



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 6IIA / pdb_00006iia
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

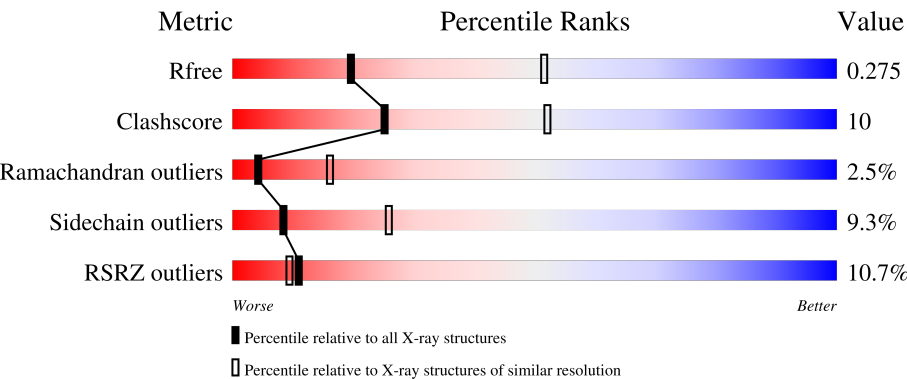
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1052	10% 69% 23% • •
1	B	1052	5% 71% 23% • •
1	C	1052	13% 65% 27% 5% •
1	D	1052	12% 71% 22% • •
1	E	1052	10% 69% 25% • • •

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Mol	Chain	Length	Quality of chain
1	F	1052	13% 71% 23%

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:

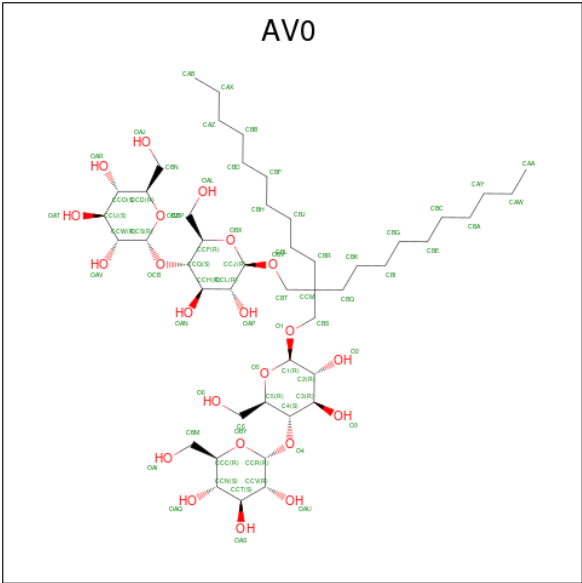
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression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

- Molecule 2 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂).

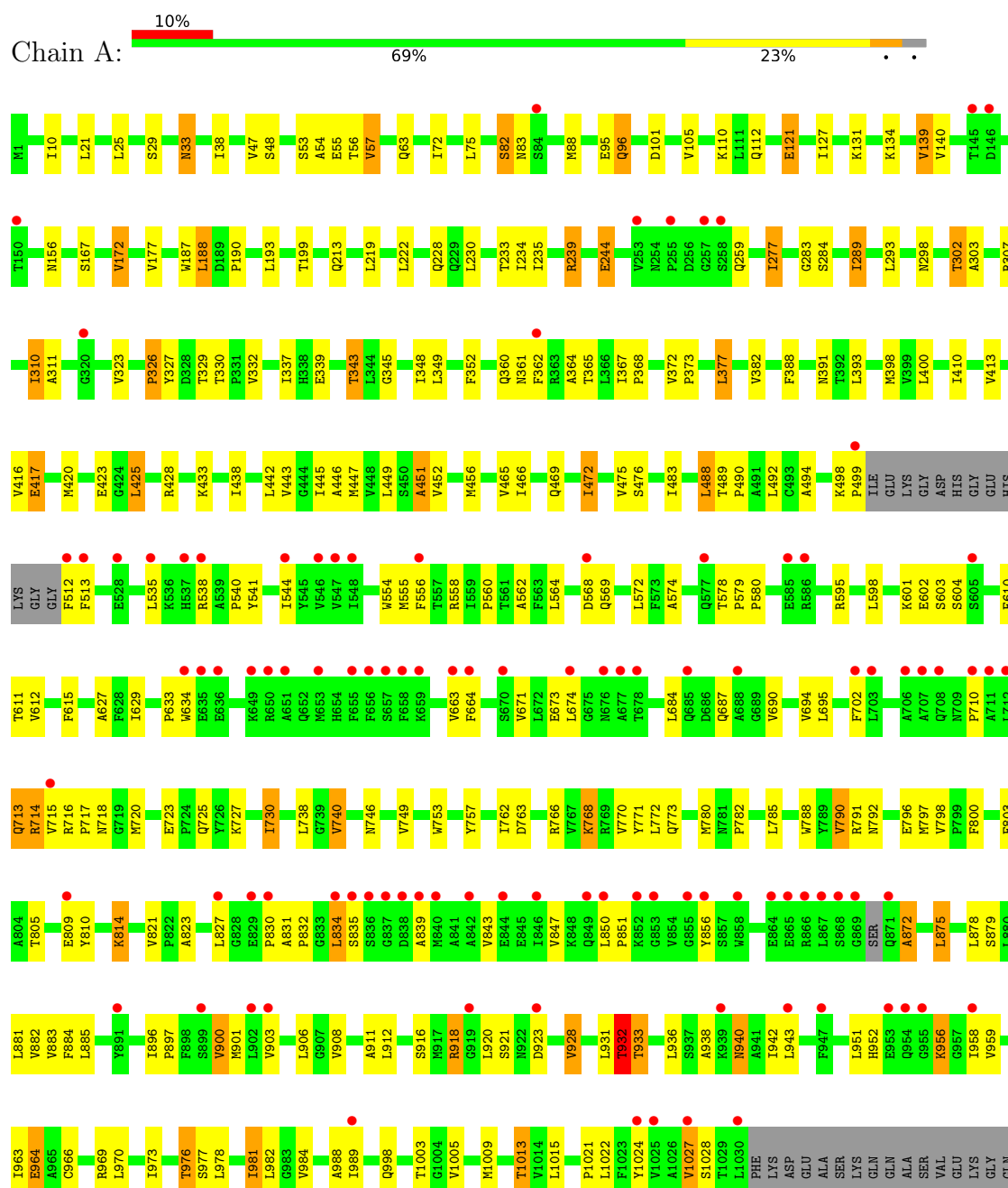


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			69	47	22		
2	E	1	Total	C	O	0	0
			69	47	22		

3 Residue-property plots

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

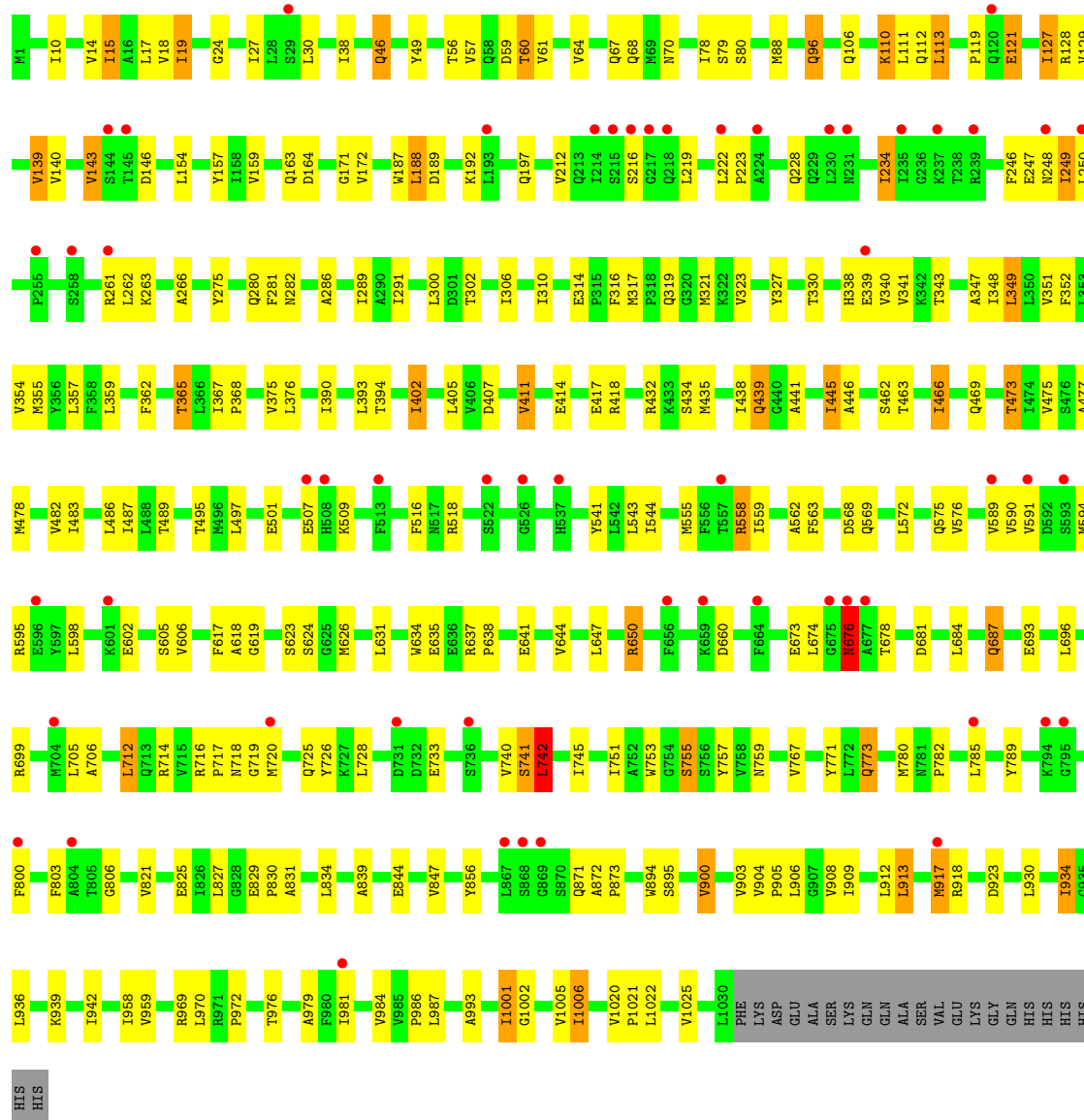
- Molecule 1: Multidrug resistance protein MexB



HIS
HIS
HIS
HIS
HIS
HIS

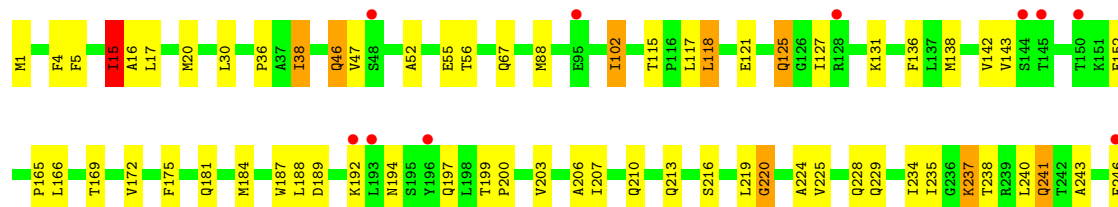
• Molecule 1: Multidrug resistance protein MexB

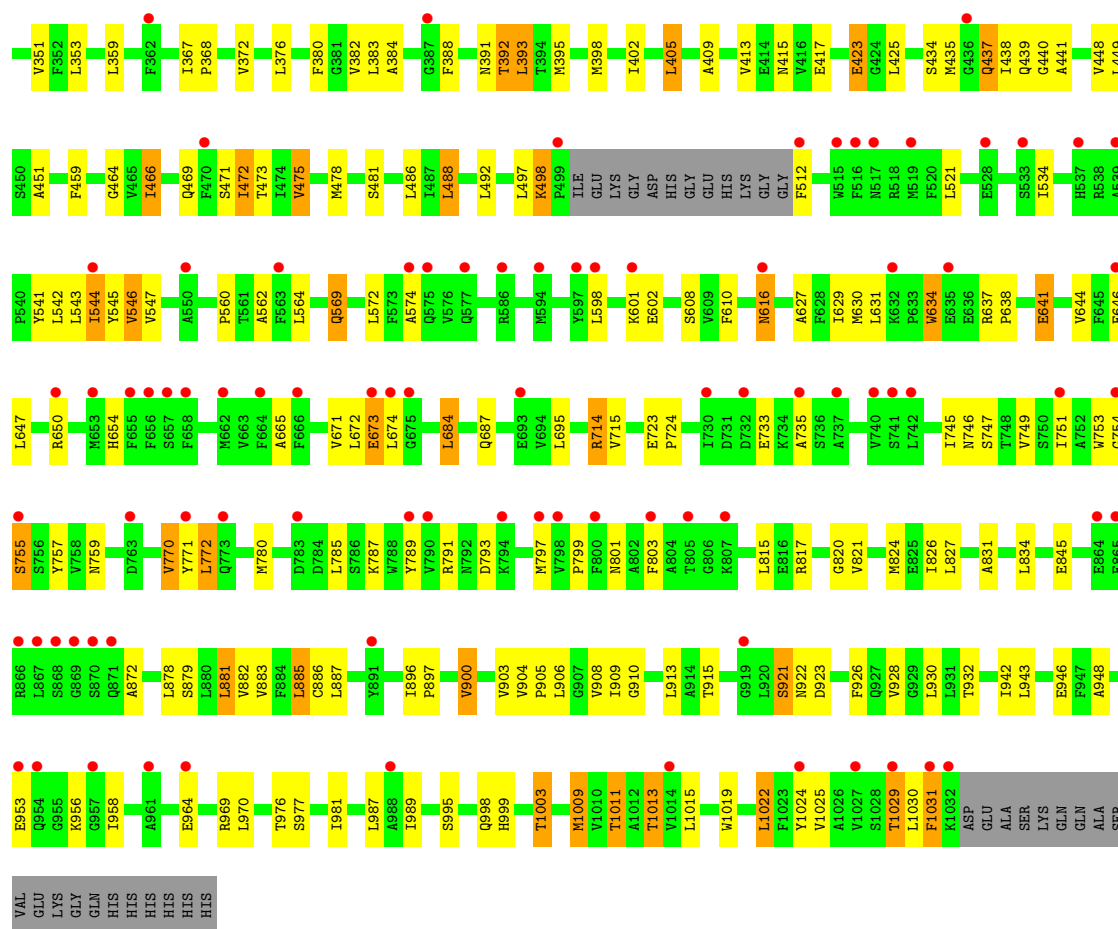
Chain B:  5% 71% 23%



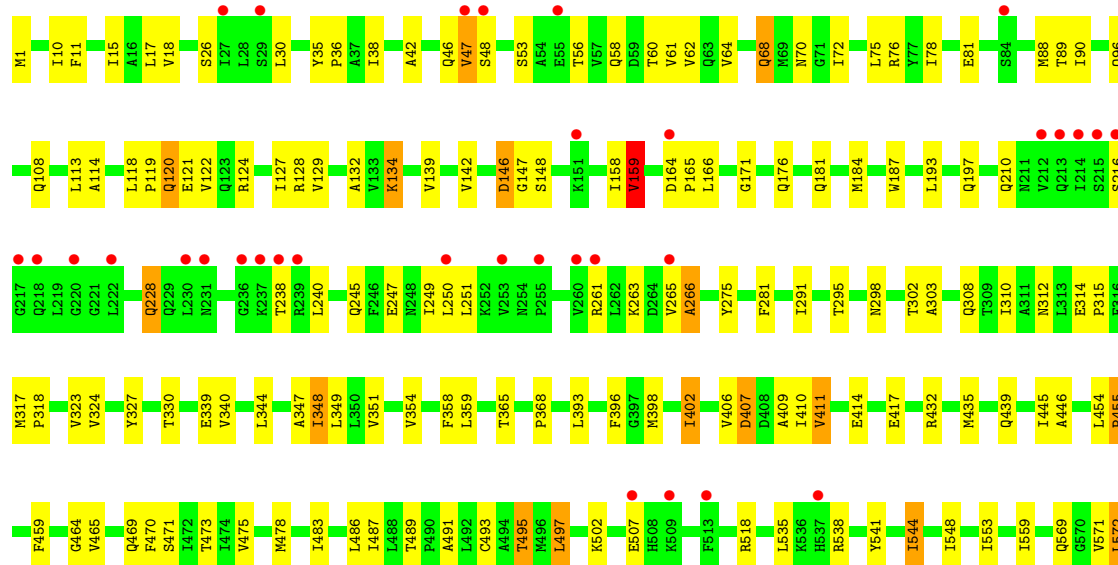
• Molecule 1: Multidrug resistance protein MexB

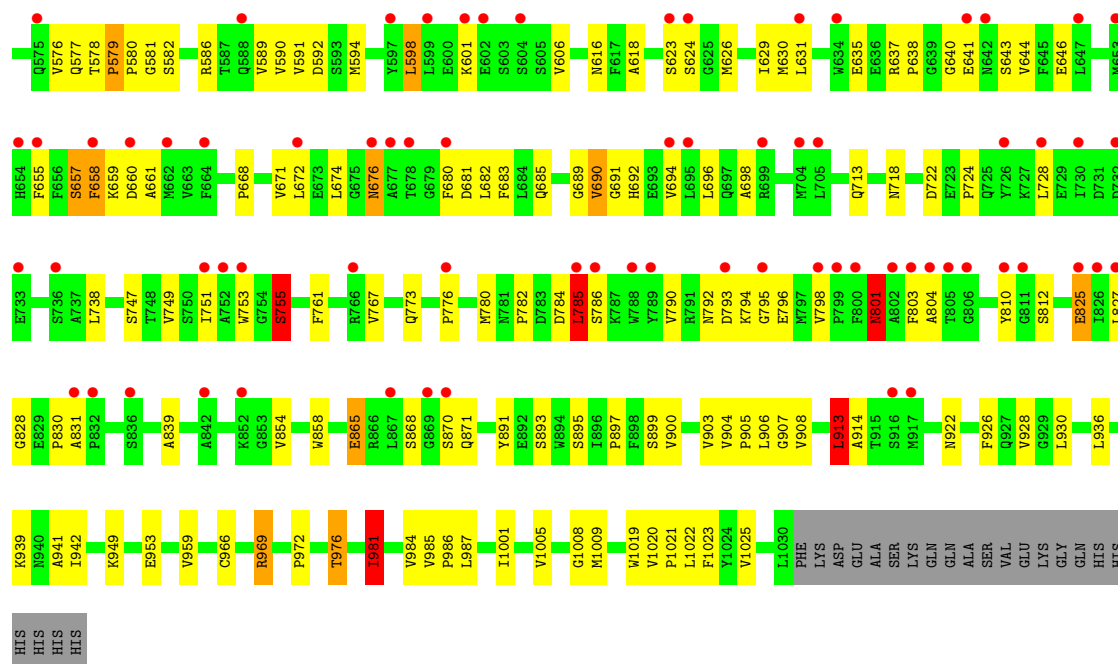
Chain C:  13% 65% 27% 5%



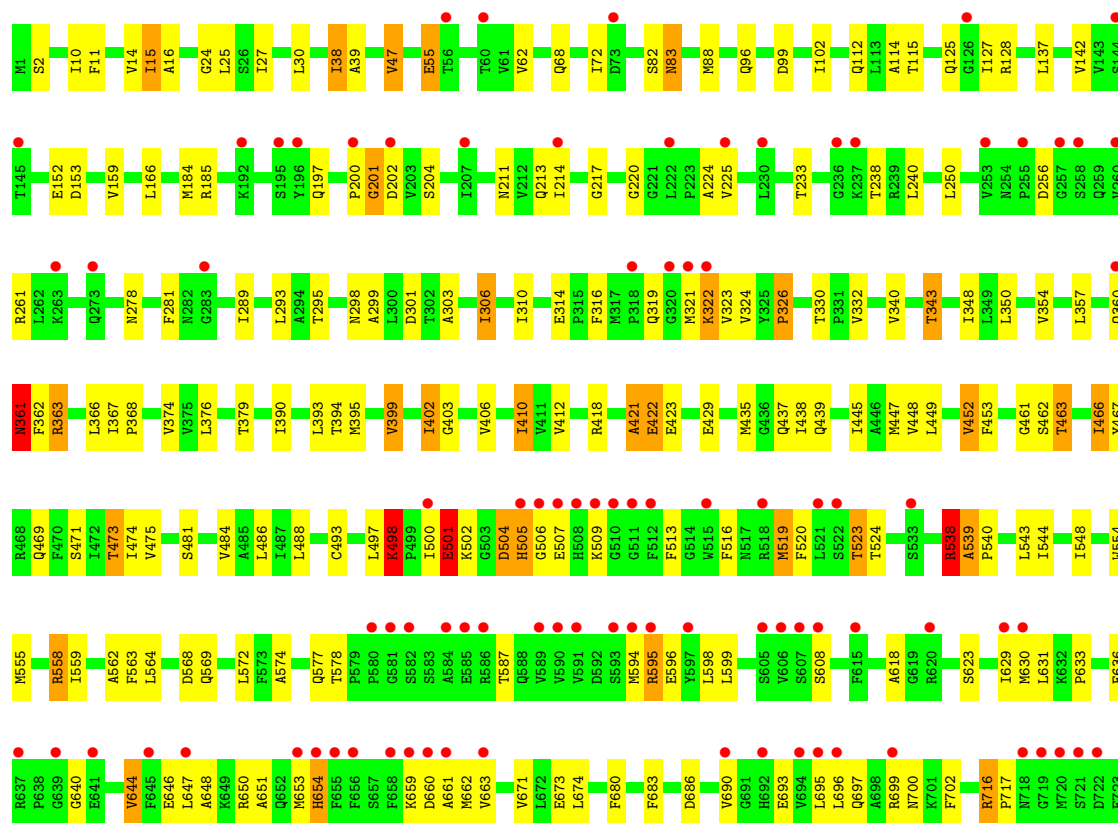


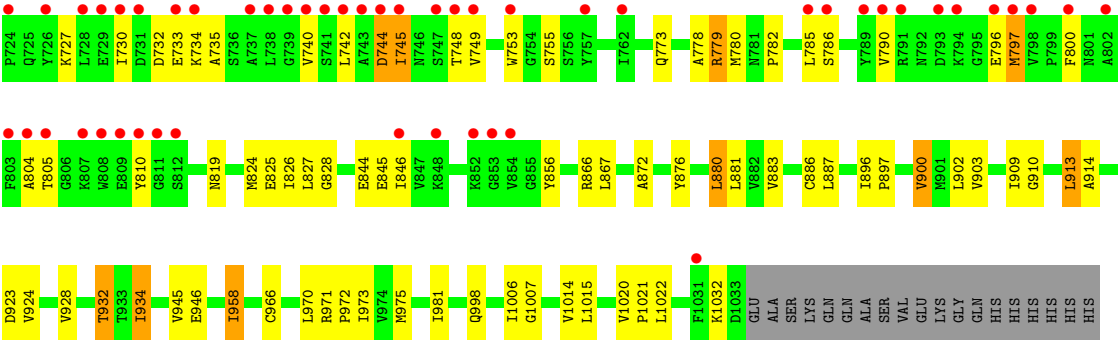
• Molecule 1: Multidrug resistance protein MexB





• Molecule 1: Multidrug resistance protein MexB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.95Å 134.34Å 149.69Å 87.53° 70.20° 89.02°	Depositor
Resolution (Å)	140.73 – 2.91 140.73 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.7 (140.73-2.91) 92.8 (140.73-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.92	1/7873 (0.0%)	1.12	12/10701 (0.1%)
1	B	0.95	0/7971	1.14	19/10833 (0.2%)
1	C	0.88	1/7971 (0.0%)	1.09	14/10833 (0.1%)
1	D	0.87	0/7901	1.08	8/10739 (0.1%)
1	E	0.87	0/7971	1.09	17/10833 (0.2%)
1	F	0.87	1/8000 (0.0%)	1.08	6/10871 (0.1%)
All	All	0.89	3/47687 (0.0%)	1.10	76/64810 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	LYS	C-O	-5.49	1.17	1.23
1	F	399	VAL	C-O	-5.37	1.18	1.24
1	A	82	SER	C-O	-5.22	1.18	1.23

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	569	GLN	N-CA-C	7.83	122.54	113.38
1	B	489	THR	CA-C-N	-7.30	111.46	119.19
1	B	489	THR	C-N-CA	-7.30	111.46	119.19
1	F	498	LYS	CA-C-N	7.08	127.11	119.89
1	F	498	LYS	C-N-CA	7.08	127.11	119.89
1	E	538	ARG	N-CA-C	6.88	118.67	111.03
1	B	569	GLN	N-CA-C	-6.79	101.39	110.55
1	F	900	VAL	N-CA-C	6.78	117.54	110.62
1	D	498	LYS	N-CA-C	6.59	124.37	109.81
1	E	411	VAL	N-CA-CB	6.41	119.25	110.54
1	E	579	PRO	N-CA-C	6.37	118.47	110.70
1	B	411	VAL	N-CA-CB	6.34	117.97	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	448	VAL	N-CA-CB	6.32	117.94	110.55
1	A	569	GLN	N-CA-C	6.14	120.36	112.86
1	C	548	ILE	CB-CA-C	-6.03	103.98	111.70
1	B	46	GLN	N-CA-C	5.96	118.92	109.50
1	F	548	ILE	CB-CA-C	-5.93	104.38	111.97
1	E	553	ILE	CB-CA-C	-5.81	104.45	111.88
1	C	909	ILE	N-CA-CB	5.69	116.83	110.51
1	C	1006	ILE	CB-CA-C	-5.66	104.63	112.04
1	E	601	LYS	N-CA-C	5.65	117.25	111.14
1	E	407	ASP	N-CA-C	5.65	117.89	111.11
1	F	924	VAL	N-CA-CB	5.63	116.76	110.51
1	A	235	ILE	CB-CA-C	5.62	118.39	111.25
1	B	15	ILE	CB-CA-C	-5.60	104.54	111.70
1	C	15	ILE	N-CA-CB	5.57	118.11	110.54
1	A	981	ILE	CB-CA-C	-5.54	104.88	111.97
1	B	15	ILE	N-CA-CB	5.53	116.43	110.62
1	D	415	ASN	N-CA-C	5.53	117.39	111.36
1	B	402	ILE	N-CA-C	5.52	116.15	110.36
1	E	626	MET	N-CA-C	5.49	116.48	108.14
1	B	1006	ILE	CB-CA-C	-5.48	104.69	111.70
1	C	709	ASN	CA-C-N	5.46	125.12	119.05
1	C	709	ASN	C-N-CA	5.46	125.12	119.05
1	C	475	VAL	N-CA-CB	5.40	117.88	110.54
1	C	821	VAL	CA-C-N	-5.39	114.41	119.85
1	C	821	VAL	C-N-CA	-5.39	114.41	119.85
1	A	872	ALA	CA-C-N	-5.38	114.13	119.56
1	A	872	ALA	C-N-CA	-5.38	114.13	119.56
1	D	348	ILE	N-CA-CB	5.37	117.44	110.57
1	E	10	ILE	N-CA-CB	5.36	116.82	110.55
1	B	773	GLN	N-CA-C	5.33	115.58	108.38
1	B	606	VAL	N-CA-C	5.33	116.26	108.58
1	B	981	ILE	N-CA-CB	5.32	116.78	110.55
1	E	159	VAL	N-CA-CB	5.31	117.77	110.54
1	C	559	ILE	N-CA-CB	5.28	114.99	110.08
1	E	801	ASN	N-CA-C	5.27	119.47	113.19
1	A	790	VAL	N-CA-C	-5.27	101.48	108.96
1	A	172	VAL	N-CA-CB	5.26	117.00	111.00
1	C	207	ILE	CB-CA-C	-5.26	105.24	111.97
1	E	358	PHE	N-CA-C	5.26	118.86	112.23
1	D	616	ASN	CB-CA-C	5.26	118.18	109.72
1	B	19	ILE	N-CA-CB	5.25	117.68	110.54
1	A	823	ALA	N-CA-C	5.23	115.26	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	GLY	CA-C-N	5.22	125.06	120.10
1	C	220	GLY	C-N-CA	5.22	125.06	120.10
1	A	277	ILE	CB-CA-C	-5.21	104.06	111.21
1	E	266	ALA	N-CA-C	5.21	116.20	108.60
1	D	163	GLN	N-CA-C	5.15	116.58	111.07
1	B	80	SER	N-CA-C	5.13	116.99	109.24
1	A	362	PHE	N-CA-CB	5.13	117.45	110.01
1	B	96	GLN	N-CA-CB	5.12	117.56	109.83
1	B	466	ILE	N-CA-CB	5.11	116.19	110.51
1	A	633	PRO	CA-C-N	5.11	127.55	120.29
1	A	633	PRO	C-N-CA	5.11	127.55	120.29
1	E	981	ILE	N-CA-CB	5.09	116.83	110.47
1	E	46	GLN	N-CA-C	5.08	117.67	108.69
1	D	546	VAL	CB-CA-C	-5.05	105.31	112.14
1	E	685	GLN	N-CA-C	5.04	117.55	108.48
1	C	46	GLN	N-CA-C	5.04	117.60	108.69
1	B	19	ILE	CB-CA-C	-5.03	105.35	112.14
1	D	107	VAL	N-CA-C	-5.02	105.95	110.82
1	E	489	THR	CA-C-N	-5.02	113.87	119.19
1	E	489	THR	C-N-CA	-5.02	113.87	119.19
1	B	895	SER	CA-C-N	5.01	123.40	120.24
1	B	895	SER	C-N-CA	5.01	123.40	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7718	0	7858	175	0
1	B	7812	0	7944	139	0
1	C	7812	0	7944	200	0
1	D	7744	0	7886	136	0
1	E	7812	0	7944	158	0
1	F	7840	0	7970	146	0
2	B	69	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	69	0	0	0	0
All	All	46876	0	47546	917	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 10.

All (917) 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:E:62:VAL:HG22	1:E:88:MET:HE2	1.58	0.83
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:A:780:MET:HE1	1:C:224:ALA:HB1	1.65	0.78
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:82:SER:C	1:F:83:ASN:HD22	2.04	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: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:46:GLN:HA	1:C:88:MET:HE3	1.77	0.65
1:C:367:ILE:HD11	1:C:496:MET:HB2	1.78	0.65
1:B:282:ASN:C	1:B:595:ARG:HD2	2.22	0.64
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:456:MET:HE3	1:A:931:LEU:HD12	1.80	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:C:418:ARG:HD2	1:C:968:MET:HE2	1.79	0.63
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: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:D:213:GLN:HG3	1:E:56:THR:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:412:VAL:HG13	1:F:435:MET:HE1	1.84	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:B:157:TYR:CG	1:B:321:MET:HE1	2.37	0.59
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: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:OAI	2:B:1101:AV0:OAQ	2.19	0.59
1:C:340:VAL:HA	1:C:343:THR:HG23	1.85	0.59
1:C:555:MET:HE2	1:C:913:LEU:HD23	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:D:780:MET:HE1	1:F:224:ALA:HB1	1.84	0.58
1:F:539:ALA:HB3	1:F:540:PRO:CD	2.32	0.58
1:C:1009:MET:HE3	1:C:1009:MET:HA	1.85	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
1:C:357:LEU:HD23	1:C:357:LEU:O	2.04	0.58
1:F:572:LEU:HB3	1:F:629:ILE:HB	1.86	0.58
1:C:357:LEU:HD23	1:C:357:LEU:C	2.29	0.57
1:F:410:ILE:C	1:F:410:ILE:HD12	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:791:ARG:HG3	1:A:797:MET:HE2	1.85	0.57
1:F:782:PRO:O	1:F:785:LEU:HG	2.05	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:D:47:VAL:HG12	1:D:88:MET:HE2	1.86	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:C:934:ILE:C	1:C:934:ILE:HD13	2.29	0.56
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:A:303:ALA:HB2	1:A:330:THR:HG21	1.86	0.56
1:A:780:MET:HE3	1:C:228:GLN:CD	2.31	0.56
1:B:317:MET:HE1	1:B:323:VAL:HG13	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:745:ILE:O	1:D:749:VAL:HG23	2.05	0.56
1:D:906:LEU:O	1:D:1011:THR:HB	2.05	0.56
1:E:303:ALA:HB2	1:E:330:THR:HG21	1.86	0.56
1:E:317:MET:HE1	1:E:323:VAL:HG13	1.86	0.56
1:E:689:GLY:O	1:E:691:GLY:N	2.38	0.56
1:A:554:TRP:CH2	1:A:558:ARG:HD2	2.40	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:E:314:GLU:HA	1:E:317:MET:HE2	1.87	0.56
1:F:568:ASP:OD1	1:F:644:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:931:LEU:C	1:A:933:THR:H	2.14	0.56
1:C:317:MET:SD	1:C:321:MET:HE2	2.47	0.55
1:D:124:ARG:NH2	1:D:757:TYR:CD2	2.74	0.55
1:D:197:GLN:HA	1:D:797:MET:SD	2.46	0.55
1:D:347:ALA:O	1:D:351:VAL:HG23	2.06	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:C:138:MET:HE1	1:C:306:ILE:HD11	1.88	0.55
1:F:447:MET:HE3	1:F:886:CYS:HB3	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:HG12	1:F:159:VAL:O	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:F:555:MET:HE2	1:F:913:LEU:HD23	1.88	0.55
1:A:634:TRP:H	1:A:634:TRP:CD1	2.24	0.54
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:47:VAL:HG12	1:A:88:MET:HE3	1.90	0.54
1:A:382:VAL:HG21	1:A:476:SER:OG	2.08	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:HH11	1:F:538:ARG:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:713:GLN:O	1:A:714:ARG:HB2	2.07	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
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:C:410:ILE:HD12	1:C:410:ILE:C	2.33	0.53
1:C:910:GLY:O	1:C:1007:GLY:C	2.51	0.53
1:E:171:GLY:HA3	1:E:302:THR:HG22	1.91	0.53
1:A:57:VAL:HG21	1:A:88:MET:HB3	1.91	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:F:184:MET:HE3	1:F:184:MET:HA	1.91	0.52
1:A:763:ASP:HB3	1:A:768:LYS:HD3	1.91	0.52
1:A:1024:TYR:O	1:A:1028:SER:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:942:ILE:HD12	1:C:942:ILE:C	2.34	0.52
1:A:562:ALA:O	1:A:923:ASP:HA	2.10	0.52
1:B:617:PHE:CD2	1:B:626:MET:HE1	2.45	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
1:A:239:ARG:HH11	1:A:239:ARG:CG	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:189:ASP:HA	1:C:775:ARG:HD3	1.91	0.52
1:C:469:GLN:O	1:C:473:THR:HG23	2.10	0.52
1:C:816:GLU:OE1	1:C:824:MET:HA	2.10	0.52
1:F:298:ASN:O	1:F:299:ALA:C	2.51	0.52
1:A:348:ILE:HD12	1:A:372:VAL:HG11	1.91	0.51
1:D:78:ILE:HD11	1:D:90:ILE:CG2	2.40	0.51
1:D:754:GLY:O	1:D:755:SER:CB	2.58	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:D:48:SER:O	1:D:125:GLN:HG2	2.11	0.51
1:D:791:ARG:HB2	1:D:797:MET:HE3	1.92	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:E:61:VAL:HG12	1:E:88:MET:HE3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:753:TRP:CZ2	1:B:785:LEU:HB3	2.46	0.51
1:B:1002:GLY:O	1:B:1006:ILE:HG12	2.11	0.51
1:C:964:GLU:O	1:C:968:MET:HG3	2.11	0.51
1:D:831:ALA:HB3	1:D:834:LEU:HD12	1.92	0.51
1:D:1009:MET:O	1:D:1013:THR:HG22	2.10	0.51
1:F:717:PRO:HA	1:F:826:ILE:HG22	1.93	0.51
1:A:101:ASP:O	1:A:105:VAL:HG23	2.11	0.51
1:A:112:GLN:HG3	1:B:112:GLN:CD	2.36	0.51
1:A:1009:MET:O	1:A:1013:THR:HG23	2.11	0.51
1:C:928:VAL:O	1:C:932:THR:HG22	2.10	0.51
1:F:321:MET:O	1:F:322:LYS:C	2.54	0.51
1:B:930:LEU:O	1:B:934:ILE:HG23	2.11	0.51
1:D:780:MET:HE2	1:F:225:VAL:HG22	1.91	0.51
1:F:211:ASN:HA	1:F:240:LEU:HD13	1.91	0.51
1:B:676:ASN:HD22	1:B:676:ASN:C	2.19	0.51
1:C:592:ASP:O	1:C:595:ARG:HG3	2.11	0.51
1:D:943:LEU:HD13	1:D:969:ARG:HH21	1.76	0.51
1:F:410:ILE:HD13	1:F:975:MET:HE2	1.93	0.51
1:F:498:LYS:HE3	1:F:498:LYS:H	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:75:LEU:C	1:A:75:LEU:HD23	2.35	0.50
1:A:140:VAL:HB	1:A:289:ILE:CD1	2.41	0.50
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.93	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:682:LEU:HD21	1:C:826:ILE:HG13	1.93	0.50
1:C:1020:VAL:HB	1:C:1021:PRO:HD3	1.93	0.50
1:F:99:ASP:HB3	1:F:102:ILE:HG12	1.94	0.50
1:F:554:TRP:CZ2	1:F:558:ARG:HD3	2.46	0.50
1:A:791:ARG:HB2	1:A:797:MET:HE1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:142:VAL:HG21	1:C:321:MET:HE3	1.94	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:407:ASP:OD1	1:E:976:THR:HG21	2.11	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:F:504:ASP:O	1:F:505:HIS:C	2.55	0.50
1:A:310:ILE:HG13	1:A:311:ALA:N	2.27	0.49
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:449:LEU:HD13	1:A:449:LEU:C	2.37	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:F:903:VAL:CG2	1:F:1020:VAL:HG22	2.43	0.49
1:D:380:PHE:CZ	1:D:398:MET:HE3	2.47	0.49
1:D:405:LEU:C	1:D:405:LEU:HD12	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:VAL:HG13	1:A:82:SER:HB3	1.95	0.49
1:A:555:MET:HB2	1:A:912:LEU:HD13	1.94	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:594:MET:HE3	1:E:655:PHE:CE2	2.47	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:718:ASN:HB2	1:A:827:LEU:HD22	1.95	0.48
1:A:746:ASN:HD21	1:C:237:LYS:HD2	1.78	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:E:657:SER:O	1:E:658:PHE:C	2.55	0.48
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.38	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
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:A:780:MET:CE	1:C:224:ALA:HB1	2.39	0.48
1:B:568:ASP:OD1	1:B:644:VAL:HG23	2.13	0.48
1:C:361:ASN:O	1:C:362:PHE:C	2.56	0.48
1:C:453:PHE:HZ	1:C:932:THR:HB	1.78	0.48
1:D:754:GLY:HA2	1:F:217:GLY:HA2	1.94	0.48
1:E:984:VAL:HG11	1:E:1005:VAL:HG21	1.95	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:B:338:HIS:C	1:B:340:VAL:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:ILE:HD13	1:B:1001:ILE:C	2.38	0.48
1:D:329:THR:O	1:D:332:VAL:HG12	2.13	0.48
1:A:780:MET:HE2	1:C:225:VAL:HG22	1.96	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:F:913:LEU:O	1:F:914:ALA:C	2.56	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:HG12	1:A:663:VAL:O	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:SER:O	1:D:340:VAL:HG23	2.12	0.47
1:D:780:MET:CE	1:F:220:GLY:HA2	2.43	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:N	1:E:127:ILE:HD12	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:F:650:ARG:O	1:F:651:ALA:C	2.56	0.47
1:B:478:MET:O	1:B:482:VAL:HG23	2.14	0.47
1:C:406:VAL:O	1:C:407:ASP:C	2.57	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:F:390:ILE:HG23	1:F:395:MET:HE3	1.96	0.47
1:F:699:ARG:HD2	1:F:824:MET:HE1	1.96	0.47
1:C:648:ALA:HA	1:C:651:ALA:HB3	1.96	0.47
1:D:630:MET:HE3	1:D:630:MET:HA	1.96	0.47
1:E:396:PHE:CD1	1:E:1001:ILE:HD11	2.50	0.47
1:F:574:ALA:HB3	1:F:594:MET:HE1	1.97	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:B:972:PRO:O	1:B:976:THR:HG22	2.15	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:F:24:GLY:O	1:F:25:LEU:C	2.58	0.47
1:F:96:GLN:CD	1:F:461:GLY:O	2.57	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:791:ARG:HD3	1:A:797:MET:HE1	1.97	0.46
1:C:102:ILE:HD12	1:C:102:ILE:C	2.40	0.46
1:C:184:MET:HE2	1:C:268:VAL:HG13	1.97	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:E:784:ASP:C	1:E:786:SER:H	2.23	0.46
1:F:438:ILE:O	1:F:439:GLN:C	2.59	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:E:985:VAL:HB	1:E:986:PRO:HD3	1.97	0.46
1:F:361:ASN:C	1:F:361:ASN:HD22	2.23	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:A:88:MET:SD	1:A:88:MET:C	2.98	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:B:46:GLN:HA	1:B:88:MET:HE3	1.96	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:B:314:GLU:HA	1:B:317:MET:HE2	1.98	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:A:791:ARG:HD3	1:A:797:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:303:ALA:C	1:F:306:ILE:HG22	2.41	0.46
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:B:830:PRO:HB3	1:B:839:ALA:HB2	1.99	0.45
1:B:984:VAL:HG21	1:B:1005:VAL:HG21	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: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:445:ILE:HD12	1:A:446:ALA:N	2.31	0.45
1:A:918:ARG:HE	1:A:1003:THR:HG21	1.82	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:F:310:ILE:C	1:F:310:ILE:HD12	2.42	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:421:ALA:O	1:F:422:GLU:C	2.59	0.45
1:F:872:ALA:HB1	1:F:876:TYR:CE2	2.51	0.45
1:A:156:ASN:OD1	1:A:768:LYS:NZ	2.48	0.45
1:A:538:ARG:HG3	1:A:1022:LEU:HD21	1.98	0.45
1:C:395:MET:HE2	1:C:398:MET:HG3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:785:LEU:HD12	1:F:786:SER:N	2.31	0.45
1:A:228:GLN:HG2	1:B:780:MET:CE	2.46	0.45
1:B:984:VAL:HG11	1:B:1005:VAL:CG2	2.46	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:A:33:ASN:O	1:A:391:ASN:HA	2.17	0.45
1:A:329:THR:O	1:A:332:VAL:HG12	2.16	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:C:175:PHE:C	1:C:175:PHE:CD1	2.95	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: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:C:449:LEU:HD12	1:C:478:MET:HE2	1.99	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:966:CYS:SG	1:A:1021:PRO:HB3	2.57	0.44
1:A:977:SER:HB3	1:A:1013:THR:HG21	1.98	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: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:B:163:GLN:O	1:B:164:ASP:C	2.60	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:244:GLU:CD	1:A:244:GLU:H	2.25	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:E:895:SER:C	1:E:897:PRO:HD2	2.42	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:60:THR:HG22	1:B:61:VAL:HG23	1.99	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: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:D:451:ALA:HB1	1:D:882:VAL:HG12	1.99	0.44
1:A:239:ARG:HH11	1:A:239:ARG:HG2	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: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:C:17:LEU:HD23	1:C:20:MET:HE3	2.00	0.44
1:C:328:ASP:OD1	1:C:328:ASP:C	2.61	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: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:454:LEU:O	1:E:455:PRO:C	2.62	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:E:327:TYR:HB2	1:E:630:MET:HE1	1.99	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:A:936:LEU:HD12	1:A:1009:MET:SD	2.59	0.43
1:B:222:LEU:HA	1:B:223:PRO:C	2.42	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:F:55:GLU:H	1:F:55:GLU:CD	2.26	0.43
1:F:654:HIS:ND1	1:F:654:HIS:C	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:ILE:HG13	1:D:910:GLY:N	2.33	0.43
1:A:63:GLN:OE1	1:C:767:VAL:HG23	2.19	0.43
1:C:399:VAL:O	1:C:402:ILE:CD1	2.66	0.43
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:453:PHE:HB3	1:C:456:MET:HE2	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:30:LEU:HD21	1:D:384:ALA:HA	2.01	0.43
1:D:254:ASN:ND2	1:D:258:SER:O	2.52	0.43
1:F:281:PHE:CE2	1:F:324:VAL:HG11	2.54	0.43
1:B:354:VAL:HG21	1:B:979:ALA:HB2	2.00	0.43
1:B:706:ALA:HB1	1:B:712:LEU:HD12	2.01	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:A:780:MET:HE3	1:C:228:GLN:OE1	2.19	0.42
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:E:26:SER:O	1:E:30:LEU:HB2	2.19	0.42
1:E:68:GLN:HG2	1:E:114:ALA:HB2	2.01	0.42
1:E:1009:MET:HA	1:E:1009:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:SER:O	1:D:57:VAL:HG12	2.19	0.42
1:D:223:PRO:HD3	1:E:275:TYR:CD2	2.54	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
1:A:417:GLU:HA	1:A:420:MET:HE2	2.01	0.42
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:O	1:B:918:ARG:HG2	2.20	0.42
1:C:1:MET:O	1:C:4:PHE:HB3	2.19	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: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:C:380:PHE:CZ	1:C:395:MET:HE1	2.54	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:E:969:ARG:C	1:E:972:PRO:HD2	2.44	0.42
1:C:1011:THR:O	1:C:1015:LEU:HB2	2.19	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:A:884:PHE:HB2	1:A:901:MET:HE2	2.02	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:380:PHE:CE1	1:D:398:MET:HE3	2.55	0.42
1:D:449:LEU:CD1	1:D:478:MET:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:LEU:HD12	1:B:275:TYR:O	2.19	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
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:D:672:LEU:O	1:D:673:GLU:C	2.63	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: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:HD12	1:A:293:LEU:HA	1.84	0.42
1:C:391:ASN:H	1:C:394:THR:HG22	1.85	0.42
1:E:88:MET:HE1	1:E:90:ILE:HD11	2.02	0.42
1:F:399:VAL:O	1:F:402:ILE:HG13	2.19	0.42
1:A:56:THR:HG23	1:C:213:GLN:HG2	2.01	0.41
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:C:547:VAL:O	1:C:550:ALA:HB3	2.20	0.41
1:D:56:THR:HG23	1:F:213:GLN:HG2	2.02	0.41
1:D:391:ASN:ND2	1:D:469:GLN:OE1	2.50	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: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:A:121:GLU:CD	1:A:121:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:452:VAL:HG22	1:A:883:VAL:HG21	2.02	0.41
1:A:981:ILE:HD11	1:A:1009:MET:HB3	2.03	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:845:GLU:C	1:C:847:VAL:H	2.27	0.41
1:C:884:PHE:CE1	1:C:897:PRO:HB2	2.55	0.41
1:D:434:SER:O	1:D:437:GLN:HG2	2.21	0.41
1:D:1030:LEU:HB3	1:D:1031:PHE:CE2	2.56	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:C:743:ALA:HB1	1:C:746:ASN:CG	2.45	0.41
1:D:110:LYS:O	1:D:111:LEU:C	2.64	0.41
1:D:560:PRO:HG2	1:D:921:SER:HB3	2.02	0.41
1:E:228:GLN:OE1	1:F:780:MET:HB3	2.21	0.41
1:E:738:LEU:HD13	1:E:798:VAL:HG11	2.03	0.41
1:F:316:PHE:N	1:F:316:PHE:CD1	2.89	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:438:ILE:HG13	1:D:439:GLN:N	2.35	0.41
1:F:749:VAL:HA	1:F:753:TRP:CZ3	2.56	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
1:A:702:PHE:CZ	1:A:843:VAL:HG13	2.54	0.41
1:A:740:VAL:HG13	1:A:790:VAL:HG11	2.01	0.41
1:A:896:ILE:N	1:A:897:PRO:HD2	2.35	0.41
1:B:57:VAL:HG11	1:B:88:MET:HB3	2.03	0.41
1:B:219:LEU:HB2	1:B:234:ILE:CG2	2.51	0.41
1:B:347:ALA:O	1:B:351:VAL:HG23	2.20	0.41
1:B:562:ALA:O	1:B:923:ASP:HA	2.21	0.41
1:B:757:TYR:HB2	1:B:771:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:TYR:CE1	1:C:1023:PHE:HZ	2.39	0.41
1:C:908:VAL:O	1:C:912:LEU:HG	2.20	0.41
1:D:310:ILE:C	1:D:312:ASN:H	2.29	0.41
1:D:330:THR:N	1:D:331:PRO:CD	2.84	0.41
1:E:184:MET:HB2	1:E:761:PHE:CZ	2.56	0.41
1:E:344:LEU:HD23	1:E:402:ILE:HG13	2.02	0.41
1:E:406:VAL:O	1:E:410:ILE:HG12	2.21	0.41
1:E:478:MET:SD	1:E:478:MET:C	3.04	0.41
1:E:792:ASN:ND2	1:E:796:GLU:HB2	2.36	0.41
1:E:794:LYS:C	1:E:796:GLU:H	2.29	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:F:410:ILE:HD13	1:F:975:MET:CE	2.51	0.41
1:F:966:CYS:SG	1:F:1021:PRO:CG	3.09	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:969:ARG:C	1:C:972:PRO:HD2	2.46	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:42:ALA:HB3	1:E:132:ALA:HB3	2.03	0.40
1:E:681:ASP:OD2	1:E:681:ASP:C	2.64	0.40
1:E:899:SER:HA	1:E:1023:PHE:HB3	2.03	0.40
1:F:630:MET:C	1:F:631:LEU:HD23	2.46	0.40
1:B:650:ARG:HH11	1:B:650:ARG:CG	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:578:THR:HG1	1:F:623:SER:HB2	1.85	0.40
1:A:762:ILE:HD11	1:B:59:ASP:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:905:PRO:HA	1:B:908:VAL:HG12	2.04	0.40
1:C:552:MET:SD	1:C:908:VAL:HB	2.61	0.40
1:C:578:THR:HG21	1:C:587:THR:HA	2.04	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:803:PHE:CD1	1:B:803:PHE:C	3.00	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:C:912:LEU:O	1:C:913:LEU:C	2.64	0.40
1:D:631:LEU:HD12	1:D:631:LEU:N	2.37	0.40
1:E:913:LEU:O	1:E:914:ALA:C	2.64	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%)	6 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1028/1052 (98%)	918 (89%)	91 (9%)	19 (2%)	6	23
1	C	1028/1052 (98%)	885 (86%)	114 (11%)	29 (3%)	4	14
1	D	1016/1052 (97%)	889 (88%)	105 (10%)	22 (2%)	5	19
1	E	1028/1052 (98%)	907 (88%)	100 (10%)	21 (2%)	6	21
1	F	1031/1052 (98%)	876 (85%)	114 (11%)	41 (4%)	2	8
All	All	6142/6312 (97%)	5384 (88%)	606 (10%)	152 (2%)	4	16

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	755 (91%)	77 (9%)	8	26
1	B	841/860 (98%)	749 (89%)	92 (11%)	6	19
1	C	841/860 (98%)	760 (90%)	81 (10%)	8	25
1	D	835/860 (97%)	762 (91%)	73 (9%)	9	28
1	E	841/860 (98%)	775 (92%)	66 (8%)	11	33
1	F	844/860 (98%)	763 (90%)	81 (10%)	8	25
All	All	5034/5160 (98%)	4564 (91%)	470 (9%)	8	26

All (470) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	25	LEU
1	A	29	SER
1	A	33	ASN
1	A	55	GLU
1	A	57	VAL
1	A	83	ASN
1	A	95	GLU
1	A	96	GLN
1	A	121	GLU
1	A	131	LYS
1	A	134	LYS
1	A	139	VAL
1	A	172	VAL
1	A	177	VAL
1	A	188	LEU
1	A	219	LEU
1	A	230	LEU
1	A	239	ARG
1	A	244	GLU
1	A	259	GLN
1	A	284	SER

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Mol	Chain	Res	Type
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	377	LEU
1	A	398	MET
1	A	417	GLU
1	A	425	LEU
1	A	433	LYS
1	A	438	ILE
1	A	442	LEU
1	A	472	ILE
1	A	475	VAL
1	A	483	ILE
1	A	488	LEU
1	A	512	PHE
1	A	556	PHE
1	A	601	LYS
1	A	612	VAL
1	A	671	VAL
1	A	674	LEU
1	A	684	LEU
1	A	687	GLN
1	A	695	LEU
1	A	730	ILE
1	A	768	LYS
1	A	770	VAL
1	A	805	THR
1	A	810	TYR
1	A	814	LYS
1	A	821	VAL
1	A	856	TYR
1	A	875	LEU
1	A	878	LEU
1	A	881	LEU
1	A	885	LEU
1	A	900	VAL
1	A	916	SER
1	A	918	ARG

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Mol	Chain	Res	Type
1	A	928	VAL
1	A	932	THR
1	A	933	THR
1	A	940	ASN
1	A	958	ILE
1	A	964	GLU
1	A	970	LEU
1	A	976	THR
1	A	978	LEU
1	A	982	LEU
1	A	989	ILE
1	A	1013	THR
1	A	1027	VAL
1	B	17	LEU
1	B	18	VAL
1	B	60	THR
1	B	64	VAL
1	B	68	GLN
1	B	78	ILE
1	B	79	SER
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	127	ILE
1	B	128	ARG
1	B	129	VAL
1	B	139	VAL
1	B	143	VAL
1	B	159	VAL
1	B	188	LEU
1	B	197	GLN
1	B	212	VAL
1	B	234	ILE
1	B	248	ASN
1	B	280	GLN
1	B	289	ILE
1	B	291	ILE
1	B	316	PHE
1	B	319	GLN

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Mol	Chain	Res	Type
1	B	341	VAL
1	B	343	THR
1	B	348	ILE
1	B	349	LEU
1	B	365	THR
1	B	376	LEU
1	B	393	LEU
1	B	402	ILE
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	495	THR
1	B	497	LEU
1	B	501	GLU
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	598	LEU
1	B	605	SER
1	B	623	SER
1	B	624	SER
1	B	635	GLU
1	B	650	ARG
1	B	674	LEU
1	B	676	ASN
1	B	678	THR
1	B	684	LEU
1	B	687	GLN
1	B	693	GLU
1	B	696	LEU
1	B	712	LEU
1	B	733	GLU

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Mol	Chain	Res	Type
1	B	742	LEU
1	B	759	ASN
1	B	767	VAL
1	B	789	TYR
1	B	800	PHE
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	934	ILE
1	B	936	LEU
1	B	959	VAL
1	B	969	ARG
1	B	970	LEU
1	B	986	PRO
1	B	1001	ILE
1	B	1022	LEU
1	C	15	ILE
1	C	30	LEU
1	C	38	ILE
1	C	55	GLU
1	C	67	GLN
1	C	102	ILE
1	C	117	LEU
1	C	118	LEU
1	C	121	GLU
1	C	125	GLN
1	C	143	VAL
1	C	152	GLU
1	C	166	LEU
1	C	237	LYS
1	C	238	THR
1	C	252	LYS
1	C	289	ILE
1	C	291	ILE
1	C	306	ILE
1	C	343	THR
1	C	348	ILE

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Mol	Chain	Res	Type
1	C	360	GLN
1	C	376	LEU
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	475	VAL
1	C	481	SER
1	C	484	VAL
1	C	486	LEU
1	C	488	LEU
1	C	495	THR
1	C	497	LEU
1	C	557	THR
1	C	567	GLU
1	C	588	GLN
1	C	592	ASP
1	C	594	MET
1	C	595	ARG
1	C	611	THR
1	C	635	GLU
1	C	646	GLU
1	C	659	LYS
1	C	685	GLN
1	C	718	ASN
1	C	730	ILE
1	C	797	MET
1	C	826	ILE
1	C	840	MET
1	C	865	GLU
1	C	867	LEU
1	C	880	LEU
1	C	881	LEU
1	C	890	LEU
1	C	896	ILE

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Mol	Chain	Res	Type
1	C	902	LEU
1	C	906	LEU
1	C	909	ILE
1	C	916	SER
1	C	920	LEU
1	C	932	THR
1	C	933	THR
1	C	934	ILE
1	C	937	SER
1	C	942	ILE
1	C	943	LEU
1	C	946	GLU
1	C	970	LEU
1	C	982	LEU
1	C	984	VAL
1	C	1009	MET
1	C	1022	LEU
1	C	1030	LEU
1	D	25	LEU
1	D	33	ASN
1	D	43	ILE
1	D	55	GLU
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	188	LEU
1	D	289	ILE
1	D	319	GLN
1	D	344	LEU
1	D	348	ILE
1	D	353	LEU
1	D	359	LEU
1	D	382	VAL
1	D	392	THR
1	D	393	LEU
1	D	405	LEU
1	D	417	GLU
1	D	423	GLU
1	D	437	GLN

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Mol	Chain	Res	Type
1	D	466	ILE
1	D	472	ILE
1	D	475	VAL
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	601	LYS
1	D	616	ASN
1	D	641	GLU
1	D	644	VAL
1	D	647	LEU
1	D	671	VAL
1	D	674	LEU
1	D	684	LEU
1	D	687	GLN
1	D	695	LEU
1	D	715	VAL
1	D	770	VAL
1	D	772	LEU
1	D	817	ARG
1	D	821	VAL
1	D	824	MET
1	D	827	LEU
1	D	845	GLU
1	D	878	LEU
1	D	881	LEU
1	D	885	LEU
1	D	900	VAL
1	D	913	LEU
1	D	921	SER
1	D	928	VAL
1	D	932	THR
1	D	958	ILE
1	D	964	GLU
1	D	970	LEU
1	D	976	THR
1	D	987	LEU
1	D	989	ILE
1	D	1003	THR

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Mol	Chain	Res	Type
1	D	1009	MET
1	D	1011	THR
1	D	1013	THR
1	D	1015	LEU
1	D	1022	LEU
1	D	1029	THR
1	D	1031	PHE
1	E	1	MET
1	E	17	LEU
1	E	18	VAL
1	E	47	VAL
1	E	48	SER
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	96	GLN
1	E	113	LEU
1	E	120	GLN
1	E	121	GLU
1	E	128	ARG
1	E	134	LYS
1	E	146	ASP
1	E	159	VAL
1	E	176	GLN
1	E	197	GLN
1	E	295	THR
1	E	308	GLN
1	E	348	ILE
1	E	349	LEU
1	E	354	VAL
1	E	365	THR
1	E	393	LEU
1	E	398	MET
1	E	402	ILE
1	E	411	VAL
1	E	414	GLU
1	E	432	ARG
1	E	455	PRO
1	E	486	LEU

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Mol	Chain	Res	Type
1	E	495	THR
1	E	497	LEU
1	E	502	LYS
1	E	544	ILE
1	E	559	ILE
1	E	572	LEU
1	E	598	LEU
1	E	635	GLU
1	E	641	GLU
1	E	659	LYS
1	E	676	ASN
1	E	682	LEU
1	E	696	LEU
1	E	722	ASP
1	E	755	SER
1	E	767	VAL
1	E	785	LEU
1	E	793	ASP
1	E	801	ASN
1	E	803	PHE
1	E	825	GLU
1	E	865	GLU
1	E	870	SER
1	E	893	SER
1	E	913	LEU
1	E	936	LEU
1	E	953	GLU
1	E	969	ARG
1	E	976	THR
1	E	981	ILE
1	E	1022	LEU
1	F	15	ILE
1	F	30	LEU
1	F	38	ILE
1	F	47	VAL
1	F	55	GLU
1	F	62	VAL
1	F	72	ILE
1	F	83	ASN
1	F	88	MET
1	F	112	GLN
1	F	115	THR

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Mol	Chain	Res	Type
1	F	125	GLN
1	F	128	ARG
1	F	142	VAL
1	F	152	GLU
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	289	ILE
1	F	295	THR
1	F	306	ILE
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	402	ILE
1	F	410	ILE
1	F	429	GLU
1	F	445	ILE
1	F	452	VAL
1	F	463	THR
1	F	466	ILE
1	F	473	THR
1	F	481	SER
1	F	484	VAL
1	F	486	LEU
1	F	488	LEU
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	538	ARG

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Mol	Chain	Res	Type
1	F	544	ILE
1	F	558	ARG
1	F	559	ILE
1	F	564	LEU
1	F	595	ARG
1	F	599	LEU
1	F	608	SER
1	F	646	GLU
1	F	654	HIS
1	F	659	LYS
1	F	695	LEU
1	F	716	ARG
1	F	730	ILE
1	F	779	ARG
1	F	797	MET
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	958	ILE
1	F	973	ILE
1	F	1022	LEU
1	F	1032	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	112	GLN
1	A	163	GLN
1	A	218	GLN
1	A	228	GLN
1	A	231	ASN
1	A	360	GLN
1	A	361	ASN
1	A	517	ASN
1	A	569	GLN

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Mol	Chain	Res	Type
1	A	700	ASN
1	A	871	GLN
1	A	940	ASN
1	B	33	ASN
1	B	67	GLN
1	B	104	GLN
1	B	106	GLN
1	B	197	GLN
1	B	361	ASN
1	B	654	HIS
1	B	676	ASN
1	B	685	GLN
1	B	687	GLN
1	B	759	ASN
1	B	781	ASN
1	B	922	ASN
1	B	927	GLN
1	B	954	GLN
1	C	34	GLN
1	C	83	ASN
1	C	104	GLN
1	C	108	GLN
1	C	218	GLN
1	C	241	GLN
1	C	259	GLN
1	C	298	ASN
1	C	312	ASN
1	C	361	ASN
1	C	391	ASN
1	C	439	GLN
1	C	537	HIS
1	C	569	GLN
1	C	588	GLN
1	C	708	GLN
1	C	709	ASN
1	C	773	GLN
1	C	781	ASN
1	D	33	ASN
1	D	34	GLN
1	D	194	ASN
1	D	213	GLN
1	D	241	GLN

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Mol	Chain	Res	Type
1	D	280	GLN
1	D	439	GLN
1	D	713	GLN
1	D	819	ASN
1	E	58	GLN
1	E	67	GLN
1	E	70	ASN
1	E	108	GLN
1	E	125	GLN
1	E	194	ASN
1	E	210	GLN
1	E	229	GLN
1	E	245	GLN
1	E	254	ASN
1	E	273	GLN
1	E	278	ASN
1	E	312	ASN
1	E	361	ASN
1	E	437	GLN
1	E	439	GLN
1	E	577	GLN
1	E	588	GLN
1	E	692	HIS
1	E	713	GLN
1	E	718	ASN
1	E	759	ASN
1	E	927	GLN
1	E	954	GLN
1	F	34	GLN
1	F	67	GLN
1	F	70	ASN
1	F	83	ASN
1	F	125	GLN
1	F	163	GLN
1	F	194	ASN
1	F	218	GLN
1	F	241	GLN
1	F	278	ASN
1	F	280	GLN
1	F	361	ASN
1	F	577	GLN
1	F	642	ASN

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Mol	Chain	Res	Type
1	F	676	ASN
1	F	713	GLN
1	F	781	ASN
1	F	792	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.47	0	92,98,98	1.18	11 (11%)
2	AV0	B	1101	-	72,72,72	0.51	0	92,98,98	1.16	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	3.45	116.39	109.96
2	B	1101	AV0	CCR-O4-C4	-2.99	110.88	117.98
2	E	1101	AV0	CCJ-OBX-CCF	-2.68	108.49	113.72
2	E	1101	AV0	CCV-CCT-CCN	-2.60	106.26	110.83
2	B	1101	AV0	OBY-CCC-CBM	2.60	112.87	106.44
2	B	1101	AV0	CCU-CCO-CCD	-2.58	105.55	110.23
2	B	1101	AV0	O4-CCR-OBY	2.54	117.37	110.69
2	B	1101	AV0	OBX-CCJ-CCL	-2.47	105.30	110.37
2	E	1101	AV0	OAU-CCV-CCT	2.30	115.80	110.38
2	E	1101	AV0	CBP-CCF-CCQ	2.29	119.83	113.38
2	E	1101	AV0	CBN-CCD-CCO	2.26	118.56	113.02
2	E	1101	AV0	OAU-CCV-CCR	-2.20	104.82	110.08
2	E	1101	AV0	O4-CCR-OBY	2.14	116.34	110.69
2	B	1101	AV0	O3-C3-C4	2.11	115.34	109.94
2	E	1101	AV0	C2-C3-C4	-2.10	104.91	109.68
2	B	1101	AV0	CCW-CCU-CCO	-2.10	107.15	110.83
2	E	1101	AV0	CCR-O4-C4	-2.06	113.09	117.98
2	B	1101	AV0	OBX-CCF-CCQ	-2.05	105.48	109.72
2	B	1101	AV0	OBX-CCJ-OBV	-2.04	105.23	110.04
2	E	1101	AV0	CCU-CCO-CCD	-2.00	106.60	110.23

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	AV0	OBV-CBT-CCM-CBQ
2	B	1101	AV0	OBV-CBT-CCM-CBR
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	OAI-CBM-CCC-OBY
2	E	1101	AV0	OAJ-CBN-CCD-OBZ
2	E	1101	AV0	OAI-CBM-CCC-OBY
2	E	1101	AV0	CBJ-CBL-CBR-CCM
2	E	1101	AV0	CCL-CCJ-OBV-CBT

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

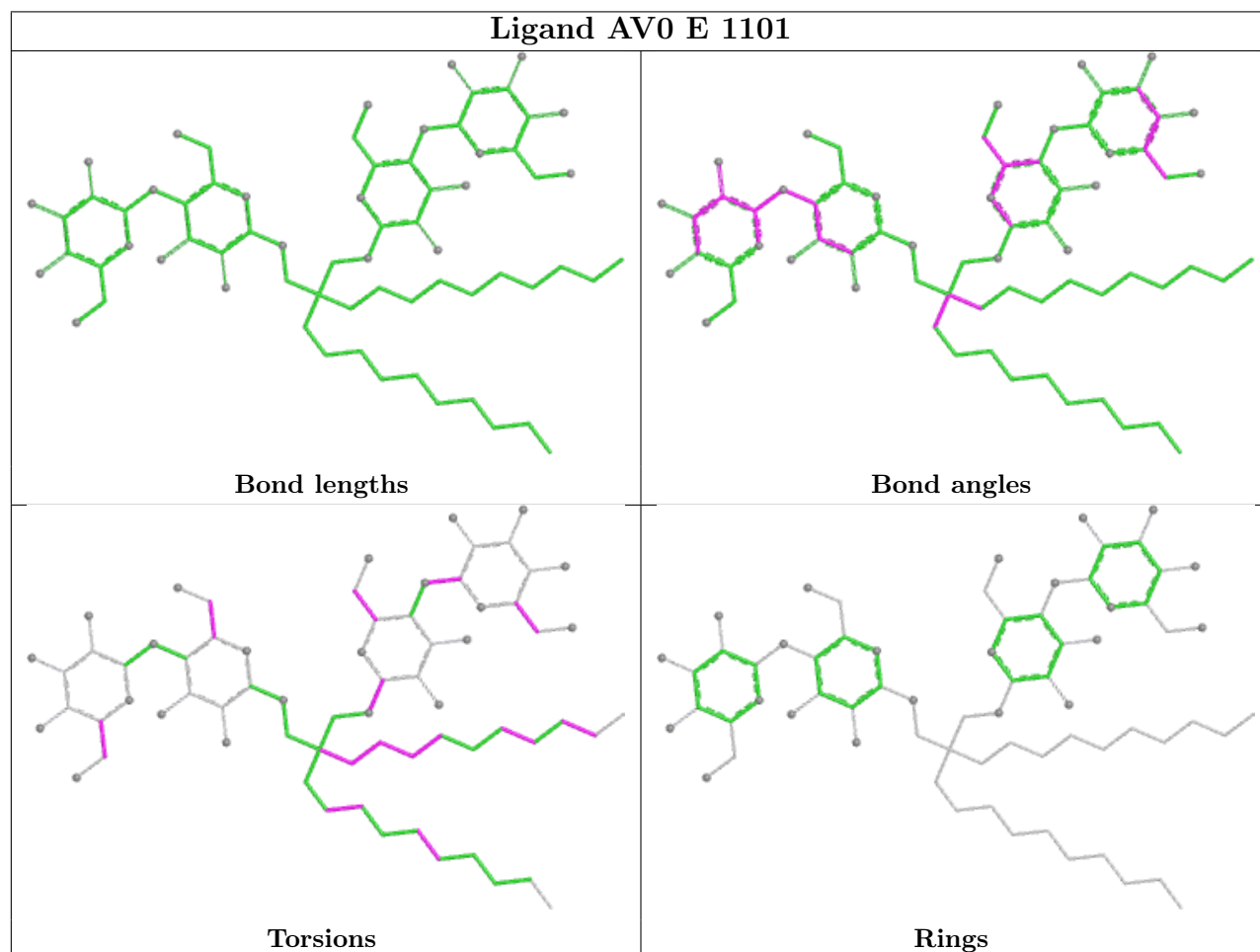
There are no ring outliers.

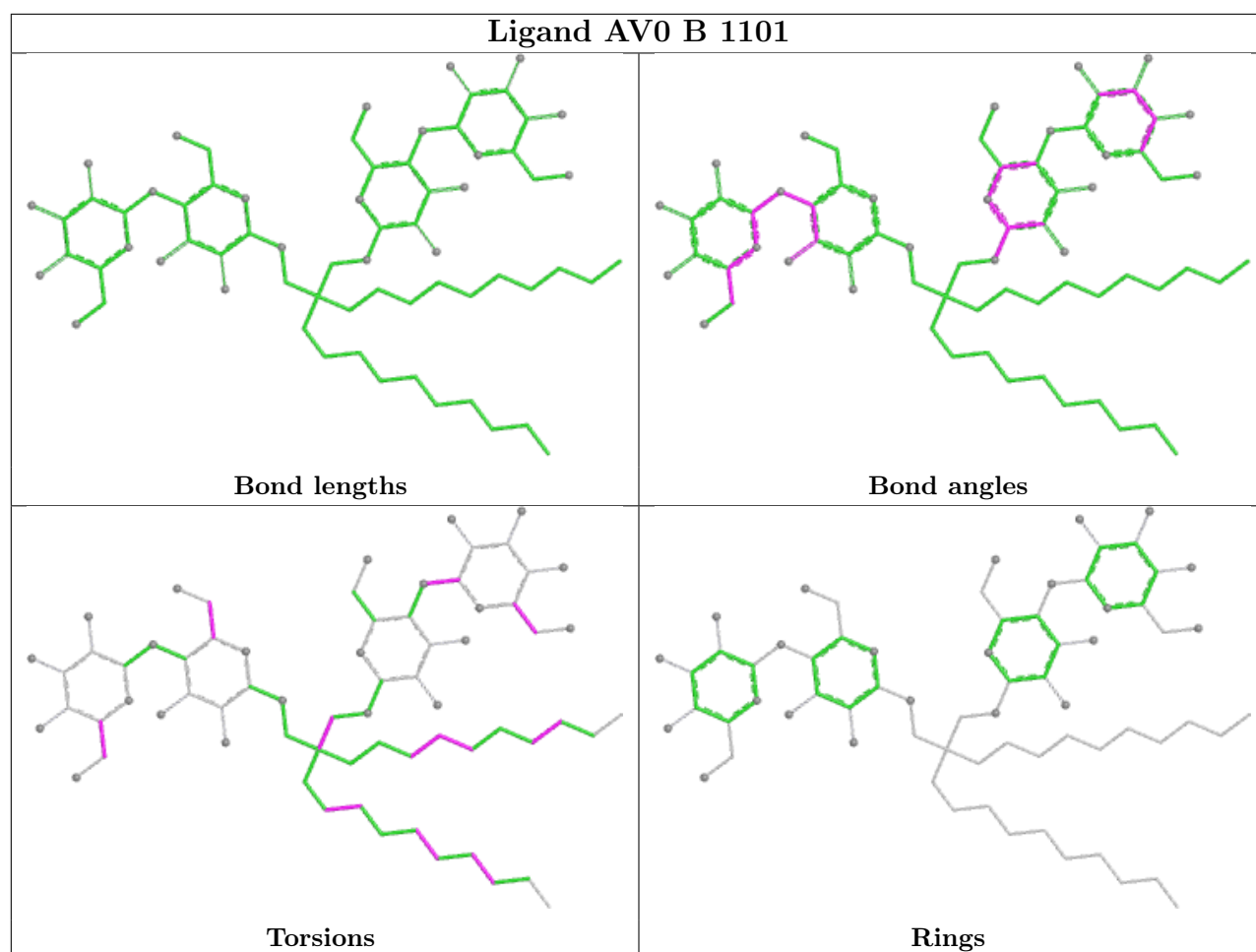
1 monomer is involved in 1 short contact:

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1017/1052 (96%)	0.61	103 (10%) 12 10	13, 47, 94, 148	0
1	B	1030/1052 (97%)	0.29	55 (5%) 32 25	12, 40, 79, 117	0
1	C	1030/1052 (97%)	0.90	135 (13%) 7 6	15, 55, 110, 162	0
1	D	1020/1052 (96%)	0.75	124 (12%) 8 7	17, 53, 97, 144	0
1	E	1030/1052 (97%)	0.63	104 (10%) 12 10	18, 52, 99, 137	0
1	F	1033/1052 (98%)	0.74	141 (13%) 7 5	21, 52, 111, 166	0
All	All	6160/6312 (97%)	0.65	662 (10%) 11 9	12, 50, 99, 166	0

All (662) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	615	PHE	8.0
1	F	742	LEU	8.0
1	C	742	LEU	7.0
1	A	656	PHE	6.9
1	A	867	LEU	6.4
1	C	738	LEU	6.4
1	F	645	PHE	6.2
1	E	237	LYS	6.1
1	D	658	PHE	6.0
1	A	839	ALA	5.9
1	D	253	VAL	5.8
1	B	216	SER	5.7
1	A	499	PRO	5.5
1	C	505	HIS	5.4
1	E	676	ASN	5.4
1	A	710	PRO	5.3
1	F	582	SER	5.3
1	A	362	PHE	5.3
1	D	219	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	645	PHE	5.1
1	F	738	LEU	5.0
1	A	636	GLU	5.0
1	C	259	GLN	4.9
1	B	145	THR	4.9
1	B	215	SER	4.8
1	F	1031	PHE	4.8
1	A	657	SER	4.8
1	C	808	TRP	4.8
1	C	755	SER	4.7
1	C	512	PHE	4.7
1	F	808	TRP	4.6
1	A	866	ARG	4.6
1	A	842	ALA	4.6
1	C	657	SER	4.6
1	A	512	PHE	4.5
1	E	537	HIS	4.5
1	F	505	HIS	4.5
1	A	711	ALA	4.4
1	F	807	LYS	4.4
1	F	597	TYR	4.3
1	F	655	PHE	4.3
1	C	753	TRP	4.3
1	D	867	LEU	4.3
1	A	568	ASP	4.3
1	E	230	LEU	4.3
1	F	753	TRP	4.3
1	C	507	GLU	4.3
1	E	623	SER	4.2
1	E	261	ARG	4.2
1	B	230	LEU	4.2
1	C	639	GLY	4.2
1	D	255	PRO	4.2
1	F	731	ASP	4.2
1	E	704	MET	4.2
1	C	597	TYR	4.1
1	C	654	HIS	4.1
1	B	794	LYS	4.1
1	E	658	PHE	4.1
1	C	994	GLY	4.1
1	C	661	ALA	4.0
1	A	659	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	235	ILE	4.0
1	C	144	SER	4.0
1	A	958	ILE	4.0
1	D	732	ASP	3.9
1	A	635	GLU	3.9
1	F	794	LYS	3.9
1	C	260	VAL	3.9
1	E	677	ALA	3.9
1	A	676	ASN	3.9
1	E	660	ASP	3.8
1	D	789	TYR	3.8
1	C	320	GLY	3.8
1	D	144	SER	3.8
1	D	362	PHE	3.8
1	D	869	GLY	3.8
1	B	656	PHE	3.8
1	C	741	SER	3.8
1	D	577	GLN	3.7
1	B	676	ASN	3.7
1	C	655	PHE	3.7
1	F	740	VAL	3.7
1	C	522	SER	3.7
1	F	230	LEU	3.7
1	F	730	ILE	3.7
1	A	258	SER	3.6
1	B	29	SER	3.6
1	E	216	SER	3.6
1	E	803	PHE	3.6
1	D	260	VAL	3.6
1	D	499	PRO	3.6
1	E	250	LEU	3.6
1	D	675	GLY	3.6
1	D	755	SER	3.6
1	E	664	PHE	3.6
1	D	187	TRP	3.6
1	E	678	THR	3.6
1	F	580	PRO	3.6
1	D	257	GLY	3.5
1	A	546	VAL	3.5
1	C	740	VAL	3.5
1	D	790	VAL	3.5
1	E	212	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	597	TYR	3.5
1	D	1032	LYS	3.5
1	A	658	PHE	3.5
1	A	947	PHE	3.5
1	C	724	PRO	3.5
1	C	506	GLY	3.5
1	D	657	SER	3.5
1	F	785	LEU	3.5
1	F	508	HIS	3.5
1	C	961	ALA	3.5
1	E	217	GLY	3.5
1	F	745	ILE	3.4
1	F	639	GLY	3.4
1	A	899	SER	3.4
1	C	524	THR	3.4
1	E	751	ILE	3.4
1	A	535	LEU	3.4
1	D	250	LEU	3.4
1	F	743	ALA	3.4
1	A	146	ASP	3.4
1	D	150	THR	3.4
1	D	953	GLU	3.4
1	F	518	ARG	3.4
1	C	721	SER	3.4
1	C	870	SER	3.4
1	E	624	SER	3.4
1	F	800	PHE	3.4
1	E	265	VAL	3.4
1	D	185	ARG	3.4
1	D	232	ALA	3.4
1	E	214	ILE	3.4
1	F	747	SER	3.4
1	B	785	LEU	3.3
1	C	723	GLU	3.3
1	A	707	ALA	3.3
1	A	577	GLN	3.3
1	F	690	VAL	3.3
1	A	869	GLY	3.3
1	D	266	ALA	3.3
1	C	656	PHE	3.3
1	F	803	PHE	3.3
1	A	320	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	722	ASP	3.3
1	F	757	TYR	3.3
1	F	789	TYR	3.3
1	B	255	PRO	3.3
1	F	594	MET	3.3
1	C	658	PHE	3.3
1	B	250	LEU	3.3
1	F	581	GLY	3.3
1	F	641	GLU	3.2
1	C	638	PRO	3.2
1	A	989	ILE	3.2
1	D	988	ALA	3.2
1	A	834	LEU	3.2
1	D	870	SER	3.2
1	B	214	ILE	3.2
1	E	730	ILE	3.2
1	D	286	ALA	3.2
1	E	804	ALA	3.2
1	A	655	PHE	3.2
1	E	798	VAL	3.2
1	A	871	GLN	3.2
1	C	805	THR	3.2
1	E	825	GLU	3.2
1	E	916	SER	3.2
1	F	812	SER	3.2
1	B	224	ALA	3.2
1	F	654	HIS	3.2
1	D	601	LYS	3.2
1	A	955	GLY	3.2
1	E	238	THR	3.2
1	E	84	SER	3.2
1	A	838	ASP	3.2
1	F	660	ASP	3.2
1	B	261	ARG	3.2
1	D	800	PHE	3.2
1	D	149	MET	3.2
1	F	728	LEU	3.1
1	F	694	VAL	3.1
1	A	837	GLY	3.1
1	F	320	GLY	3.1
1	F	522	SER	3.1
1	D	267	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	656	PHE	3.1
1	E	236	GLY	3.1
1	F	214	ILE	3.1
1	C	613	THR	3.1
1	C	513	PHE	3.1
1	D	254	ASN	3.1
1	D	575	GLN	3.1
1	D	954	GLN	3.1
1	B	237	LYS	3.1
1	D	674	LEU	3.1
1	E	831	ALA	3.0
1	C	256	ASP	3.0
1	F	283	GLY	3.0
1	C	321	MET	3.0
1	D	515	TRP	3.0
1	D	210	GLN	3.0
1	D	252	LYS	3.0
1	F	585	GLU	3.0
1	F	145	THR	3.0
1	A	840	MET	3.0
1	E	917	MET	3.0
1	F	515	TRP	3.0
1	C	500	ILE	3.0
1	F	257	GLY	3.0
1	F	509	LYS	3.0
1	F	721	SER	3.0
1	F	512	PHE	3.0
1	E	826	ILE	3.0
1	E	799	PRO	3.0
1	A	702	PHE	3.0
1	C	277	ILE	2.9
1	B	217	GLY	2.9
1	E	785	LEU	2.9
1	F	653	MET	2.9
1	C	252	LYS	2.9
1	F	734	LYS	2.9
1	C	647	LEU	2.9
1	E	705	LEU	2.9
1	A	868	SER	2.9
1	C	990	SER	2.9
1	D	258	SER	2.9
1	A	145	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	537	HIS	2.9
1	D	650	ARG	2.9
1	F	236	GLY	2.9
1	D	871	GLN	2.9
1	E	218	GLN	2.9
1	B	231	ASN	2.9
1	D	735	ALA	2.9
1	E	786	SER	2.9
1	F	656	PHE	2.9
1	F	620	ARG	2.9
1	C	754	GLY	2.9
1	C	519	MET	2.9
1	C	278	ASN	2.9
1	F	718	ASN	2.9
1	E	260	VAL	2.9
1	F	854	VAL	2.9
1	D	866	ARG	2.9
1	F	741	SER	2.9
1	F	805	THR	2.9
1	C	728	LEU	2.9
1	C	640	GLY	2.8
1	E	588	GLN	2.8
1	D	632	LYS	2.8
1	E	810	TYR	2.8
1	F	733	GLU	2.8
1	C	735	ALA	2.8
1	D	517	ASN	2.8
1	F	202	ASP	2.8
1	A	836	SER	2.8
1	D	754	GLY	2.8
1	F	719	GLY	2.8
1	F	507	GLU	2.8
1	E	253	VAL	2.8
1	F	225	VAL	2.8
1	B	981	ILE	2.8
1	C	508	HIS	2.8
1	C	521	LEU	2.8
1	D	186	ILE	2.8
1	B	522	SER	2.8
1	C	604	SER	2.8
1	E	736	SER	2.8
1	E	653	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	773	GLN	2.8
1	C	789	TYR	2.8
1	C	665	ALA	2.8
1	E	827	LEU	2.8
1	B	144	SER	2.8
1	F	255	PRO	2.8
1	F	595	ARG	2.8
1	F	804	ALA	2.8
1	D	537	HIS	2.8
1	C	991	THR	2.8
1	C	719	GLY	2.8
1	A	865	GLU	2.7
1	C	636	GLU	2.7
1	D	268	VAL	2.7
1	C	193	LEU	2.7
1	C	649	LYS	2.7
1	D	320	GLY	2.7
1	E	215	SER	2.7
1	C	602	GLU	2.7
1	D	673	GLU	2.7
1	E	507	GLU	2.7
1	A	715	VAL	2.7
1	C	663	VAL	2.7
1	A	712	LEU	2.7
1	E	800	PHE	2.7
1	A	939	LYS	2.7
1	E	805	THR	2.7
1	B	869	GLY	2.7
1	C	276	SER	2.7
1	F	144	SER	2.7
1	F	260	VAL	2.7
1	E	728	LEU	2.7
1	A	257	GLY	2.7
1	D	145	THR	2.7
1	C	732	ASP	2.7
1	F	793	ASP	2.7
1	B	593	SER	2.7
1	D	237	LYS	2.7
1	F	720	MET	2.7
1	B	239	ARG	2.7
1	E	793	ASP	2.7
1	F	744	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	218	GLN	2.7
1	C	547	VAL	2.7
1	E	641	GLU	2.7
1	C	599	LEU	2.7
1	C	279	ALA	2.6
1	D	512	PHE	2.6
1	E	752	ALA	2.6
1	F	661	ALA	2.6
1	C	253	VAL	2.6
1	C	790	VAL	2.6
1	F	222	LEU	2.6
1	F	659	LYS	2.6
1	A	513	PHE	2.6
1	B	258	SER	2.6
1	D	868	SER	2.6
1	F	321	MET	2.6
1	F	593	SER	2.6
1	C	196	TYR	2.6
1	C	791	ARG	2.6
1	E	699	ARG	2.6
1	F	726	TYR	2.6
1	D	964	GLU	2.6
1	F	500	ILE	2.6
1	D	539	ALA	2.6
1	D	148	SER	2.6
1	F	195	SER	2.6
1	E	788	TRP	2.6
1	F	729	GLU	2.6
1	B	731	ASP	2.6
1	F	737	ALA	2.6
1	E	654	HIS	2.6
1	C	779	ARG	2.6
1	D	220	GLY	2.6
1	A	903	VAL	2.6
1	F	748	THR	2.6
1	F	749	VAL	2.6
1	F	797	MET	2.6
1	C	743	ALA	2.6
1	C	258	SER	2.5
1	E	634	TRP	2.5
1	E	672	LEU	2.5
1	A	544	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	663	VAL	2.5
1	B	513	PHE	2.5
1	E	766	ARG	2.5
1	C	812	SER	2.5
1	F	695	LEU	2.5
1	C	917	MET	2.5
1	C	958	ILE	2.5
1	A	1024	TYR	2.5
1	A	556	PHE	2.5
1	D	516	PHE	2.5
1	D	655	PHE	2.5
1	D	773	GLN	2.5
1	F	658	PHE	2.5
1	C	667	ALA	2.5
1	D	961	ALA	2.5
1	C	653	MET	2.5
1	C	913	LEU	2.5
1	E	222	LEU	2.5
1	E	753	TRP	2.5
1	A	864	GLU	2.5
1	C	734	LYS	2.5
1	F	630	MET	2.5
1	F	647	LEU	2.5
1	A	548	ILE	2.5
1	D	147	GLY	2.5
1	D	533	SER	2.5
1	F	607	SER	2.5
1	D	666	PHE	2.5
1	E	602	GLU	2.5
1	A	649	LYS	2.5
1	F	237	LYS	2.5
1	F	263	LYS	2.5
1	E	231	ASN	2.5
1	A	902	LEU	2.4
1	E	647	LEU	2.4
1	A	846	ILE	2.4
1	F	724	PRO	2.4
1	A	1025	VAL	2.4
1	A	1027	VAL	2.4
1	D	436	GLY	2.4
1	D	919	GLY	2.4
1	F	253	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	858	TRP	2.4
1	D	865	GLU	2.4
1	A	706	ALA	2.4
1	B	804	ALA	2.4
1	E	509	LYS	2.4
1	A	703	LEU	2.4
1	E	631	LEU	2.4
1	A	923	ASP	2.4
1	C	710	PRO	2.4
1	D	1027	VAL	2.4
1	E	806	GLY	2.4
1	B	868	SER	2.4
1	C	995	SER	2.4
1	C	95	GLU	2.4
1	E	733	GLU	2.4
1	F	322	LYS	2.4
1	A	651	ALA	2.4
1	C	295	THR	2.4
1	A	1030	LEU	2.4
1	E	662	MET	2.4
1	C	730	ILE	2.4
1	C	846	ILE	2.4
1	F	207	ILE	2.4
1	C	739	GLY	2.4
1	D	263	LYS	2.4
1	B	507	GLU	2.4
1	D	646	GLU	2.4
1	D	864	GLU	2.4
1	A	685	GLN	2.4
1	A	856	TYR	2.4
1	D	797	MET	2.4
1	F	762	ILE	2.4
1	A	855	GLY	2.4
1	B	659	LYS	2.4
1	C	660	ASP	2.4
1	E	151	LYS	2.4
1	F	699	ARG	2.4
1	E	513	PHE	2.4
1	C	677	ALA	2.4
1	F	802	ALA	2.4
1	E	29	SER	2.4
1	E	604	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	786	SER	2.4
1	B	917	MET	2.4
1	A	827	LEU	2.4
1	B	193	LEU	2.4
1	C	598	LEU	2.4
1	E	867	LEU	2.4
1	D	730	ILE	2.4
1	F	846	ILE	2.4
1	F	318	PRO	2.4
1	D	807	LYS	2.3
1	D	272	GLY	2.3
1	C	666	PHE	2.3
1	C	793	ASP	2.3
1	D	737	ALA	2.3
1	A	670	SER	2.3
1	B	720	MET	2.3
1	F	533	SER	2.3
1	C	810	TYR	2.3
1	F	852	LYS	2.3
1	E	239	ARG	2.3
1	F	591	VAL	2.3
1	F	798	VAL	2.3
1	C	257	GLY	2.3
1	D	1031	PHE	2.3
1	B	339	GLU	2.3
1	D	550	ALA	2.3
1	E	842	ALA	2.3
1	C	687	GLN	2.3
1	D	519	MET	2.3
1	A	605	SER	2.3
1	F	696	LEU	2.3
1	A	547	VAL	2.3
1	B	675	GLY	2.3
1	E	795	GLY	2.3
1	F	511	GLY	2.3
1	F	739	GLY	2.3
1	F	853	GLY	2.3
1	C	642	ASN	2.3
1	D	662	MET	2.3
1	A	943	LEU	2.3
1	B	222	LEU	2.3
1	D	193	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	598	LEU	2.3
1	E	575	GLN	2.3
1	C	525	HIS	2.3
1	B	736	SER	2.3
1	E	27	ILE	2.3
1	F	192	LYS	2.3
1	F	60	THR	2.3
1	E	597	TYR	2.3
1	E	776	PRO	2.3
1	B	664	PHE	2.3
1	D	664	PHE	2.3
1	F	521	LEU	2.3
1	C	659	LYS	2.3
1	C	410	ILE	2.3
1	E	48	SER	2.3
1	F	56	THR	2.3
1	D	157	TYR	2.3
1	C	589	VAL	2.3
1	E	255	PRO	2.3
1	C	581	GLY	2.3
1	A	664	PHE	2.2
1	A	809	GLU	2.2
1	C	729	GLU	2.2
1	C	695	LEU	2.2
1	A	852	LYS	2.2
1	C	192	LYS	2.2
1	A	538	ARG	2.2
1	B	508	HIS	2.2
1	F	692	HIS	2.2
1	A	634	TRP	2.2
1	A	255	PRO	2.2
1	C	1014	VAL	2.2
1	D	271	GLY	2.2
1	F	811	GLY	2.2
1	A	653	MET	2.2
1	D	594	MET	2.2
1	E	695	LEU	2.2
1	F	809	GLU	2.2
1	F	273	GLN	2.2
1	F	586	ARG	2.2
1	F	637	ARG	2.2
1	F	791	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	145	THR	2.2
1	D	1029	THR	2.2
1	F	606	VAL	2.2
1	D	741	SER	2.2
1	D	771	TYR	2.2
1	E	726	TYR	2.2
1	E	789	TYR	2.2
1	F	258	SER	2.2
1	A	919	GLY	2.2
1	D	957	GLY	2.2
1	D	794	LYS	2.2
1	F	796	GLU	2.2
1	C	439	GLN	2.2
1	B	537	HIS	2.2
1	C	566	ASP	2.2
1	C	731	ASP	2.2
1	C	285	PRO	2.2
1	C	324	VAL	2.2
1	D	1014	VAL	2.2
1	A	678	THR	2.2
1	A	891	TYR	2.2
1	B	795	GLY	2.2
1	D	891	TYR	2.2
1	E	220	GLY	2.2
1	E	870	SER	2.2
1	F	126	GLY	2.2
1	C	520	PHE	2.2
1	C	698	ALA	2.2
1	D	528	GLU	2.2
1	C	909	ILE	2.2
1	D	337	ILE	2.2
1	C	576	VAL	2.2
1	C	612	VAL	2.2
1	F	810	TYR	2.2
1	C	1015	LEU	2.2
1	D	742	LEU	2.2
1	F	605	SER	2.2
1	A	953	GLU	2.2
1	D	693	GLU	2.2
1	F	629	ILE	2.1
1	A	849	GLN	2.1
1	E	213	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	900	VAL	2.1
1	E	694	VAL	2.1
1	B	704	MET	2.1
1	A	150	THR	2.1
1	E	601	LYS	2.1
1	C	554	TRP	2.1
1	A	84	SER	2.1
1	B	677	ALA	2.1
1	A	650	ARG	2.1
1	A	829	GLU	2.1
1	D	751	ILE	2.1
1	F	360	GLN	2.1
1	B	248	ASN	2.1
1	C	517	ASN	2.1
1	D	616	ASN	2.1
1	B	591	VAL	2.1
1	A	853	GLY	2.1
1	D	563	PHE	2.1
1	E	599	LEU	2.1
1	A	677	ALA	2.1
1	E	802	ALA	2.1
1	C	829	GLU	2.1
1	D	635	GLU	2.1
1	E	55	GLU	2.1
1	E	836	SER	2.1
1	D	653	MET	2.1
1	E	832	PRO	2.1
1	F	200	PRO	2.1
1	B	867	LEU	2.1
1	C	785	LEU	2.1
1	D	387	GLY	2.1
1	E	869	GLY	2.1
1	B	557	THR	2.1
1	D	574	ALA	2.1
1	A	528	GLU	2.1
1	D	216	SER	2.1
1	B	120	GLN	2.1
1	F	589	VAL	2.1
1	A	850	LEU	2.1
1	D	251	LEU	2.1
1	D	803	PHE	2.1
1	E	680	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	506	GLY	2.1
1	F	615	PHE	2.1
1	D	763	ASP	2.1
1	E	164	ASP	2.1
1	F	584	ALA	2.1
1	A	844	GLU	2.1
1	D	1024	TYR	2.1
1	C	48	SER	2.0
1	A	708	GLN	2.0
1	D	192	LYS	2.0
1	A	663	VAL	2.0
1	F	790	VAL	2.0
1	A	830	PRO	2.0
1	C	776	PRO	2.0
1	E	642	ASN	2.0
1	E	655	PHE	2.0
1	F	510	GLY	2.0
1	C	150	THR	2.0
1	C	745	ILE	2.0
1	C	751	ILE	2.0
1	D	233	THR	2.0
1	D	805	THR	2.0
1	A	688	ALA	2.0
1	B	596	GLU	2.0
1	C	641	GLU	2.0
1	E	852	LYS	2.0
1	F	848	LYS	2.0
1	C	496	MET	2.0
1	A	253	VAL	2.0
1	A	835	SER	2.0
1	A	954	GLN	2.0
1	B	589	VAL	2.0
1	D	798	VAL	2.0
1	E	47	VAL	2.0
1	F	590	VAL	2.0
1	F	608	SER	2.0
1	A	674	LEU	2.0
1	A	586	ARG	2.0
1	C	128	ARG	2.0
1	D	586	ARG	2.0
1	B	526	GLY	2.0
1	B	800	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	246	PHE	2.0
1	D	470	PHE	2.0
1	E	811	GLY	2.0
1	D	544	ILE	2.0
1	A	585	GLU	2.0
1	B	601	LYS	2.0
1	C	247	GLU	2.0
1	D	783	ASP	2.0
1	E	732	ASP	2.0
1	F	73	ASP	2.0
1	F	196	TYR	2.0
1	C	690	VAL	2.0
1	D	740	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

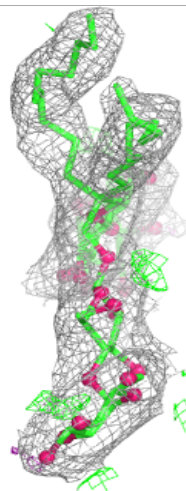
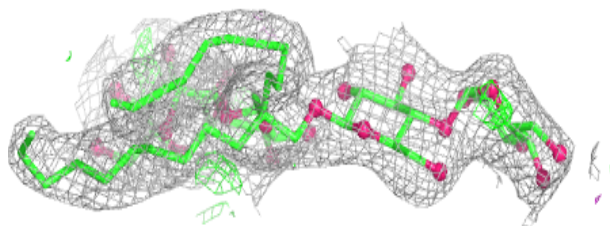
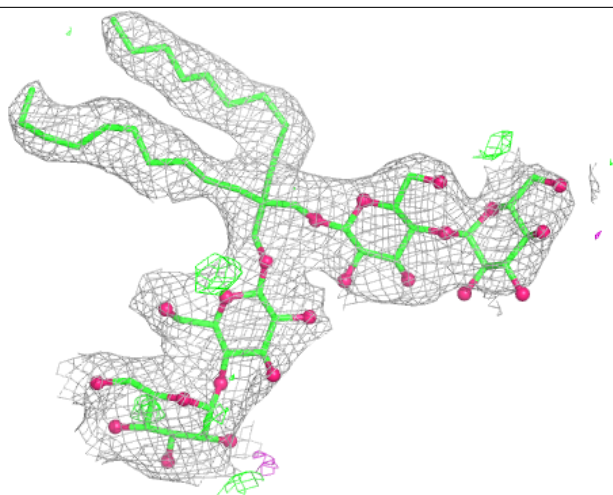
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	1101	69/69	0.92	0.12	29,46,63,70	0
2	AV0	E	1101	69/69	0.92	0.11	30,49,65,69	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.

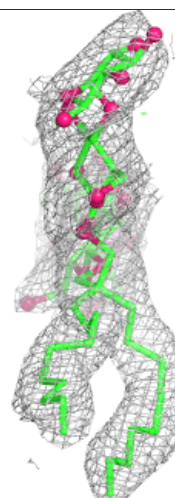
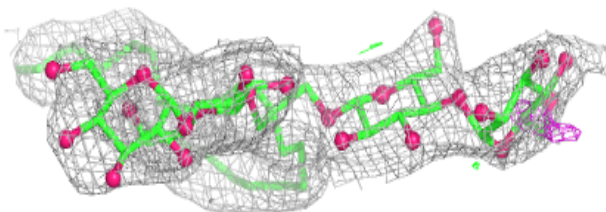
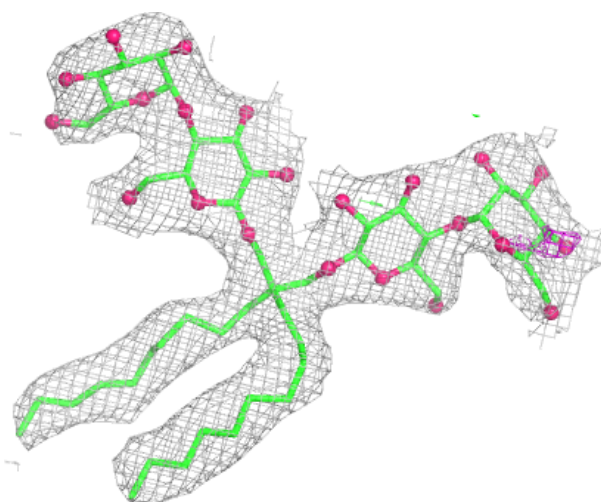
Electron density around AV0 B 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AV0 E 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.