1:E:581:GLY:N	2.54	0.40
1:E:907:GLY:O	1:E:1008:GLY:HA2	2.21	0.40
1:F:11:PHE:HD2	1:F:11:PHE:O	2.04	0.40
1:F:310:ILE:HD12	1:F:310:ILE:C	2.42	0.40
1:A:762:ILE:HD11	1:B:59:ASP:HB3	2.03	0.40
1:A:875:LEU:CD2	1:A:931:LEU:HD11	2.48	0.40
1:B:357:LEU:HD11	1:B:516:PHE:CE1	2.56	0.40
1:D:439:GLN:HG3	1:D:486:LEU:HD22	2.02	0.40
1:E:139:VAL:HG22	1:E:327:TYR:HB3	2.03	0.40
1:A:352:PHE:CE1	1:A:365:THR:HG22	2.56	0.40
1:A:720:MET:HG3	1:A:814:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:PRO:HA	1:B:908:VAL:HG12	2.04	0.40
1:C:578:THR:HG21	1:C:587:THR:HA	2.04	0.40
1:C:552:MET:SD	1:C:908:VAL:HB	2.61	0.40
1:E:493:CYS:CA	1:E:497:LEU:HD22	2.52	0.40
1:F:314:GLU:OE2	1:F:323:VAL:HG12	2.21	0.40
1:A:373:PRO:O	1:A:377:LEU:HB2	2.21	0.40
1:A:690:VAL:CG2	1:A:694:VAL:HB	2.52	0.40
1:A:830:PRO:HB3	1:A:839:ALA:HB2	2.02	0.40
1:B:250:LEU:CD2	1:B:261:ARG:HG3	2.52	0.40
1:B:394:THR:HA	1:B:473:THR:HG21	2.04	0.40
1:B:904:VAL:O	1:B:908:VAL:HG12	2.21	0.40
1:C:530:GLY:O	1:C:534:ILE:HD13	2.21	0.40
1:C:660:ASP:O	1:C:661:ALA:HB2	2.22	0.40
1:C:699:ARG:HH12	1:C:721:SER:HA	1.87	0.40
1:D:631:LEU:N	1:D:631:LEU:HD12	2.37	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	A	1011/1052 (96%)	909 (90%)	82 (8%)	20 (2%)	7	26
1	B	1028/1052 (98%)	918 (89%)	91 (9%)	19 (2%)	8	28
1	C	1028/1052 (98%)	885 (86%)	114 (11%)	29 (3%)	5	17
1	D	1016/1052 (97%)	889 (88%)	105 (10%)	22 (2%)	6	23
1	E	1028/1052 (98%)	907 (88%)	100 (10%)	21 (2%)	7	26
1	F	1031/1052 (98%)	876 (85%)	114 (11%)	41 (4%)	3	10
All	All	6142/6312 (97%)	5384 (88%)	606 (10%)	152 (2%)	5	20

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	A	714	ARG
1	A	715	VAL
1	A	740	VAL
1	A	872	ALA
1	B	140	VAL
1	B	249	ILE
1	B	439	GLN
1	B	558	ARG
1	B	660	ASP
1	B	741	SER
1	C	125	GLN
1	C	276	SER
1	C	501	GLU
1	C	602	GLU
1	C	633	PRO
1	C	659	LYS
1	C	661	ALA
1	D	872	ALA
1	D	953	GLU
1	E	147	GLY
1	E	228	GLN
1	E	238	THR
1	E	582	SER
1	E	618	ALA
1	E	690	VAL
1	E	785	LEU
1	F	319	GLN
1	F	363	ARG
1	F	422	GLU
1	F	501	GLU
1	F	539	ALA
1	F	796	GLU
1	F	958	ILE
1	A	673	GLU
1	A	835	SER
1	B	146	ASP
1	B	509	LYS
1	B	705	LEU
1	B	719	GLY
1	B	742	LEU
1	C	258	SER
1	C	361	ASN

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Mol	Chain	Res	Type
1	C	598	LEU
1	C	663	VAL
1	C	687	GLN
1	C	737	ALA
1	D	147	GLY
1	D	440	GLY
1	D	441	ALA
1	D	654	HIS
1	D	673	GLU
1	D	733	GLU
1	D	922	ASN
1	E	657	SER
1	E	658	PHE
1	E	728	LEU
1	E	790	VAL
1	F	201	GLY
1	F	326	PRO
1	F	462	SER
1	F	505	HIS
1	F	598	LEU
1	F	636	GLU
1	F	744	ASP
1	F	778	ALA
1	F	805	THR
1	F	913	LEU
1	A	603	SER
1	A	956	LYS
1	B	438	ILE
1	B	676	ASN
1	B	755	SER
1	C	422	GLU
1	C	582	SER
1	C	662	MET
1	C	714	ARG
1	C	755	SER
1	C	804	ALA
1	D	239	ARG
1	D	498	LYS
1	D	634	TRP
1	D	755	SER
1	D	995	SER
1	E	318	PRO

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Mol	Chain	Res	Type
1	E	580	PRO
1	E	623	SER
1	F	618	ALA
1	F	644	VAL
1	F	660	ASP
1	F	661	ALA
1	F	690	VAL
1	F	742	LEU
1	F	745	ILE
1	F	810	TYR
1	A	564	LEU
1	A	713	GLN
1	A	834	LEU
1	A	932	THR
1	B	216	SER
1	C	240	LEU
1	C	241	GLN
1	C	742	LEU
1	D	564	LEU
1	D	793	ASP
1	E	339	GLU
1	E	755	SER
1	E	913	LEU
1	F	322	LYS
1	F	421	ALA
1	F	538	ARG
1	F	663	VAL
1	F	727	LYS
1	F	755	SER
1	A	451	ALA
1	A	832	PRO
1	B	127	ILE
1	B	339	GLU
1	B	673	GLU
1	C	647	LEU
1	C	743	ALA
1	C	917	MET
1	C	1017	ILE
1	D	61	VAL
1	D	801	ASN
1	D	946	GLU
1	D	956	LYS

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Mol	Chain	Res	Type
1	E	676	ASN
1	F	202	ASP
1	F	361	ASN
1	F	504	ASP
1	F	633	PRO
1	F	647	LEU
1	F	819	ASN
1	A	54	ALA
1	A	717	PRO
1	A	851	PRO
1	A	952	HIS
1	A	1027	VAL
1	B	228	GLN
1	C	639	GLY
1	D	714	ARG
1	E	216	SER
1	F	238	THR
1	F	845	GLU
1	F	330	THR
1	C	326	PRO
1	D	372	VAL
1	F	640	GLY
1	E	795	GLY
1	C	873	PRO
1	E	340	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	832/860 (97%)	757 (91%)	75 (9%)	9	27
1	B	841/860 (98%)	749 (89%)	92 (11%)	6	18
1	C	841/860 (98%)	766 (91%)	75 (9%)	9	28
1	D	835/860 (97%)	768 (92%)	67 (8%)	12	32
1	E	841/860 (98%)	775 (92%)	66 (8%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	844/860 (98%)	772 (92%)	72 (8%)	10	30
All	All	5034/5160 (98%)	4587 (91%)	447 (9%)	9	28

All (447) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	21	LEU
1	A	25	LEU
1	A	29	SER
1	A	33	ASN
1	A	49	TYR
1	A	83	ASN
1	A	88	MET
1	A	95	GLU
1	A	96	GLN
1	A	139	VAL
1	A	177	VAL
1	A	188	LEU
1	A	205	SER
1	A	219	LEU
1	A	230	LEU
1	A	239	ARG
1	A	259	GLN
1	A	289	ILE
1	A	302	THR
1	A	307	ARG
1	A	310	ILE
1	A	337	ILE
1	A	343	THR
1	A	349	LEU
1	A	356	TYR
1	A	377	LEU
1	A	417	GLU
1	A	433	LYS
1	A	438	ILE
1	A	442	LEU
1	A	472	ILE
1	A	483	ILE
1	A	488	LEU
1	A	512	PHE
1	A	525	HIS

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Mol	Chain	Res	Type
1	A	556	PHE
1	A	595	ARG
1	A	601	LYS
1	A	612	VAL
1	A	643	SER
1	A	659	LYS
1	A	671	VAL
1	A	674	LEU
1	A	687	GLN
1	A	695	LEU
1	A	716	ARG
1	A	730	ILE
1	A	768	LYS
1	A	770	VAL
1	A	800	PHE
1	A	805	THR
1	A	810	TYR
1	A	814	LYS
1	A	817	ARG
1	A	821	VAL
1	A	856	TYR
1	A	861	LEU
1	A	875	LEU
1	A	878	LEU
1	A	881	LEU
1	A	900	VAL
1	A	916	SER
1	A	918	ARG
1	A	928	VAL
1	A	932	THR
1	A	939	LYS
1	A	940	ASN
1	A	950	GLU
1	A	958	ILE
1	A	964	GLU
1	A	976	THR
1	A	982	LEU
1	A	1013	THR
1	A	1027	VAL
1	B	11	PHE
1	B	17	LEU
1	B	18	VAL

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Mol	Chain	Res	Type
1	B	49	TYR
1	B	60	THR
1	B	64	VAL
1	B	68	GLN
1	B	79	SER
1	B	88	MET
1	B	96	GLN
1	B	106	GLN
1	B	110	LYS
1	B	111	LEU
1	B	113	LEU
1	B	121	GLU
1	B	128	ARG
1	B	129	VAL
1	B	134	LYS
1	B	139	VAL
1	B	159	VAL
1	B	188	LEU
1	B	197	GLN
1	B	215	SER
1	B	248	ASN
1	B	280	GLN
1	B	289	ILE
1	B	291	ILE
1	B	316	PHE
1	B	319	GLN
1	B	341	VAL
1	B	343	THR
1	B	348	ILE
1	B	365	THR
1	B	393	LEU
1	B	411	VAL
1	B	414	GLU
1	B	418	ARG
1	B	432	ARG
1	B	434	SER
1	B	445	ILE
1	B	462	SER
1	B	473	THR
1	B	475	VAL
1	B	486	LEU
1	B	497	LEU

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Mol	Chain	Res	Type
1	B	501	GLU
1	B	525	HIS
1	B	543	LEU
1	B	558	ARG
1	B	559	ILE
1	B	572	LEU
1	B	575	GLN
1	B	589	VAL
1	B	601	LYS
1	B	605	SER
1	B	610	PHE
1	B	623	SER
1	B	624	SER
1	B	635	GLU
1	B	641	GLU
1	B	650	ARG
1	B	658	PHE
1	B	662	MET
1	B	674	LEU
1	B	676	ASN
1	B	684	LEU
1	B	687	GLN
1	B	693	GLU
1	B	696	LEU
1	B	712	LEU
1	B	716	ARG
1	B	725	GLN
1	B	757	TYR
1	B	759	ASN
1	B	784	ASP
1	B	789	TYR
1	B	800	PHE
1	B	801	ASN
1	B	827	LEU
1	B	844	GLU
1	B	871	GLN
1	B	900	VAL
1	B	906	LEU
1	B	909	ILE
1	B	913	LEU
1	B	917	MET
1	B	922	ASN

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Mol	Chain	Res	Type
1	B	936	LEU
1	B	969	ARG
1	B	970	LEU
1	B	1001	ILE
1	B	1022	LEU
1	C	11	PHE
1	C	15	ILE
1	C	30	LEU
1	C	38	ILE
1	C	67	GLN
1	C	88	MET
1	C	102	ILE
1	C	112	GLN
1	C	117	LEU
1	C	118	LEU
1	C	125	GLN
1	C	143	VAL
1	C	152	GLU
1	C	166	LEU
1	C	238	THR
1	C	291	ILE
1	C	298	ASN
1	C	306	ILE
1	C	343	THR
1	C	348	ILE
1	C	360	GLN
1	C	361	ASN
1	C	376	LEU
1	C	391	ASN
1	C	394	THR
1	C	402	ILE
1	C	408	ASP
1	C	410	ILE
1	C	434	SER
1	C	435	MET
1	C	439	GLN
1	C	448	VAL
1	C	452	VAL
1	C	463	THR
1	C	466	ILE
1	C	481	SER
1	C	484	VAL

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Mol	Chain	Res	Type
1	C	486	LEU
1	C	497	LEU
1	C	557	THR
1	C	588	GLN
1	C	592	ASP
1	C	594	MET
1	C	595	ARG
1	C	611	THR
1	C	645	PHE
1	C	646	GLU
1	C	650	ARG
1	C	659	LYS
1	C	685	GLN
1	C	730	ILE
1	C	785	LEU
1	C	797	MET
1	C	814	LYS
1	C	840	MET
1	C	867	LEU
1	C	880	LEU
1	C	881	LEU
1	C	890	LEU
1	C	896	ILE
1	C	898	PHE
1	C	902	LEU
1	C	906	LEU
1	C	916	SER
1	C	920	LEU
1	C	932	THR
1	C	933	THR
1	C	934	ILE
1	C	943	LEU
1	C	946	GLU
1	C	969	ARG
1	C	984	VAL
1	C	1009	MET
1	C	1022	LEU
1	C	1030	LEU
1	D	11	PHE
1	D	25	LEU
1	D	33	ASN
1	D	43	ILE

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Mol	Chain	Res	Type
1	D	49	TYR
1	D	55	GLU
1	D	88	MET
1	D	96	GLN
1	D	121	GLU
1	D	134	LYS
1	D	145	THR
1	D	166	LEU
1	D	172	VAL
1	D	289	ILE
1	D	319	GLN
1	D	348	ILE
1	D	353	LEU
1	D	359	LEU
1	D	362	PHE
1	D	392	THR
1	D	393	LEU
1	D	405	LEU
1	D	417	GLU
1	D	437	GLN
1	D	472	ILE
1	D	481	SER
1	D	488	LEU
1	D	497	LEU
1	D	512	PHE
1	D	521	LEU
1	D	544	ILE
1	D	586	ARG
1	D	592	ASP
1	D	601	LYS
1	D	616	ASN
1	D	644	VAL
1	D	647	LEU
1	D	664	PHE
1	D	674	LEU
1	D	687	GLN
1	D	695	LEU
1	D	716	ARG
1	D	772	LEU
1	D	784	ASP
1	D	800	PHE
1	D	817	ARG

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Mol	Chain	Res	Type
1	D	824	MET
1	D	827	LEU
1	D	845	GLU
1	D	861	LEU
1	D	863	TYR
1	D	878	LEU
1	D	881	LEU
1	D	885	LEU
1	D	913	LEU
1	D	921	SER
1	D	932	THR
1	D	958	ILE
1	D	964	GLU
1	D	970	LEU
1	D	987	LEU
1	D	989	ILE
1	D	1009	MET
1	D	1011	THR
1	D	1013	THR
1	D	1022	LEU
1	D	1031	PHE
1	E	11	PHE
1	E	17	LEU
1	E	18	VAL
1	E	33	ASN
1	E	47	VAL
1	E	48	SER
1	E	49	TYR
1	E	55	GLU
1	E	58	GLN
1	E	68	GLN
1	E	70	ASN
1	E	78	ILE
1	E	81	GLU
1	E	89	THR
1	E	113	LEU
1	E	120	GLN
1	E	125	GLN
1	E	128	ARG
1	E	134	LYS
1	E	146	ASP
1	E	159	VAL

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Mol	Chain	Res	Type
1	E	176	GLN
1	E	197	GLN
1	E	261	ARG
1	E	308	GLN
1	E	348	ILE
1	E	354	VAL
1	E	365	THR
1	E	393	LEU
1	E	398	MET
1	E	402	ILE
1	E	414	GLU
1	E	432	ARG
1	E	486	LEU
1	E	495	THR
1	E	497	LEU
1	E	544	ILE
1	E	556	PHE
1	E	559	ILE
1	E	572	LEU
1	E	592	ASP
1	E	635	GLU
1	E	641	GLU
1	E	659	LYS
1	E	666	PHE
1	E	676	ASN
1	E	682	LEU
1	E	696	LEU
1	E	716	ARG
1	E	722	ASP
1	E	755	SER
1	E	759	ASN
1	E	785	LEU
1	E	801	ASN
1	E	803	PHE
1	E	825	GLU
1	E	856	TYR
1	E	865	GLU
1	E	870	SER
1	E	893	SER
1	E	913	LEU
1	E	936	LEU
1	E	956	LYS

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Mol	Chain	Res	Type
1	E	969	ARG
1	E	976	THR
1	E	1022	LEU
1	F	11	PHE
1	F	15	ILE
1	F	38	ILE
1	F	47	VAL
1	F	49	TYR
1	F	67	GLN
1	F	83	ASN
1	F	88	MET
1	F	112	GLN
1	F	125	GLN
1	F	128	ARG
1	F	142	VAL
1	F	153	ASP
1	F	166	LEU
1	F	185	ARG
1	F	233	THR
1	F	256	ASP
1	F	278	ASN
1	F	295	THR
1	F	306	ILE
1	F	316	PHE
1	F	343	THR
1	F	348	ILE
1	F	357	LEU
1	F	361	ASN
1	F	366	LEU
1	F	374	VAL
1	F	376	LEU
1	F	379	THR
1	F	394	THR
1	F	410	ILE
1	F	429	GLU
1	F	445	ILE
1	F	463	THR
1	F	466	ILE
1	F	473	THR
1	F	481	SER
1	F	486	LEU
1	F	488	LEU

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Mol	Chain	Res	Type
1	F	498	LYS
1	F	501	GLU
1	F	502	LYS
1	F	507	GLU
1	F	509	LYS
1	F	519	MET
1	F	523	THR
1	F	544	ILE
1	F	558	ARG
1	F	564	LEU
1	F	595	ARG
1	F	599	LEU
1	F	608	SER
1	F	646	GLU
1	F	659	LYS
1	F	695	LEU
1	F	699	ARG
1	F	716	ARG
1	F	730	ILE
1	F	779	ARG
1	F	793	ASP
1	F	797	MET
1	F	807	LYS
1	F	846	ILE
1	F	856	TYR
1	F	880	LEU
1	F	881	LEU
1	F	902	LEU
1	F	909	ILE
1	F	932	THR
1	F	934	ILE
1	F	946	GLU
1	F	1032	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	106	GLN
1	A	112	GLN
1	A	228	GLN
1	A	700	ASN

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Mol	Chain	Res	Type
1	A	922	ASN
1	A	940	ASN
1	B	46	GLN
1	B	67	GLN
1	B	68	GLN
1	B	104	GLN
1	B	106	GLN
1	B	194	ASN
1	B	210	GLN
1	B	319	GLN
1	B	676	ASN
1	B	922	ASN
1	B	927	GLN
1	C	63	GLN
1	C	67	GLN
1	C	83	ASN
1	C	125	GLN
1	C	241	GLN
1	C	248	ASN
1	C	361	ASN
1	C	439	GLN
1	C	692	HIS
1	C	849	GLN
1	D	33	ASN
1	D	96	GLN
1	D	213	GLN
1	D	241	GLN
1	D	622	GLN
1	D	642	ASN
1	E	58	GLN
1	E	70	ASN
1	E	125	GLN
1	E	210	GLN
1	E	229	GLN
1	E	273	GLN
1	E	278	ASN
1	E	312	ASN
1	E	319	GLN
1	E	361	ASN
1	E	577	GLN
1	E	588	GLN
1	E	692	HIS

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Mol	Chain	Res	Type
1	E	713	GLN
1	E	718	ASN
1	E	922	ASN
1	E	927	GLN
1	E	954	GLN
1	F	34	GLN
1	F	68	GLN
1	F	83	ASN
1	F	125	GLN
1	F	176	GLN
1	F	194	ASN
1	F	241	GLN
1	F	361	ASN
1	F	569	GLN

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AV0	E	1101	-	72,72,72	0.48	0	96,98,98	1.19	11 (11%)
2	AV0	B	1101	-	72,72,72	0.51	0	96,98,98	1.13	9 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AV0	E	1101	-	-	22/50/130/130	0/4/4/4
2	AV0	B	1101	-	-	15/50/130/130	0/4/4/4

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	AV0	CBR-CCM-CBQ	3.43	116.39	109.97
2	B	1101	AV0	CCR-O4-C4	-2.86	110.88	117.96
2	E	1101	AV0	CCJ-OBX-CCF	-2.65	108.49	113.69
2	B	1101	AV0	CCU-CCO-CCD	-2.63	105.55	110.24
2	E	1101	AV0	CCV-CCT-CCN	-2.61	106.26	110.82
2	B	1101	AV0	OBY-CCC-CBM	2.59	112.87	106.44
2	E	1101	AV0	CBQ-CCM-CBT	-2.41	103.69	109.40
2	B	1101	AV0	O4-CCR-OBY	2.40	117.37	110.67
2	B	1101	AV0	OBX-CCJ-CCL	-2.38	105.30	110.35
2	E	1101	AV0	CBN-CCD-CCO	2.37	118.56	113.00
2	E	1101	AV0	OAU-CCV-CCT	2.36	115.80	110.35
2	E	1101	AV0	CBP-CCF-CCQ	2.23	119.83	113.33
2	E	1101	AV0	OAU-CCV-CCR	-2.15	104.82	110.05
2	B	1101	AV0	CCW-CCU-CCO	-2.10	107.15	110.82
2	E	1101	AV0	C2-C3-C4	-2.09	104.91	109.68
2	E	1101	AV0	CCU-CCO-CCD	-2.04	106.60	110.24
2	B	1101	AV0	O3-C3-C4	2.04	115.34	109.94
2	E	1101	AV0	O4-CCR-OBY	2.03	116.34	110.67
2	B	1101	AV0	OBX-CCF-CCQ	-2.02	105.48	109.75
2	B	1101	AV0	OBX-CCJ-OBV	-2.00	105.23	109.97

There are no chirality outliers.

All (37) torsion outliers are listed below:

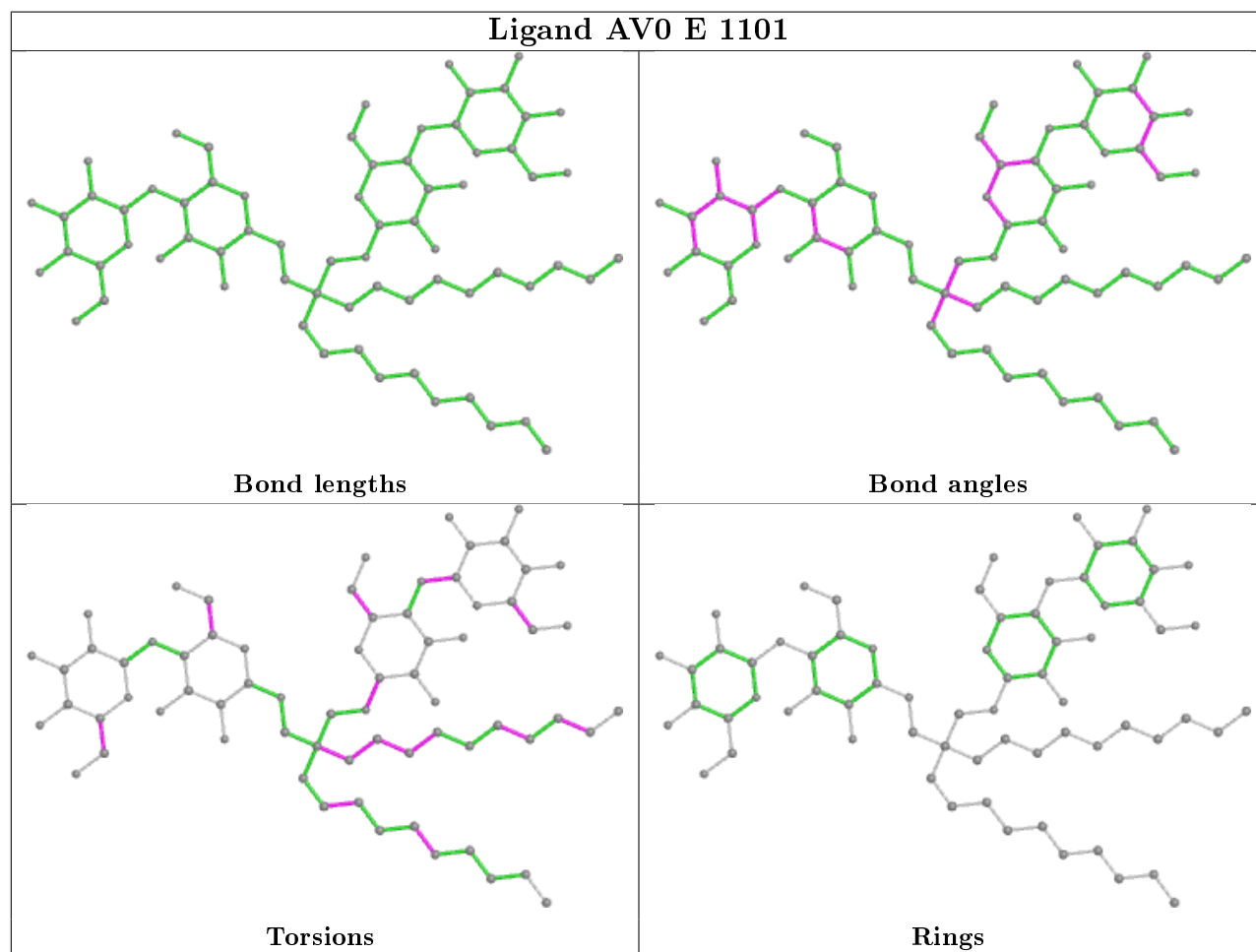
Mol	Chain	Res	Type	Atoms
2	E	1101	AV0	CBL-CBR-CCM-CBQ
2	E	1101	AV0	CBL-CBR-CCM-CBS
2	E	1101	AV0	CBL-CBR-CCM-CBT
2	B	1101	AV0	OBV-CBT-CCM-CBQ
2	B	1101	AV0	OBV-CBT-CCM-CBR
2	E	1101	AV0	OAJ-CBN-CCD-OBZ
2	B	1101	AV0	OAI-CBM-CCC-OBY
2	E	1101	AV0	OAI-CBM-CCC-OBY
2	E	1101	AV0	CBJ-CBL-CBR-CCM
2	B	1101	AV0	OAI-CBM-CCC-CCN
2	B	1101	AV0	OBV-CBT-CCM-CBS
2	E	1101	AV0	C4-C5-C6-O6
2	B	1101	AV0	CAX-CAZ-CBB-CBD
2	E	1101	AV0	CCL-CCJ-OBV-CBT
2	B	1101	AV0	CBA-CBC-CBE-CBG
2	B	1101	AV0	CBG-CBI-CBK-CBQ
2	E	1101	AV0	OAL-CBP-CCF-CCQ
2	B	1101	AV0	CBD-CBF-CBH-CBJ
2	B	1101	AV0	OAJ-CBN-CCD-OBZ
2	E	1101	AV0	CBG-CBI-CBK-CBQ
2	E	1101	AV0	OAJ-CBN-CCD-CCO
2	B	1101	AV0	CBF-CBH-CBJ-CBL
2	E	1101	AV0	OAL-CBP-CCF-OBX
2	E	1101	AV0	O5-C5-C6-O6
2	E	1101	AV0	OBZ-CCS-OCB-CCQ
2	E	1101	AV0	OBX-CCJ-OBV-CBT
2	B	1101	AV0	O5-C5-C6-O6
2	B	1101	AV0	OBZ-CCS-OCB-CCQ
2	E	1101	AV0	CBA-CBC-CBE-CBG
2	E	1101	AV0	CBH-CBJ-CBL-CBR
2	E	1101	AV0	CAB-CAX-CAZ-CBB
2	E	1101	AV0	CAZ-CBB-CBD-CBF
2	E	1101	AV0	OAI-CBM-CCC-CCN
2	B	1101	AV0	CAW-CAY-CBA-CBC
2	B	1101	AV0	CCW-CCS-OCB-CCQ
2	E	1101	AV0	CCW-CCS-OCB-CCQ
2	E	1101	AV0	CBF-CBH-CBJ-CBL

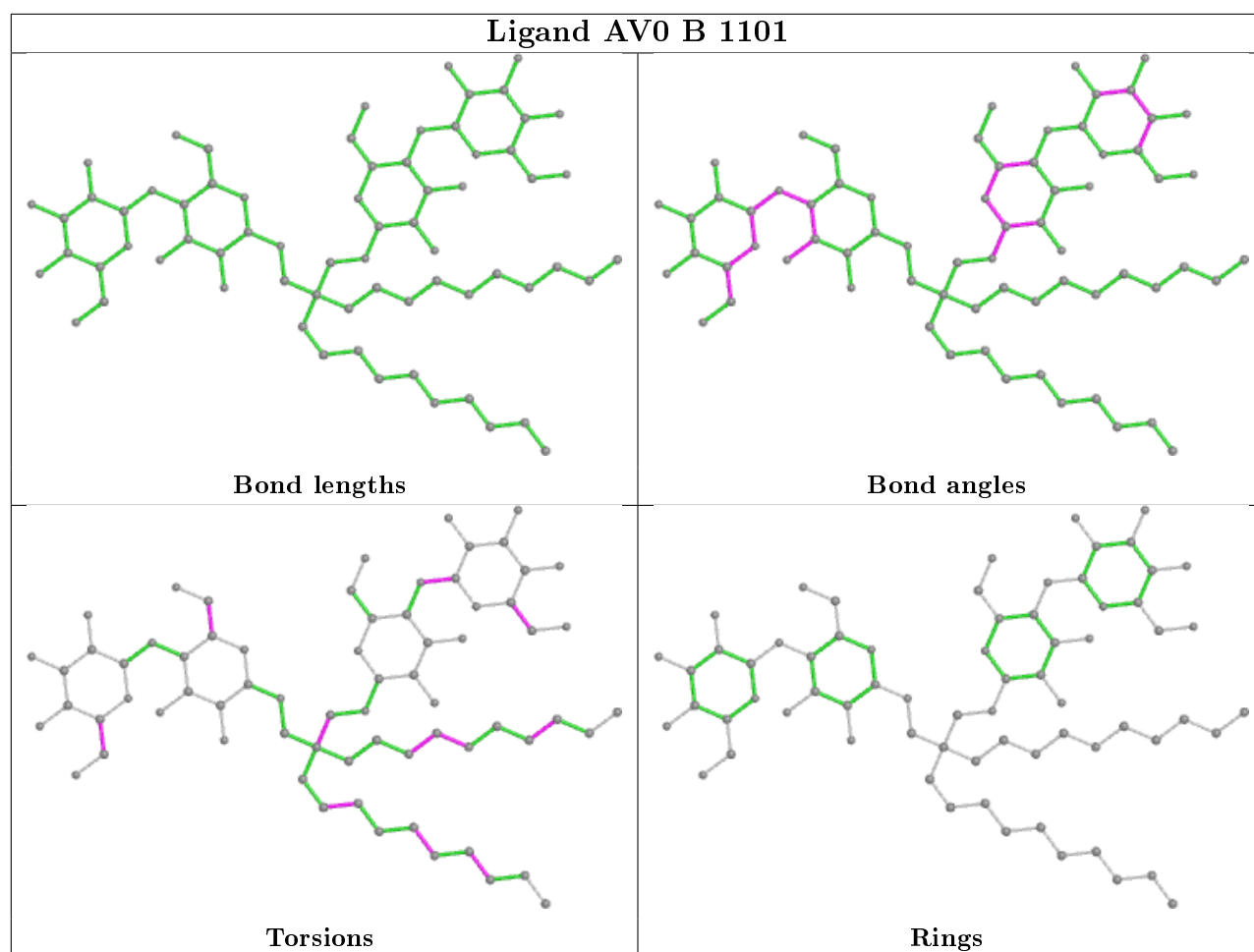
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	AV0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	1017/1052 (96%)	0.00	36 (3%)	44	40	13, 47, 94, 148	0
1	B	1030/1052 (97%)	-0.04	33 (3%)	47	44	12, 40, 79, 117	0
1	C	1030/1052 (97%)	0.29	63 (6%)	21	18	15, 55, 110, 162	0
1	D	1020/1052 (96%)	0.10	52 (5%)	28	24	17, 53, 97, 144	0
1	E	1030/1052 (97%)	0.11	51 (4%)	28	25	18, 52, 99, 137	0
1	F	1033/1052 (98%)	0.17	69 (6%)	17	14	21, 52, 111, 166	0
All	All	6160/6312 (97%)	0.11	304 (4%)	29	26	12, 50, 99, 166	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	742	LEU	12.3
1	F	742	LEU	9.2
1	A	955	GLY	8.9
1	C	657	SER	8.1
1	C	259	GLN	7.4
1	C	258	SER	7.3
1	F	741	SER	7.0
1	E	704	MET	6.3
1	C	738	LEU	6.3
1	D	870	SER	6.1
1	A	656	PHE	6.0
1	E	708	GLN	5.9
1	F	739	GLY	5.8
1	E	804	ALA	5.8
1	F	796	GLU	5.7
1	F	257	GLY	5.4
1	F	597	TYR	5.4
1	E	676	ASN	5.4
1	D	149	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	753	TRP	5.2
1	C	257	GLY	5.0
1	C	256	ASP	5.0
1	D	1032	LYS	4.9
1	D	732	ASP	4.8
1	F	505	HIS	4.8
1	F	258	SER	4.8
1	D	1031	PHE	4.8
1	C	507	GLU	4.7
1	C	254	ASN	4.7
1	D	954	GLN	4.6
1	A	145	THR	4.6
1	C	739	GLY	4.6
1	F	789	TYR	4.5
1	F	733	GLU	4.5
1	E	537	HIS	4.4
1	B	145	THR	4.4
1	A	869	GLY	4.4
1	C	639	GLY	4.4
1	F	734	LYS	4.4
1	A	636	GLU	4.3
1	C	512	PHE	4.3
1	B	216	SER	4.3
1	D	1030	LEU	4.3
1	B	224	ALA	4.3
1	E	740	VAL	4.2
1	F	255	PRO	4.2
1	B	258	SER	4.2
1	F	639	GLY	4.2
1	C	740	VAL	4.2
1	F	253	VAL	4.2
1	A	657	SER	4.2
1	C	638	PRO	4.1
1	D	537	HIS	4.1
1	C	656	PHE	4.1
1	C	794	LYS	4.1
1	D	144	SER	4.0
1	C	513	PHE	4.0
1	D	253	VAL	4.0
1	B	261	ARG	4.0
1	F	803	PHE	4.0
1	D	267	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	225	VAL	3.9
1	F	791	ARG	3.9
1	C	554	TRP	3.9
1	E	789	TYR	3.8
1	F	802	ALA	3.8
1	E	710	PRO	3.8
1	F	655	PHE	3.8
1	C	741	SER	3.7
1	D	150	THR	3.7
1	A	635	GLU	3.7
1	F	800	PHE	3.7
1	F	645	PHE	3.6
1	F	1033	ASP	3.6
1	E	801	ASN	3.6
1	F	656	PHE	3.6
1	C	505	HIS	3.6
1	C	687	GLN	3.6
1	E	850	LEU	3.6
1	F	259	GLN	3.6
1	F	797	MET	3.6
1	D	259	GLN	3.5
1	A	146	ASP	3.5
1	F	801	ASN	3.5
1	C	796	GLU	3.5
1	A	605	SER	3.5
1	E	216	SER	3.5
1	E	217	GLY	3.4
1	F	252	LYS	3.4
1	A	1030	LEU	3.4
1	F	738	LEU	3.4
1	F	790	VAL	3.4
1	B	256	ASP	3.3
1	C	791	ARG	3.3
1	F	794	LYS	3.3
1	D	661	ALA	3.3
1	D	601	LYS	3.3
1	B	264	ASP	3.3
1	F	740	VAL	3.2
1	A	515	TRP	3.2
1	C	736	SER	3.2
1	E	705	LEU	3.2
1	F	661	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	601	LYS	3.2
1	C	733	GLU	3.2
1	F	653	MET	3.2
1	F	198	LEU	3.1
1	C	732	ASP	3.1
1	D	515	TRP	3.1
1	D	789	TYR	3.1
1	F	256	ASP	3.1
1	F	641	GLU	3.1
1	A	320	GLY	3.1
1	C	589	VAL	3.1
1	D	641	GLU	3.1
1	D	321	MET	3.1
1	E	810	TYR	3.1
1	D	143	VAL	3.0
1	E	786	SER	3.0
1	B	263	LYS	3.0
1	D	740	VAL	3.0
1	C	802	ALA	3.0
1	C	255	PRO	3.0
1	D	597	TYR	3.0
1	F	260	VAL	3.0
1	F	735	ALA	3.0
1	F	1031	PHE	3.0
1	D	252	LYS	3.0
1	C	734	LYS	3.0
1	B	230	LEU	3.0
1	B	249	ILE	3.0
1	D	790	VAL	3.0
1	C	597	TYR	3.0
1	C	506	GLY	3.0
1	E	660	ASP	3.0
1	B	255	PRO	2.9
1	D	362	PHE	2.9
1	C	144	SER	2.9
1	A	954	GLN	2.9
1	B	251	LEU	2.9
1	D	145	THR	2.9
1	D	657	SER	2.9
1	B	229	GLN	2.9
1	D	658	PHE	2.9
1	B	257	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	1030	LEU	2.9
1	F	745	ILE	2.9
1	E	800	PHE	2.9
1	A	868	SER	2.9
1	E	261	ARG	2.9
1	B	322	LYS	2.9
1	D	257	GLY	2.9
1	D	148	SER	2.8
1	B	254	ASN	2.8
1	C	753	TRP	2.8
1	E	799	PRO	2.8
1	D	539	ALA	2.8
1	A	255	PRO	2.8
1	D	533	SER	2.8
1	F	799	PRO	2.8
1	B	537	HIS	2.8
1	B	193	LEU	2.8
1	C	600	GLU	2.8
1	E	709	ASN	2.8
1	A	499	PRO	2.8
1	C	803	PHE	2.8
1	A	834	LEU	2.8
1	F	196	TYR	2.8
1	D	258	SER	2.7
1	D	577	GLN	2.7
1	F	743	ALA	2.7
1	B	253	VAL	2.7
1	E	599	LEU	2.7
1	F	792	ASN	2.7
1	B	250	LEU	2.7
1	F	660	ASP	2.7
1	C	708	GLN	2.6
1	E	805	THR	2.6
1	D	783	ASP	2.6
1	D	254	ASN	2.6
1	F	319	GLN	2.6
1	F	808	TRP	2.6
1	F	793	ASP	2.6
1	B	194	ASN	2.6
1	E	641	GLU	2.6
1	C	522	SER	2.6
1	A	711	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	839	ALA	2.6
1	E	254	ASN	2.6
1	E	678	THR	2.6
1	D	793	ASP	2.6
1	B	362	PHE	2.6
1	E	706	ALA	2.6
1	C	808	TRP	2.5
1	E	197	GLN	2.5
1	A	537	HIS	2.5
1	C	735	ALA	2.5
1	C	704	MET	2.5
1	F	798	VAL	2.5
1	F	195	SER	2.5
1	C	321	MET	2.5
1	A	535	LEU	2.5
1	B	710	PRO	2.5
1	F	657	SER	2.5
1	F	230	LEU	2.5
1	C	196	TYR	2.4
1	C	252	LYS	2.4
1	E	849	GLN	2.4
1	C	805	THR	2.4
1	D	147	GLY	2.4
1	F	512	PHE	2.4
1	A	538	ARG	2.4
1	F	658	PHE	2.4
1	A	840	MET	2.4
1	C	28	LEU	2.4
1	A	1027	VAL	2.4
1	A	871	GLN	2.4
1	D	1029	THR	2.4
1	E	797	MET	2.4
1	D	517	ASN	2.4
1	A	894	TRP	2.4
1	E	707	ALA	2.4
1	A	263	LYS	2.4
1	C	615	PHE	2.3
1	A	362	PHE	2.3
1	E	739	GLY	2.3
1	B	260	VAL	2.3
1	F	254	ASN	2.3
1	C	260	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	214	ILE	2.3
1	E	195	SER	2.3
1	E	600	GLU	2.3
1	A	710	PRO	2.3
1	E	712	LEU	2.3
1	B	513	PHE	2.3
1	C	653	MET	2.3
1	D	598	LEU	2.3
1	E	230	LEU	2.3
1	C	268	VAL	2.2
1	F	145	THR	2.2
1	C	709	ASN	2.2
1	F	854	VAL	2.2
1	B	835	SER	2.2
1	F	264	ASP	2.2
1	D	955	GLY	2.2
1	E	539	ALA	2.2
1	E	513	PHE	2.2
1	E	253	VAL	2.2
1	B	315	PRO	2.2
1	E	845	GLU	2.2
1	F	647	LEU	2.2
1	E	989	ILE	2.2
1	E	733	GLU	2.2
1	C	319	GLN	2.2
1	C	320	GLY	2.2
1	C	792	ASN	2.2
1	C	601	LYS	2.2
1	F	748	THR	2.2
1	D	640	GLY	2.2
1	F	522	SER	2.2
1	F	594	MET	2.2
1	F	511	GLY	2.2
1	E	658	PHE	2.2
1	D	534	ILE	2.2
1	F	601	LYS	2.2
1	D	894	TRP	2.1
1	F	515	TRP	2.1
1	D	244	GLU	2.1
1	E	255	PRO	2.1
1	A	257	GLY	2.1
1	C	852	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	853	GLY	2.1
1	E	791	ARG	2.1
1	A	603	SER	2.1
1	F	606	VAL	2.1
1	A	319	GLN	2.1
1	B	149	MET	2.1
1	E	639	GLY	2.1
1	C	557	THR	2.1
1	A	253	VAL	2.1
1	B	338	HIS	2.1
1	C	777	ASP	2.1
1	D	639	GLY	2.1
1	B	252	LYS	2.1
1	B	506	GLY	2.1
1	C	775	ARG	2.1
1	F	718	ASN	2.1
1	A	849	GLN	2.0
1	D	535	LEU	2.0
1	A	891	TYR	2.0
1	C	641	GLU	2.0
1	C	524	THR	2.0
1	E	194	ASN	2.0
1	D	796	GLU	2.0
1	E	795	GLY	2.0
1	F	747	SER	2.0
1	E	260	VAL	2.0
1	A	867	LEU	2.0
1	B	197	GLN	2.0
1	C	776	PRO	2.0
1	D	869	GLY	2.0
1	D	961	ALA	2.0
1	B	196	TYR	2.0
1	D	655	PHE	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 ⓘ

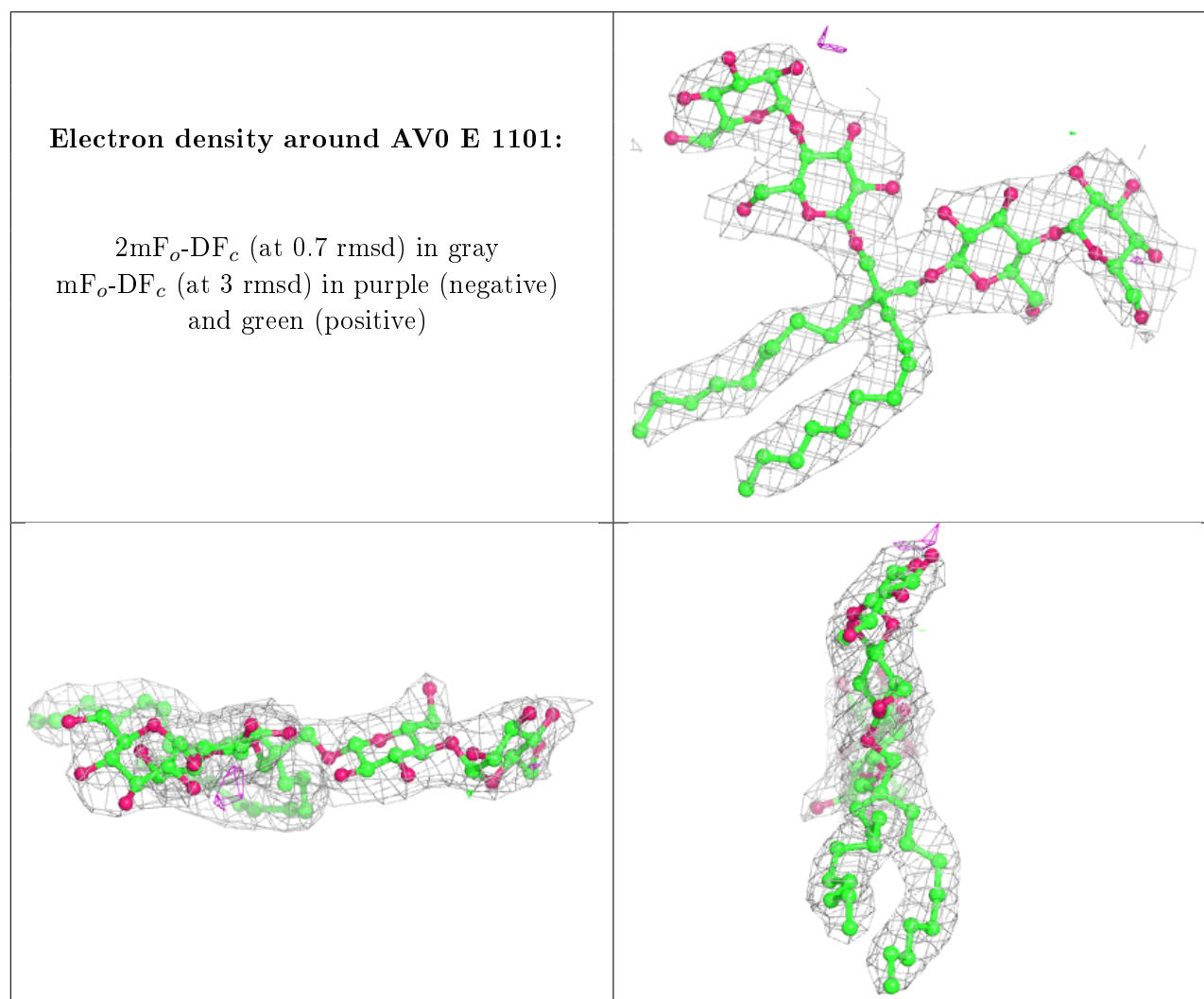
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

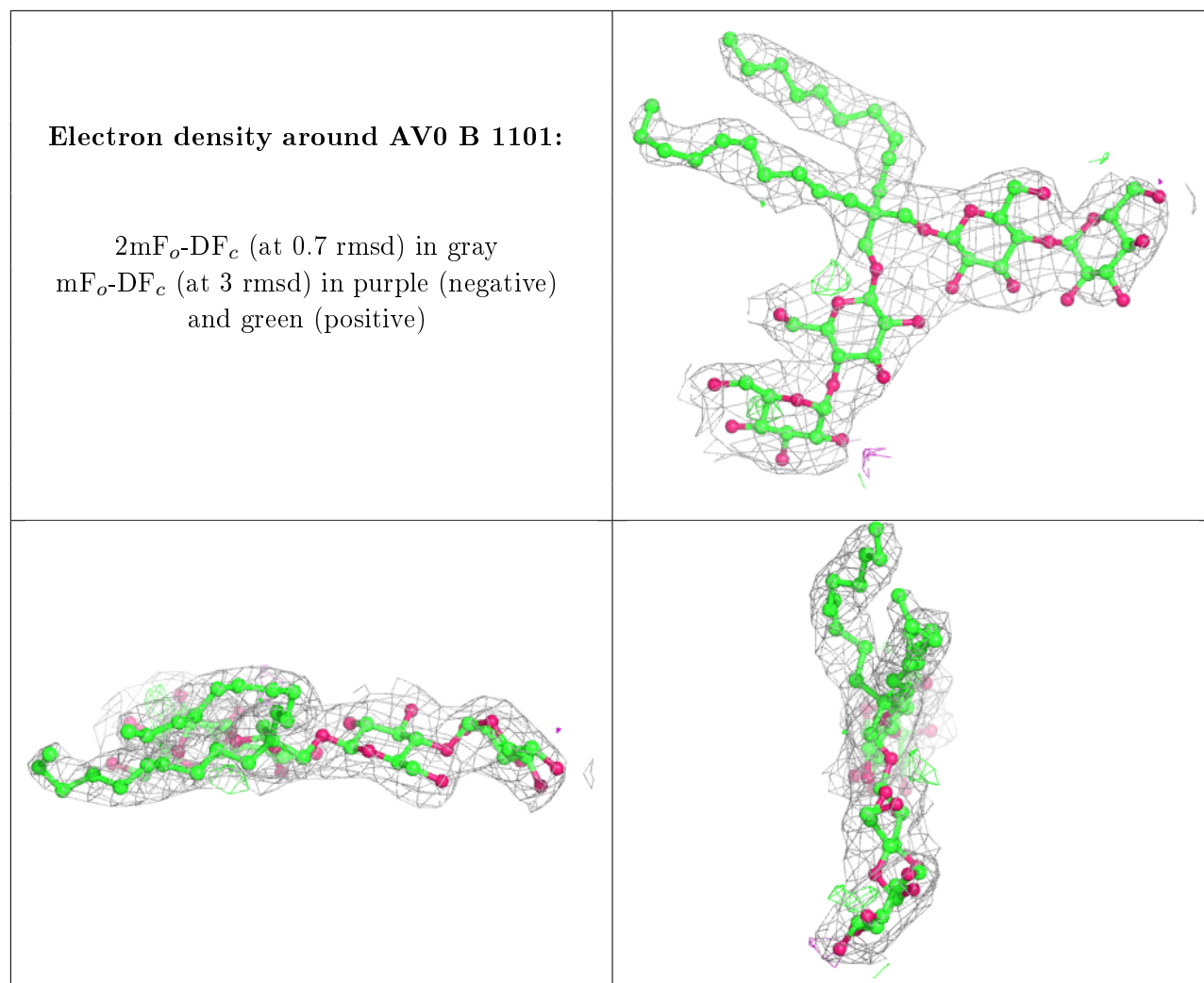
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AV0	E	1101	69/69	0.93	0.18	30,49,65,69	0
2	AV0	B	1101	69/69	0.93	0.19	29,46,63,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.