Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 04:48 PM EDT

PDB ID	:	3T9N
Title	:	Crystal structure of a membrane protein
Authors	:	Yang, M.; Zhang, X.; Ge, J.; Wang, J.
Deposited on	:	2011-08-03
Resolution	:	3.46 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:

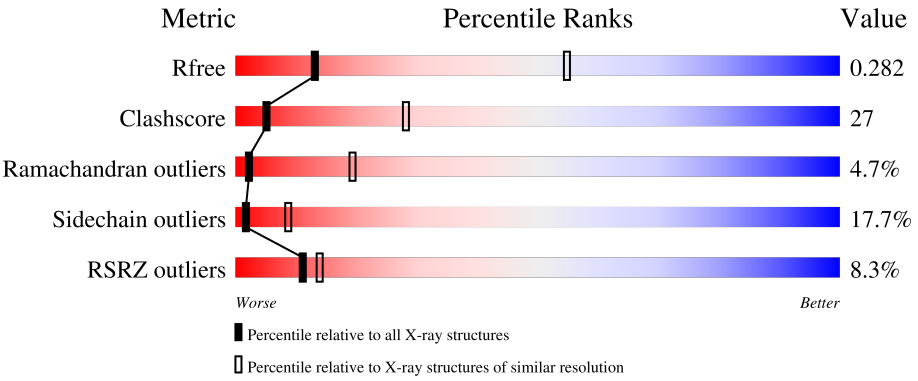
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.46 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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 <=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	282	8% 46% 37% 10% · 6%
1	B	282	7% 45% 36% 12% · 6%
1	C	282	7% 44% 37% 12% · 6%
1	D	282	9% 43% 37% 13% · 6%
1	E	282	9% 43% 37% 13% · 6%

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Mol	Chain	Length	Quality of chain
1	F	282	9% 46% 35% 11% • 6%
1	G	282	6% 47% 34% 12% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	283	-	-	-	X
2	LMT	F	283	-	-	-	X

2 Entry composition

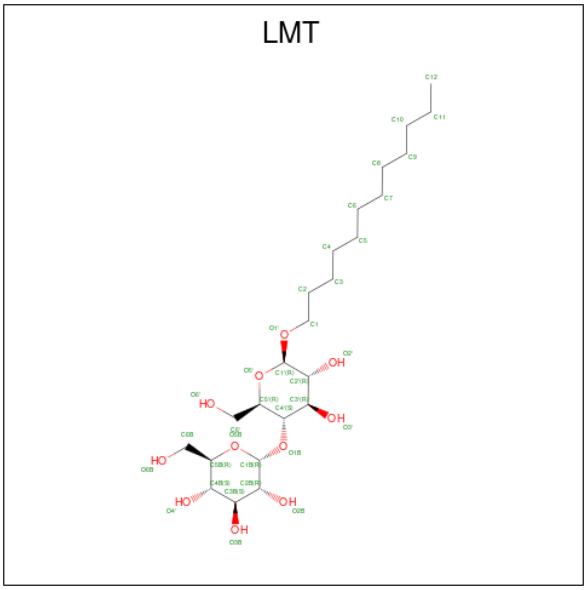
There are 2 unique types of molecules in this entry. The entry contains 14789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Small-conductance mechanosensitive channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2116	1382	341	383	10			
1	B	264	Total	C	N	O	S	0	0	0
			2099	1373	339	377	10			
1	C	264	Total	C	N	O	S	0	0	0
			2099	1373	339	377	10			
1	D	265	Total	C	N	O	S	0	0	0
			2108	1378	340	380	10			
1	E	264	Total	C	N	O	S	0	0	0
			2099	1373	339	377	10			
1	F	264	Total	C	N	O	S	0	0	0
			2099	1373	339	377	10			
1	G	264	Total	C	N	O	S	0	0	0
			2099	1373	339	377	10			

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



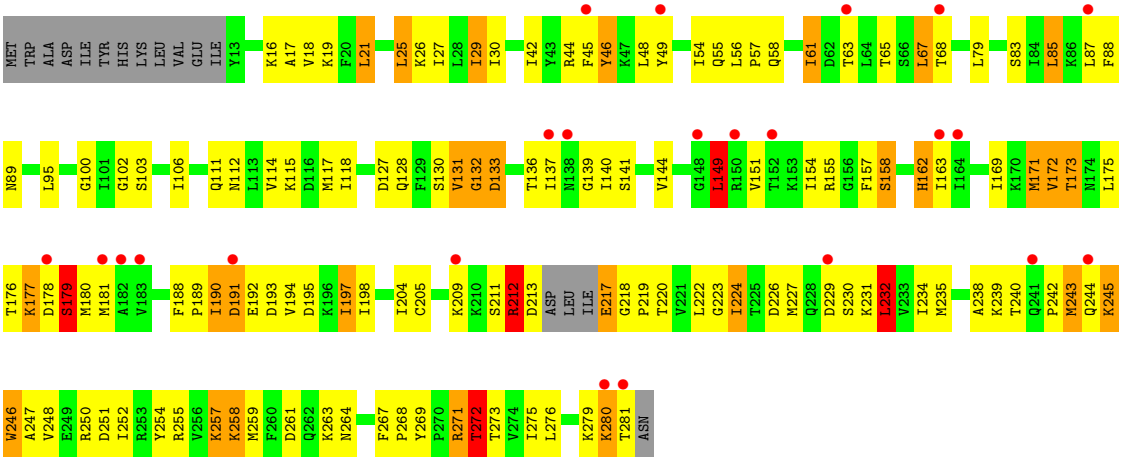
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 35	C 24	O 11	0	0
2	F	1	Total 35	C 24	O 11	0	0

3 Residue-property plots (i)

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.

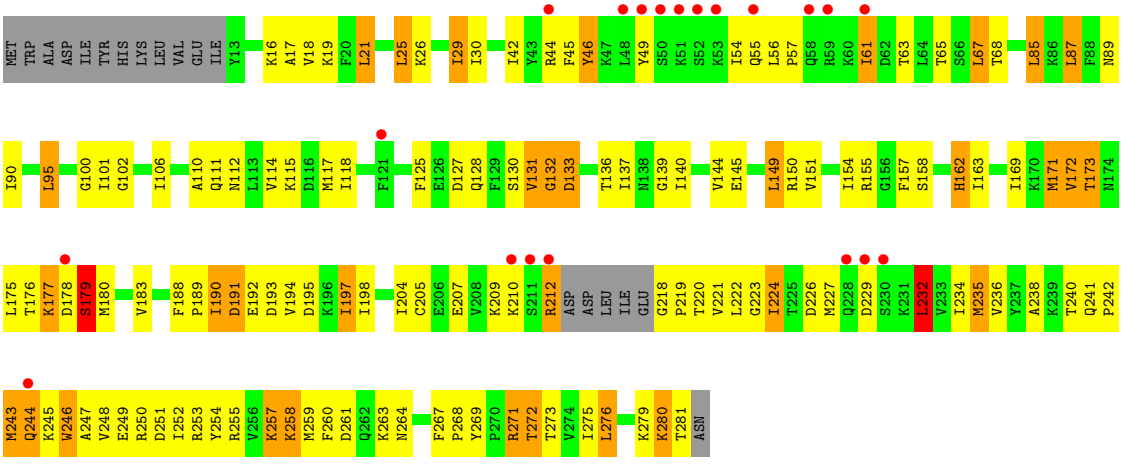
• Molecule 1: Small-conductance mechanosensitive channel

Chain A:



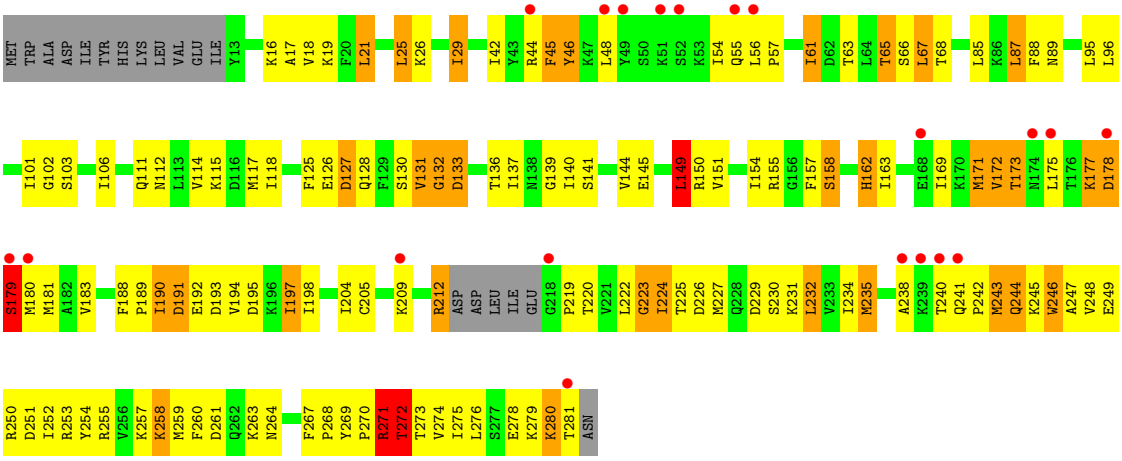
• Molecule 1: Small-conductance mechanosensitive channel

Chain B:



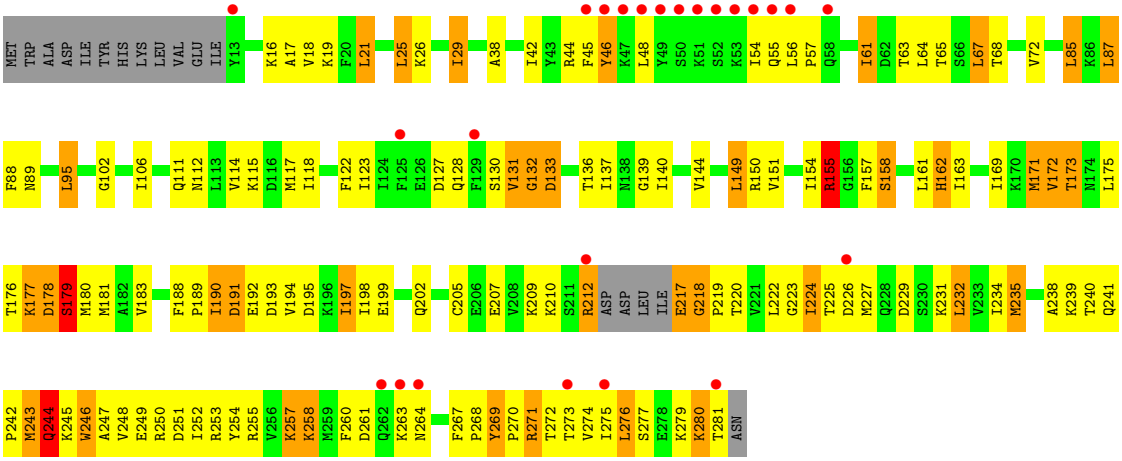
• Molecule 1: Small-conductance mechanosensitive channel

Chain C:



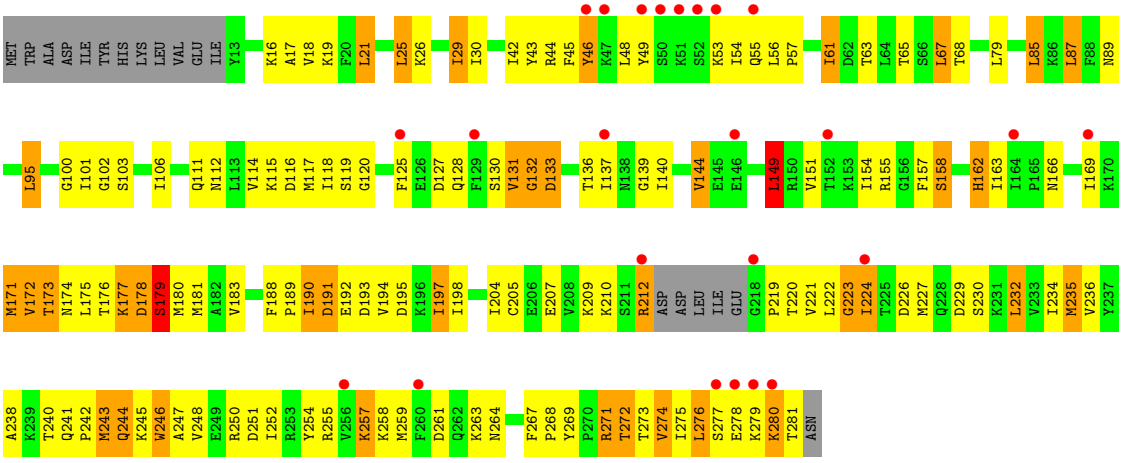
• Molecule 1: Small-conductance mechanosensitive channel

Chain D:



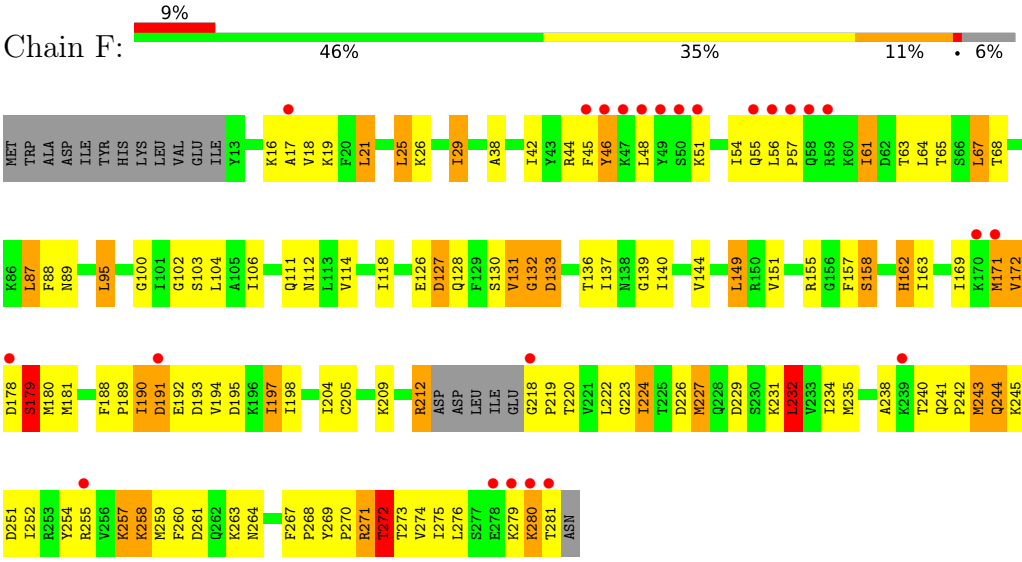
• Molecule 1: Small-conductance mechanosensitive channel

Chain E:



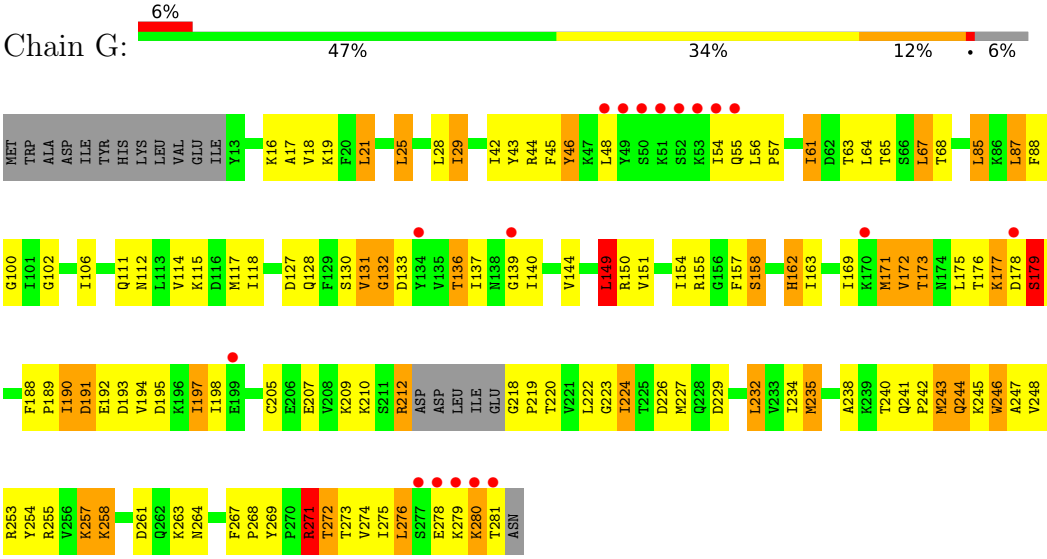
• Molecule 1: Small-conductance mechanosensitive channel

Chain F:



• Molecule 1: Small-conductance mechanosensitive channel

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.03Å 138.63Å 214.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.74 – 3.46 38.74 – 3.46	Depositor EDS
% Data completeness (in resolution range)	95.4 (38.74-3.46) 95.4 (38.74-3.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.253 , 0.288 0.252 , 0.282	Depositor DCC
R_{free} test set	1802 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	110.0	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 94.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14789	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LMT

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	0.54	0/2150	0.75	6/2894 (0.2%)
1	B	0.52	0/2133	0.72	4/2871 (0.1%)
1	C	0.51	0/2133	0.73	4/2871 (0.1%)
1	D	0.55	1/2142 (0.0%)	0.89	3/2883 (0.1%)
1	E	0.54	0/2133	0.69	1/2871 (0.0%)
1	F	0.51	0/2133	0.73	5/2871 (0.2%)
1	G	0.53	0/2133	0.94	6/2871 (0.2%)
All	All	0.53	1/14957 (0.0%)	0.78	29/20132 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	244	GLN	CG-CD	5.09	1.62	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	250	ARG	NE-CZ-NH2	-23.17	108.72	120.30
1	G	250	ARG	NE-CZ-NH1	20.29	130.44	120.30
1	D	155	ARG	NE-CZ-NH1	-19.53	110.53	120.30
1	D	155	ARG	NE-CZ-NH2	19.11	129.86	120.30
1	G	250	ARG	CD-NE-CZ	10.23	137.92	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	155	ARG	CD-NE-CZ	9.30	136.62	123.60
1	G	271	ARG	CB-CA-C	-9.17	92.06	110.40
1	C	272	THR	N-CA-C	-8.35	88.47	111.00
1	B	271	ARG	CB-CA-C	-7.97	94.45	110.40
1	B	272	THR	N-CA-C	-7.62	90.43	111.00
1	F	272	THR	N-CA-C	-7.61	90.45	111.00
1	G	272	THR	N-CA-C	-7.21	91.53	111.00
1	C	272	THR	CB-CA-C	6.96	130.40	111.60
1	A	212	ARG	N-CA-C	6.86	129.53	111.00
1	A	271	ARG	CB-CA-C	-6.68	97.05	110.40
1	F	271	ARG	CB-CA-C	-6.57	97.26	110.40
1	F	272	THR	CB-CA-C	5.90	127.54	111.60
1	A	149	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	272	THR	N-CA-C	-5.68	95.66	111.00
1	A	245	LYS	N-CA-C	5.67	126.31	111.00
1	C	149	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	272	THR	CB-CA-C	5.53	126.53	111.60
1	A	232	LEU	CA-CB-CG	5.46	127.86	115.30
1	F	232	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	271	ARG	CB-CA-C	-5.32	99.76	110.40
1	E	149	LEU	CA-CB-CG	5.24	127.34	115.30
1	F	149	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	232	LEU	CA-CB-CG	5.09	127.00	115.30
1	G	149	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	SER	Peptide
1	A	212	ARG	Mainchain

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	2116	0	2222	128	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2099	0	2212	127	0
1	C	2099	0	2212	140	0
1	D	2108	0	2218	166	2
1	E	2099	0	2212	142	5
1	F	2099	0	2212	125	3
1	G	2099	0	2212	133	4
2	B	35	0	46	3	1
2	F	35	0	46	10	0
All	All	14789	0	15592	817	9

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 27.

All (817) 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:273:THR:HG22	1:G:275:ILE:HB	1.24	1.17
1:A:273:THR:HG22	1:D:275:ILE:HB	1.11	1.08
1:C:275:ILE:HB	1:F:273:THR:HG22	1.35	1.07
1:A:269:TYR:OH	1:D:191:ASP:HB2	1.58	1.04
1:D:267:PHE:HB2	1:D:269:TYR:CE1	1.93	1.04
1:D:217:GLU:HB2	1:D:239:LYS:HB3	1.49	0.94
1:D:189:PRO:HB3	1:D:271:ARG:NH1	1.82	0.94
1:D:189:PRO:HB3	1:D:271:ARG:HH12	1.29	0.93
1:A:217:GLU:HB2	1:A:239:LYS:HB3	1.50	0.93
1:D:241:GLN:HG3	1:D:242:PRO:HD2	1.54	0.90
1:D:274:VAL:HG13	1:E:275:ILE:O	1.70	0.90
1:B:241:GLN:HG3	1:B:242:PRO:HD2	1.54	0.90
1:A:275:ILE:HB	1:B:273:THR:HG22	1.51	0.89
1:E:241:GLN:HG3	1:E:242:PRO:HD2	1.53	0.89
1:F:241:GLN:HG3	1:F:242:PRO:HD2	1.54	0.89
1:A:257:LYS:HE2	1:D:194:VAL:HG23	1.55	0.87
1:A:212:ARG:HH11	1:A:212:ARG:CG	1.87	0.87
1:B:275:ILE:HB	1:G:273:THR:HG22	1.56	0.87
1:D:257:LYS:HE2	1:E:194:VAL:HG23	1.57	0.86
1:C:241:GLN:HG3	1:C:242:PRO:HD2	1.58	0.86
1:B:212:ARG:CG	1:B:212:ARG:HH11	1.89	0.85
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.41	0.85
1:D:269:TYR:OH	1:E:191:ASP:HB2	1.76	0.85
1:D:250:ARG:CZ	1:E:222:LEU:HD11	2.07	0.84
1:E:212:ARG:HH11	1:E:212:ARG:CG	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:ARG:HB3	1:E:273:THR:OG1	1.75	0.84
1:F:212:ARG:HH11	1:F:212:ARG:CG	1.91	0.84
1:A:273:THR:CG2	1:D:275:ILE:HB	2.01	0.84
1:C:269:TYR:OH	1:G:191:ASP:HB2	1.77	0.83
1:D:155:ARG:HH22	1:E:177:LYS:HB3	1.43	0.83
1:G:241:GLN:HG3	1:G:242:PRO:HD2	1.57	0.83
1:C:251:ASP:OD1	1:C:255:ARG:NH1	2.12	0.83
1:D:212:ARG:CG	1:D:212:ARG:HH11	1.92	0.83
1:G:212:ARG:CG	1:G:212:ARG:HH11	1.91	0.82
1:F:251:ASP:OD1	1:F:255:ARG:NH1	2.13	0.81
1:E:212:ARG:HH11	1:E:212:ARG:HG2	1.45	0.81
1:C:212:ARG:HH11	1:C:212:ARG:CG	1.93	0.81
1:B:212:ARG:HH11	1:B:212:ARG:HG2	1.46	0.80
1:F:212:ARG:HH11	1:F:212:ARG:HG2	1.46	0.80
1:D:217:GLU:HB2	1:D:239:LYS:CB	2.12	0.80
1:E:251:ASP:OD1	1:E:255:ARG:NH1	2.15	0.80
1:G:212:ARG:HH11	1:G:212:ARG:HG2	1.46	0.80
1:B:224:ILE:HD13	1:B:224:ILE:H	1.47	0.79
1:A:271:ARG:HB3	1:D:273:THR:OG1	1.81	0.79
1:G:224:ILE:HD13	1:G:224:ILE:H	1.48	0.79
1:E:177:LYS:O	1:E:179:SER:N	2.16	0.78
1:D:267:PHE:CB	1:D:269:TYR:CE1	2.66	0.78
1:A:212:ARG:HD3	1:A:213:ASP:H	1.49	0.78
1:D:251:ASP:OD1	1:D:255:ARG:NH1	2.17	0.78
1:B:177:LYS:O	1:B:179:SER:N	2.18	0.77
1:C:273:THR:CG2	1:G:275:ILE:HB	2.12	0.77
1:G:251:ASP:OD1	1:G:255:ARG:NH1	2.17	0.77
1:C:257:LYS:HE2	1:G:194:VAL:HG23	1.66	0.77
1:D:189:PRO:CB	1:D:271:ARG:HH12	1.97	0.77
1:D:269:TYR:CD2	1:E:271:ARG:HG3	2.19	0.77
1:E:224:ILE:HD13	1:E:224:ILE:H	1.50	0.77
1:A:217:GLU:HB2	1:A:239:LYS:CB	2.15	0.76
1:D:244:GLN:O	1:D:248:VAL:HG23	1.85	0.76
1:D:267:PHE:HB2	1:D:269:TYR:HE1	1.51	0.74
1:B:251:ASP:OD1	1:B:255:ARG:NH1	2.19	0.74
1:F:100:GLY:CA	2:F:283:LMT:H2B	2.17	0.74
1:D:267:PHE:CB	1:D:269:TYR:HE1	2.00	0.74
1:D:274:VAL:HG22	1:D:274:VAL:O	1.84	0.74
1:C:212:ARG:HH11	1:C:212:ARG:HG2	1.51	0.74
1:A:269:TYR:HH	1:D:191:ASP:HB2	1.50	0.73
1:B:244:GLN:O	1:B:248:VAL:HG23	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:O	1:D:192:GLU:HB2	1.89	0.72
1:B:177:LYS:HB3	1:G:155:ARG:HH22	1.54	0.72
1:C:244:GLN:O	1:C:248:VAL:HG23	1.89	0.72
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.03	0.72
1:E:189:PRO:O	1:E:192:GLU:HB2	1.90	0.72
1:A:224:ILE:HD11	1:B:254:TYR:HB2	1.71	0.72
1:A:247:ALA:HA	1:A:250:ARG:NH2	2.05	0.72
1:C:191:ASP:HB2	1:F:269:TYR:OH	1.90	0.71
1:G:177:LYS:O	1:G:179:SER:N	2.23	0.71
1:A:251:ASP:OD1	1:A:255:ARG:NH1	2.24	0.71
1:E:257:LYS:HE2	1:F:194:VAL:HG23	1.73	0.70
1:E:274:VAL:HG23	1:E:275:ILE:N	2.05	0.70
1:B:222:LEU:HD11	1:G:250:ARG:CZ	2.22	0.70
1:D:274:VAL:O	1:D:274:VAL:CG2	2.38	0.70
1:A:224:ILE:HD13	1:A:224:ILE:H	1.55	0.70
1:F:189:PRO:O	1:F:192:GLU:HB2	1.92	0.70
1:F:244:GLN:O	1:F:248:VAL:HG23	1.92	0.70
1:E:190:ILE:O	1:E:192:GLU:N	2.23	0.70
1:G:244:GLN:O	1:G:248:VAL:HG23	1.92	0.70
1:C:224:ILE:HD13	1:C:224:ILE:H	1.57	0.69
1:D:224:ILE:HD13	1:D:224:ILE:H	1.56	0.69
1:G:189:PRO:O	1:G:192:GLU:HB2	1.93	0.69
1:D:190:ILE:O	1:D:192:GLU:N	2.24	0.69
1:A:231:LYS:HD3	1:D:229:ASP:OD1	1.92	0.69
1:C:224:ILE:HG22	1:C:234:ILE:HG12	1.73	0.69
1:D:269:TYR:CE2	1:E:271:ARG:HG3	2.29	0.69
1:E:269:TYR:OH	1:F:191:ASP:HB2	1.92	0.69
1:A:177:LYS:O	1:A:179:SER:N	2.22	0.68
1:F:177:LYS:O	1:F:179:SER:N	2.24	0.68
1:C:177:LYS:O	1:C:179:SER:N	2.26	0.68
2:F:283:LMT:H51	1:G:100:GLY:HA3	1.76	0.67
1:E:130:SER:O	1:E:132:GLY:N	2.27	0.67
1:G:212:ARG:HG2	1:G:212:ARG:NH1	2.08	0.67
1:A:212:ARG:HD3	1:A:213:ASP:N	2.08	0.67
1:D:276:LEU:HD12	1:E:276:LEU:HD21	1.76	0.67
1:A:244:GLN:O	1:A:248:VAL:HG23	1.95	0.66
1:B:241:GLN:HG3	1:B:242:PRO:CD	2.25	0.66
1:F:224:ILE:H	1:F:224:ILE:HD13	1.59	0.66
1:E:241:GLN:HG3	1:E:242:PRO:CD	2.24	0.66
1:A:189:PRO:O	1:A:192:GLU:HB2	1.96	0.66
1:E:212:ARG:HG2	1:E:212:ARG:NH1	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:LYS:O	1:D:179:SER:N	2.26	0.66
1:D:212:ARG:HH11	1:D:212:ARG:HG2	1.61	0.66
1:F:104:LEU:HG	2:F:283:LMT:O3B	1.96	0.66
1:E:230:SER:HB2	1:E:271:ARG:HD2	1.79	0.65
1:C:54:ILE:HG22	1:C:55:GLN:HG3	1.77	0.65
1:E:244:GLN:O	1:E:248:VAL:HG23	1.96	0.65
1:B:114:VAL:O	1:B:118:ILE:HG13	1.95	0.65
1:D:54:ILE:HG22	1:D:55:GLN:HG3	1.79	0.65
1:G:21:LEU:O	1:G:25:LEU:HB2	1.97	0.64
1:G:54:ILE:HG22	1:G:55:GLN:HG3	1.79	0.64
1:D:254:TYR:OH	1:E:195:ASP:OD1	2.15	0.64
1:E:195:ASP:HA	1:E:198:ILE:HG22	1.79	0.64
1:F:212:ARG:HG2	1:F:212:ARG:NH1	2.08	0.64
1:A:273:THR:HG22	1:D:275:ILE:CB	2.07	0.64
1:G:130:SER:O	1:G:132:GLY:N	2.31	0.64
1:A:191:ASP:HB2	1:B:269:TYR:OH	1.98	0.63
1:B:54:ILE:HG22	1:B:55:GLN:HG3	1.79	0.63
1:A:194:VAL:HG23	1:B:257:LYS:HE2	1.80	0.63
1:F:100:GLY:HA3	2:F:283:LMT:H2B	1.79	0.63
1:C:222:LEU:HD11	1:F:250:ARG:CZ	2.29	0.63
1:C:250:ARG:CZ	1:G:222:LEU:HD11	2.28	0.63
1:E:54:ILE:HG22	1:E:55:GLN:HG3	1.79	0.63
1:F:241:GLN:HG3	1:F:242:PRO:CD	2.27	0.63
1:G:136:THR:HG22	1:G:175:LEU:HD13	1.80	0.63
1:F:195:ASP:HA	1:F:198:ILE:HG22	1.81	0.63
1:B:212:ARG:HG2	1:B:212:ARG:NH1	2.07	0.63
1:B:279:LYS:HB3	1:G:275:ILE:CG2	2.29	0.63
1:B:114:VAL:HG11	1:G:106:ILE:HA	1.80	0.63
1:E:254:TYR:HB2	1:F:224:ILE:HD11	1.81	0.63
1:B:189:PRO:O	1:B:192:GLU:HB2	1.99	0.62
1:G:139:GLY:O	1:G:140:ILE:HD12	1.99	0.62
1:C:195:ASP:HA	1:C:198:ILE:HG22	1.81	0.62
1:D:130:SER:O	1:D:132:GLY:N	2.27	0.62
1:A:21:LEU:O	1:A:25:LEU:HB2	2.00	0.62
1:B:224:ILE:HD11	1:G:254:TYR:HB2	1.81	0.62
1:C:16:LYS:O	1:C:18:VAL:N	2.33	0.62
1:C:248:VAL:O	1:C:252:ILE:HG13	2.00	0.62
1:B:194:VAL:HG23	1:G:257:LYS:HE2	1.81	0.62
1:F:151:VAL:HG11	1:F:163:ILE:HG23	1.81	0.62
1:C:224:ILE:HD11	1:F:254:TYR:HB2	1.82	0.62
1:D:240:THR:HG21	1:D:248:VAL:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:GLY:O	1:C:140:ILE:HD12	1.99	0.62
1:D:136:THR:HG22	1:D:175:LEU:HD13	1.81	0.62
1:D:241:GLN:HG3	1:D:242:PRO:CD	2.29	0.62
1:A:195:ASP:HA	1:A:198:ILE:HG22	1.81	0.62
1:C:280:LYS:HG2	1:C:281:THR:H	1.64	0.62
1:D:212:ARG:HG2	1:D:212:ARG:NH1	2.14	0.62
1:F:54:ILE:HG22	1:F:55:GLN:HG3	1.80	0.62
1:D:21:LEU:O	1:D:25:LEU:HB2	2.00	0.61
1:C:257:LYS:NZ	1:G:190:ILE:O	2.33	0.61
1:B:137:ILE:HD12	1:B:154:ILE:HD11	1.82	0.61
1:B:191:ASP:HB2	1:G:269:TYR:OH	2.00	0.61
1:G:195:ASP:HA	1:G:198:ILE:HG22	1.83	0.61
1:B:136:THR:HG23	1:B:173:THR:HG23	1.83	0.61
1:C:194:VAL:HG23	1:F:257:LYS:HE2	1.82	0.61
1:C:269:TYR:CD1	1:G:271:ARG:HG3	2.35	0.61
1:F:25:LEU:O	1:F:29:ILE:HG23	2.00	0.61
1:C:151:VAL:HG11	1:C:163:ILE:HG23	1.83	0.61
1:E:274:VAL:CG2	1:E:275:ILE:N	2.61	0.61
1:B:25:LEU:O	1:B:29:ILE:HG23	2.00	0.61
1:F:100:GLY:HA3	2:F:283:LMT:C2B	2.31	0.61
1:A:54:ILE:HG22	1:A:55:GLN:HG3	1.81	0.60
1:A:224:ILE:HG22	1:A:234:ILE:HG12	1.83	0.60
1:G:240:THR:HG21	1:G:248:VAL:HG21	1.82	0.60
1:F:248:VAL:O	1:F:252:ILE:HG13	2.02	0.60
1:C:16:LYS:O	1:C:19:LYS:N	2.35	0.60
1:B:195:ASP:HA	1:B:198:ILE:HG22	1.82	0.60
1:A:190:ILE:HD11	1:A:229:ASP:O	2.02	0.60
1:B:280:LYS:HG2	1:B:281:THR:H	1.66	0.60
1:C:212:ARG:HG2	1:C:212:ARG:NH1	2.12	0.60
1:E:190:ILE:HD11	1:E:229:ASP:O	2.01	0.60
1:G:248:VAL:O	1:G:252:ILE:HG13	2.01	0.60
1:A:250:ARG:CZ	1:D:222:LEU:HD11	2.32	0.59
1:A:190:ILE:O	1:A:192:GLU:N	2.34	0.59
1:A:280:LYS:HG2	1:A:281:THR:H	1.66	0.59
1:B:151:VAL:HG11	1:B:163:ILE:HG23	1.84	0.59
1:G:117:MET:HG2	1:G:149:LEU:HD13	1.85	0.59
1:C:254:TYR:HB2	1:G:224:ILE:HD11	1.82	0.59
1:F:100:GLY:HA2	2:F:283:LMT:H2B	1.84	0.59
1:D:195:ASP:HA	1:D:198:ILE:HG22	1.82	0.59
1:D:212:ARG:HH11	1:D:212:ARG:HG3	1.67	0.59
1:B:188:PHE:HE2	1:B:234:ILE:HG13	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:O	1:C:29:ILE:HG23	2.02	0.59
1:F:21:LEU:O	1:F:25:LEU:HB2	2.02	0.59
1:B:130:SER:O	1:B:132:GLY:N	2.32	0.58
1:B:219:PRO:HB3	1:B:238:ALA:HB2	1.85	0.58
1:C:130:SER:O	1:C:132:GLY:N	2.32	0.58
1:F:103:SER:HB2	2:F:283:LMT:O3B	2.03	0.58
1:F:176:THR:HG22	1:F:180:MET:HE2	1.85	0.58
1:F:280:LYS:HG2	1:F:281:THR:H	1.68	0.58
1:C:21:LEU:O	1:C:25:LEU:HB2	2.04	0.58
1:C:136:THR:HG23	1:C:173:THR:HG23	1.84	0.58
1:C:241:GLN:HG3	1:C:242:PRO:CD	2.31	0.58
1:D:111:GLN:HG3	1:D:112:ASN:N	2.18	0.58
1:A:16:LYS:O	1:A:19:LYS:N	2.37	0.58
1:A:118:ILE:HG12	2:B:283:LMT:H41	1.85	0.58
1:B:176:THR:HG22	1:B:180:MET:HE2	1.84	0.58
1:G:151:VAL:HG11	1:G:163:ILE:HG23	1.85	0.58
1:F:136:THR:HG22	1:F:175:LEU:HD13	1.86	0.58
1:D:224:ILE:HG22	1:D:234:ILE:HG12	1.86	0.58
1:A:222:LEU:HD11	1:B:250:ARG:CZ	2.34	0.58
1:G:188:PHE:HE2	1:G:234:ILE:HG13	1.68	0.58
1:A:254:TYR:HB2	1:D:224:ILE:HD11	1.85	0.57
1:B:21:LEU:O	1:B:25:LEU:HB2	2.04	0.57
1:C:247:ALA:HA	1:C:250:ARG:NH2	2.18	0.57
1:C:275:ILE:HB	1:F:273:THR:CG2	2.24	0.57
1:E:21:LEU:O	1:E:25:LEU:HB2	2.02	0.57
1:F:111:GLN:HG3	1:F:112:ASN:N	2.19	0.57
1:D:248:VAL:O	1:D:252:ILE:HG13	2.04	0.57
1:F:190:ILE:O	1:F:192:GLU:N	2.38	0.57
1:A:209:LYS:HG3	1:A:219:PRO:HD2	1.86	0.57
1:B:16:LYS:O	1:B:19:LYS:N	2.38	0.57
1:B:125:PHE:CZ	1:G:64:LEU:HD12	2.39	0.57
1:E:136:THR:HG23	1:E:173:THR:HG23	1.85	0.57
1:D:280:LYS:HG2	1:D:281:THR:H	1.67	0.57
1:G:247:ALA:HA	1:G:250:ARG:NH2	2.19	0.57
1:A:130:SER:O	1:A:132:GLY:N	2.32	0.57
1:B:16:LYS:O	1:B:18:VAL:N	2.37	0.57
1:B:136:THR:HG22	1:B:175:LEU:HD13	1.85	0.57
1:E:280:LYS:HG2	1:E:281:THR:H	1.68	0.57
1:F:136:THR:HG23	1:F:173:THR:HG23	1.86	0.57
1:A:136:THR:HG23	1:A:173:THR:HG23	1.86	0.57
1:C:272:THR:O	1:G:274:VAL:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:HB1	2:B:283:LMT:H101	1.85	0.57
1:E:273:THR:OG1	1:E:273:THR:O	2.23	0.57
1:D:151:VAL:HG11	1:D:163:ILE:HG23	1.87	0.57
1:E:139:GLY:O	1:E:140:ILE:HD12	2.05	0.57
1:F:16:LYS:O	1:F:19:LYS:N	2.38	0.57
1:F:209:LYS:HG3	1:F:219:PRO:HD2	1.87	0.57
1:A:25:LEU:O	1:A:29:ILE:HG23	2.05	0.56
1:A:188:PHE:HD2	1:A:232:LEU:HD23	1.70	0.56
1:A:217:GLU:CB	1:A:239:LYS:CB	2.82	0.56
1:B:183:VAL:CG2	1:G:158:SER:HB2	2.35	0.56
1:F:130:SER:O	1:F:132:GLY:N	2.34	0.56
1:G:190:ILE:O	1:G:192:GLU:N	2.38	0.56
1:E:16:LYS:O	1:E:19:LYS:N	2.39	0.56
1:E:205:CYS:HB3	1:E:219:PRO:O	2.05	0.56
1:D:16:LYS:O	1:D:19:LYS:N	2.39	0.56
1:F:224:ILE:HG22	1:F:234:ILE:HG12	1.86	0.56
1:G:176:THR:HG22	1:G:180:MET:HE2	1.88	0.56
1:A:248:VAL:O	1:A:252:ILE:HG13	2.06	0.56
1:B:190:ILE:O	1:B:192:GLU:N	2.38	0.56
1:D:139:GLY:O	1:D:140:ILE:HD12	2.04	0.56
1:A:111:GLN:HG3	1:A:112:ASN:N	2.21	0.56
1:A:205:CYS:HB3	1:A:219:PRO:O	2.06	0.56
1:C:189:PRO:O	1:C:192:GLU:HB2	2.05	0.56
1:E:224:ILE:HG22	1:E:234:ILE:HG12	1.88	0.56
1:G:241:GLN:HG3	1:G:242:PRO:CD	2.31	0.56
1:B:100:GLY:HA3	2:F:283:LMT:H101	1.88	0.56
1:C:114:VAL:O	1:C:118:ILE:HG13	2.05	0.56
1:E:111:GLN:HG3	1:E:112:ASN:N	2.21	0.56
1:G:280:LYS:HG2	1:G:281:THR:H	1.69	0.56
1:G:16:LYS:O	1:G:18:VAL:N	2.39	0.56
1:D:254:TYR:HB2	1:E:224:ILE:HD11	1.87	0.56
1:G:212:ARG:CG	1:G:212:ARG:NH1	2.60	0.56
1:A:136:THR:HG22	1:A:175:LEU:HD13	1.87	0.55
1:A:151:VAL:HG11	1:A:163:ILE:HG23	1.88	0.55
1:C:114:VAL:HG11	1:F:106:ILE:HA	1.88	0.55
1:A:158:SER:HA	1:D:181:MET:HB3	1.87	0.55
1:G:111:GLN:HG3	1:G:112:ASN:N	2.21	0.55
1:G:137:ILE:HD12	1:G:154:ILE:HD11	1.89	0.55
1:E:136:THR:HG22	1:E:175:LEU:HD13	1.89	0.55
1:C:103:SER:HB2	2:F:283:LMT:O2'	2.07	0.55
1:A:16:LYS:O	1:A:18:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:CYS:HB3	1:D:219:PRO:O	2.06	0.55
1:B:139:GLY:O	1:B:140:ILE:HD12	2.07	0.55
1:D:25:LEU:O	1:D:29:ILE:HG23	2.07	0.55
1:D:158:SER:HA	1:E:181:MET:HB3	1.87	0.55
1:D:269:TYR:CD1	1:D:269:TYR:N	2.74	0.55
1:C:188:PHE:HD2	1:C:232:LEU:HD23	1.72	0.55
1:C:240:THR:HG21	1:C:248:VAL:HG21	1.88	0.55
1:G:16:LYS:O	1:G:19:LYS:N	2.40	0.55
1:B:26:LYS:HE3	1:G:89:ASN:ND2	2.21	0.55
1:D:161:LEU:O	1:E:174:ASN:N	2.34	0.55
1:D:271:ARG:HB3	1:E:273:THR:O	2.07	0.55
1:E:188:PHE:HE2	1:E:234:ILE:HG13	1.72	0.55
1:B:257:LYS:HE3	1:B:261:ASP:OD2	2.06	0.54
1:D:217:GLU:CB	1:D:239:LYS:CB	2.84	0.54
1:C:209:LYS:HG3	1:C:219:PRO:HD2	1.88	0.54
1:D:269:TYR:N	1:D:269:TYR:HD1	2.04	0.54
1:G:188:PHE:HD2	1:G:232:LEU:HD23	1.73	0.54
1:G:219:PRO:HB3	1:G:238:ALA:HB2	1.89	0.54
1:C:231:LYS:HD3	1:G:229:ASP:OD1	2.07	0.54
1:F:190:ILE:HD11	1:F:229:ASP:O	2.06	0.54
1:A:275:ILE:HG12	1:D:277:SER:HB3	1.89	0.54
1:F:219:PRO:HB3	1:F:238:ALA:HB2	1.89	0.54
1:B:111:GLN:HG3	1:B:112:ASN:N	2.21	0.54
1:D:16:LYS:O	1:D:18:VAL:N	2.40	0.54
1:D:89:ASN:ND2	1:E:26:LYS:HE3	2.23	0.54
1:D:188:PHE:HE2	1:D:234:ILE:HG13	1.73	0.54
1:D:190:ILE:HD11	1:D:229:ASP:O	2.08	0.54
1:D:276:LEU:HD12	1:E:276:LEU:CD2	2.37	0.54
1:E:248:VAL:O	1:E:252:ILE:HG13	2.07	0.54
1:F:114:VAL:O	1:F:118:ILE:HG13	2.08	0.54
1:B:209:LYS:HG3	1:B:219:PRO:HD2	1.89	0.54
1:F:188:PHE:HE2	1:F:234:ILE:HG13	1.73	0.54
1:G:193:ASP:O	1:G:197:ILE:HG12	2.08	0.54
1:E:151:VAL:HG11	1:E:163:ILE:HG23	1.89	0.54
1:E:250:ARG:CZ	1:F:222:LEU:HD11	2.37	0.54
1:B:235:MET:HG3	1:B:235:MET:O	2.08	0.54
1:A:176:THR:HG22	1:A:180:MET:HE2	1.89	0.54
1:G:224:ILE:HG22	1:G:234:ILE:HG12	1.90	0.54
1:B:205:CYS:HB3	1:B:219:PRO:O	2.07	0.53
1:B:240:THR:HG21	1:B:248:VAL:HG21	1.91	0.53
1:C:111:GLN:HG3	1:C:112:ASN:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:LYS:HG3	1:D:219:PRO:HD2	1.89	0.53
1:D:188:PHE:HD2	1:D:232:LEU:HD23	1.73	0.53
1:E:257:LYS:C	1:E:257:LYS:HD3	2.29	0.53
1:D:133:ASP:OD1	1:D:133:ASP:N	2.40	0.53
1:B:247:ALA:HA	1:B:250:ARG:NH2	2.24	0.53
1:C:183:VAL:CG2	1:F:158:SER:HB2	2.39	0.53
1:C:271:ARG:HG3	1:F:269:TYR:CD1	2.43	0.53
1:A:155:ARG:HH22	1:D:177:LYS:HB3	1.74	0.53
1:D:106:ILE:HA	1:E:114:VAL:HG11	1.91	0.53
1:G:257:LYS:HE3	1:G:261:ASP:OD2	2.09	0.53
1:A:279:LYS:HB3	1:B:275:ILE:CG2	2.39	0.53
1:C:158:SER:HB2	1:G:183:VAL:CG2	2.39	0.53
1:B:188:PHE:HD2	1:B:232:LEU:HD23	1.74	0.53
1:D:219:PRO:HB3	1:D:238:ALA:HB2	1.89	0.53
1:E:189:PRO:HB3	1:E:271:ARG:NH1	2.24	0.53
1:C:128:GLN:OE1	1:C:172:VAL:HG11	2.09	0.53
1:C:205:CYS:HB3	1:C:219:PRO:O	2.09	0.53
1:E:176:THR:HG22	1:E:180:MET:HE2	1.90	0.53
1:E:209:LYS:HG3	1:E:219:PRO:HD2	1.91	0.53
1:F:139:GLY:O	1:F:140:ILE:HD12	2.08	0.53
1:A:217:GLU:CB	1:A:239:LYS:HB2	2.39	0.52
1:B:102:GLY:O	1:B:106:ILE:HG12	2.09	0.52
1:E:25:LEU:O	1:E:29:ILE:HG23	2.09	0.52
1:B:257:LYS:HD3	1:B:257:LYS:C	2.30	0.52
1:C:26:LYS:HE3	1:F:89:ASN:ND2	2.25	0.52
1:D:128:GLN:OE1	1:D:172:VAL:HG11	2.09	0.52
1:G:209:LYS:HG3	1:G:219:PRO:HD2	1.90	0.52
1:G:257:LYS:HD3	1:G:257:LYS:C	2.30	0.52
1:A:169:ILE:O	1:A:169:ILE:HG22	2.10	0.52
1:B:177:LYS:HB3	1:G:155:ARG:NH2	2.23	0.52
1:D:131:VAL:HG12	1:D:131:VAL:O	2.10	0.52
1:D:276:LEU:CD1	1:E:276:LEU:HD21	2.39	0.52
1:E:191:ASP:HB3	1:E:271:ARG:NH1	2.25	0.52
1:B:190:ILE:HD11	1:B:229:ASP:O	2.09	0.52
1:C:102:GLY:O	1:C:106:ILE:HG12	2.10	0.52
1:C:136:THR:HG22	1:C:175:LEU:HD13	1.92	0.52
1:A:257:LYS:HE3	1:A:261:ASP:OD2	2.10	0.52
1:D:89:ASN:HD21	1:E:26:LYS:HE3	1.75	0.52
1:D:247:ALA:HA	1:D:250:ARG:NH2	2.24	0.52
1:E:16:LYS:O	1:E:18:VAL:N	2.43	0.52
1:F:169:ILE:O	1:F:169:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:279:LYS:HG3	1:F:280:LYS:H	1.73	0.52
1:A:79:LEU:HD21	1:B:95:LEU:HA	1.90	0.52
1:D:179:SER:OG	1:D:180:MET:N	2.43	0.52
1:D:217:GLU:CB	1:D:239:LYS:HB2	2.40	0.52
1:E:128:GLN:OE1	1:E:172:VAL:HG11	2.10	0.52
1:D:257:LYS:HD3	1:D:257:LYS:C	2.30	0.52
1:F:16:LYS:O	1:F:18:VAL:N	2.43	0.52
1:F:205:CYS:HB3	1:F:219:PRO:O	2.09	0.52
1:F:257:LYS:HD3	1:F:257:LYS:C	2.29	0.52
1:E:188:PHE:HD2	1:E:232:LEU:HD23	1.73	0.52
1:B:179:SER:OG	1:B:180:MET:N	2.43	0.51
1:G:205:CYS:HB3	1:G:219:PRO:O	2.10	0.51
1:B:183:VAL:HG23	1:G:158:SER:HB2	1.92	0.51
1:A:57:PRO:O	1:A:61:ILE:HG22	2.10	0.51
1:C:137:ILE:HD12	1:C:154:ILE:HD11	1.91	0.51
1:G:114:VAL:O	1:G:118:ILE:HG13	2.10	0.51
1:F:102:GLY:O	1:F:106:ILE:HG12	2.10	0.51
1:F:188:PHE:HD2	1:F:232:LEU:HD23	1.75	0.51
1:G:242:PRO:O	1:G:243:MET:HB2	2.11	0.51
1:C:279:LYS:HG3	1:C:280:LYS:H	1.76	0.51
1:E:204:ILE:HD11	1:E:259:MET:HB2	1.92	0.51
1:F:179:SER:OG	1:F:180:MET:N	2.42	0.51
1:A:257:LYS:HD3	1:A:257:LYS:C	2.31	0.51
1:A:279:LYS:HG3	1:A:280:LYS:H	1.76	0.51
1:C:242:PRO:O	1:C:243:MET:HB2	2.11	0.51
1:A:254:TYR:OH	1:D:195:ASP:OD1	2.24	0.51
1:B:42:ILE:O	1:B:46:TYR:HB2	2.11	0.51
1:C:191:ASP:HB3	1:C:271:ARG:HH11	1.76	0.51
1:C:106:ILE:HA	1:G:114:VAL:HG11	1.91	0.51
1:D:117:MET:HG2	1:D:149:LEU:HD13	1.93	0.51
1:E:42:ILE:O	1:E:46:TYR:HB2	2.11	0.51
1:A:177:LYS:HB3	1:B:155:ARG:HH22	1.76	0.51
1:E:219:PRO:HB3	1:E:238:ALA:HB2	1.93	0.51
1:G:176:THR:HG22	1:G:180:MET:CE	2.41	0.51
1:B:257:LYS:HD3	1:B:257:LYS:O	2.11	0.51
1:E:279:LYS:HG3	1:E:280:LYS:H	1.76	0.51
1:G:128:GLN:OE1	1:G:172:VAL:HG11	2.11	0.51
1:A:102:GLY:O	1:A:106:ILE:HG12	2.10	0.50
1:C:257:LYS:HE3	1:C:261:ASP:OD2	2.11	0.50
1:D:102:GLY:O	1:D:106:ILE:HG12	2.10	0.50
1:D:158:SER:HB2	1:E:183:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:O	1:C:46:TYR:HB2	2.12	0.50
1:D:137:ILE:HD12	1:D:154:ILE:HD11	1.92	0.50
1:C:190:ILE:O	1:C:192:GLU:N	2.43	0.50
1:F:257:LYS:HD3	1:F:257:LYS:O	2.12	0.50
1:A:258:LYS:HE3	1:D:195:ASP:OD2	2.12	0.50
1:B:224:ILE:HG22	1:B:234:ILE:HG12	1.93	0.50
1:D:158:SER:HB2	1:E:183:VAL:HG23	1.94	0.50
1:B:117:MET:HG2	1:B:149:LEU:HD13	1.93	0.50
1:F:269:TYR:CE2	1:G:275:ILE:HD12	2.46	0.50
1:B:188:PHE:CE2	1:B:234:ILE:HG13	2.46	0.50
1:C:190:ILE:HD11	1:C:229:ASP:O	2.11	0.50
1:D:279:LYS:HG3	1:D:280:LYS:H	1.76	0.50
1:C:257:LYS:HD3	1:C:257:LYS:C	2.32	0.50
1:E:133:ASP:OD1	1:E:133:ASP:N	2.43	0.50
1:E:240:THR:HG21	1:E:248:VAL:HG21	1.93	0.50
1:F:254:TYR:CE2	1:F:258:LYS:HG3	2.47	0.50
1:A:128:GLN:OE1	1:A:172:VAL:HG11	2.11	0.49
1:A:212:ARG:C	1:A:213:ASP:CG	2.71	0.49
1:B:151:VAL:HG11	1:B:163:ILE:CG2	2.42	0.49
1:G:279:LYS:HG3	1:G:280:LYS:H	1.76	0.49
1:A:117:MET:HG2	1:A:149:LEU:HD13	1.94	0.49
1:D:258:LYS:HE3	1:E:195:ASP:OD2	2.12	0.49
1:A:212:ARG:O	1:A:213:ASP:OD1	2.30	0.49
1:E:243:MET:C	1:E:245:LYS:H	2.15	0.49
1:G:190:ILE:HD11	1:G:229:ASP:O	2.12	0.49
1:C:44:ARG:C	1:C:46:TYR:N	2.64	0.49
1:C:193:ASP:O	1:C:197:ILE:HG12	2.11	0.49
1:C:226:ASP:OD2	1:C:227:MET:N	2.46	0.49
1:D:176:THR:HG22	1:D:180:MET:HE2	1.93	0.49
1:F:42:ILE:O	1:F:46:TYR:HB2	2.13	0.49
1:F:151:VAL:HG11	1:F:163:ILE:CG2	2.42	0.49
1:F:242:PRO:O	1:F:243:MET:HB2	2.12	0.49
1:G:42:ILE:O	1:G:46:TYR:HB2	2.13	0.49
1:G:136:THR:HG23	1:G:173:THR:HG23	1.94	0.49
1:A:240:THR:HG21	1:A:248:VAL:HG21	1.93	0.49
1:A:273:THR:HA	1:D:275:ILE:O	2.13	0.49
1:B:133:ASP:OD1	1:B:133:ASP:N	2.39	0.49
1:G:249:GLU:O	1:G:253:ARG:HG3	2.13	0.49
1:A:106:ILE:HA	1:D:114:VAL:HG11	1.94	0.49
1:A:193:ASP:O	1:A:197:ILE:HG12	2.11	0.49
1:F:240:THR:HG21	1:F:248:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:SER:OG	1:A:180:MET:N	2.42	0.49
1:A:191:ASP:HB3	1:A:271:ARG:HH11	1.77	0.49
1:A:219:PRO:HB3	1:A:238:ALA:HB2	1.94	0.49
1:A:191:ASP:HB3	1:A:271:ARG:NH1	2.28	0.49
1:C:137:ILE:HD12	1:C:154:ILE:CD1	2.42	0.49
1:D:193:ASP:O	1:D:197:ILE:HG12	2.13	0.49
1:E:137:ILE:HD12	1:E:154:ILE:HD11	1.94	0.49
1:A:140:ILE:O	1:A:140:ILE:HG22	2.13	0.49
1:B:57:PRO:O	1:B:61:ILE:HG22	2.13	0.49
1:C:191:ASP:HB3	1:C:271:ARG:NH1	2.27	0.49
1:C:179:SER:OG	1:C:180:MET:N	2.45	0.49
1:E:102:GLY:O	1:E:106:ILE:HG12	2.13	0.49
1:G:191:ASP:HB3	1:G:271:ARG:NH1	2.28	0.49
1:C:219:PRO:HB3	1:C:238:ALA:HB2	1.94	0.48
1:F:257:LYS:HE3	1:F:261:ASP:OD2	2.13	0.48
1:B:137:ILE:HD12	1:B:154:ILE:CD1	2.43	0.48
1:D:257:LYS:HE3	1:D:261:ASP:OD2	2.13	0.48
1:E:57:PRO:O	1:E:61:ILE:HG22	2.13	0.48
1:A:115:LYS:HB2	1:A:115:LYS:HE3	1.64	0.48
1:C:279:LYS:HB3	1:F:275:ILE:CG2	2.43	0.48
1:E:257:LYS:HD3	1:E:257:LYS:O	2.13	0.48
1:A:44:ARG:C	1:A:46:TYR:N	2.66	0.48
1:A:242:PRO:O	1:A:243:MET:HB2	2.13	0.48
1:C:269:TYR:CE1	1:G:271:ARG:HG3	2.48	0.48
1:C:96:LEU:HD11	2:F:283:LMT:H2'	1.95	0.48
1:A:212:ARG:HH11	1:A:212:ARG:HG3	1.76	0.48
1:C:267:PHE:CD2	1:G:190:ILE:HD12	2.48	0.48
1:D:257:LYS:HG3	1:E:194:VAL:HG21	1.94	0.48
1:G:179:SER:OG	1:G:180:MET:N	2.47	0.48
1:B:248:VAL:O	1:B:252:ILE:HG13	2.13	0.48
1:C:169:ILE:HG22	1:C:169:ILE:O	2.12	0.48
1:D:88:PHE:CD1	1:E:30:ILE:HB	2.49	0.48
1:E:85:LEU:HD12	1:E:85:LEU:HA	1.74	0.48
1:F:128:GLN:OE1	1:F:172:VAL:HG11	2.14	0.48
1:G:188:PHE:CE2	1:G:234:ILE:HG13	2.47	0.48
1:C:271:ARG:HG3	1:F:269:TYR:CE1	2.48	0.47
1:C:273:THR:HA	1:G:275:ILE:O	2.14	0.47
1:D:271:ARG:CB	1:E:273:THR:O	2.62	0.47
1:G:254:TYR:CE2	1:G:258:LYS:HG3	2.49	0.47
1:A:137:ILE:HG23	1:A:169:ILE:HG13	1.96	0.47
1:B:44:ARG:C	1:B:46:TYR:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:MET:CE	1:C:243:MET:H	2.27	0.47
1:D:42:ILE:O	1:D:46:TYR:HB2	2.14	0.47
1:A:246:TRP:N	1:A:246:TRP:CD1	2.82	0.47
1:A:257:LYS:CE	1:D:194:VAL:HG23	2.37	0.47
1:C:44:ARG:C	1:C:46:TYR:H	2.17	0.47
1:C:145:GLU:OE2	1:C:155:ARG:HD2	2.14	0.47
1:E:235:MET:O	1:E:235:MET:HG3	2.12	0.47
1:E:247:ALA:HA	1:E:250:ARG:NH2	2.30	0.47
1:B:169:ILE:HG22	1:B:169:ILE:O	2.14	0.47
1:B:193:ASP:O	1:B:197:ILE:HG12	2.14	0.47
1:C:235:MET:O	1:C:235:MET:HG3	2.15	0.47
1:E:44:ARG:C	1:E:46:TYR:N	2.68	0.47
1:F:191:ASP:HB3	1:F:271:ARG:NH1	2.30	0.47
1:G:57:PRO:O	1:G:61:ILE:HG22	2.14	0.47
1:B:176:THR:HG22	1:B:180:MET:CE	2.45	0.47
1:C:180:MET:HE3	1:C:242:PRO:HA	1.97	0.47
1:F:95:LEU:HD22	1:F:95:LEU:O	2.14	0.47
1:G:226:ASP:OD2	1:G:227:MET:N	2.47	0.47
1:A:42:ILE:O	1:A:46:TYR:HB2	2.13	0.47
1:A:188:PHE:HE2	1:A:234:ILE:HG13	1.79	0.47
1:E:67:LEU:HD22	1:E:67:LEU:HA	1.65	0.47
1:B:276:LEU:HD21	1:G:276:LEU:HD12	1.97	0.46
1:E:177:LYS:C	1:E:179:SER:N	2.68	0.46
1:E:179:SER:OG	1:E:180:MET:N	2.46	0.46
1:F:226:ASP:OD2	1:F:227:MET:N	2.48	0.46
1:C:57:PRO:O	1:C:61:ILE:HG22	2.15	0.46
1:G:243:MET:C	1:G:245:LYS:H	2.19	0.46
1:B:128:GLN:OE1	1:B:172:VAL:HG11	2.15	0.46
1:C:115:LYS:HB2	1:C:115:LYS:HE3	1.61	0.46
1:G:87:LEU:HD12	1:G:87:LEU:HA	1.75	0.46
1:G:169:ILE:HG22	1:G:169:ILE:O	2.14	0.46
1:D:44:ARG:C	1:D:46:TYR:N	2.69	0.46
1:F:193:ASP:O	1:F:197:ILE:HG12	2.15	0.46
1:F:247:ALA:HA	1:F:250:ARG:NH2	2.30	0.46
1:G:257:LYS:HD3	1:G:257:LYS:O	2.15	0.46
1:A:155:ARG:NH2	1:D:177:LYS:HB3	2.31	0.46
1:D:57:PRO:O	1:D:61:ILE:HG22	2.16	0.46
1:D:162:HIS:HA	1:E:173:THR:HA	1.98	0.46
1:E:188:PHE:CE2	1:E:234:ILE:HG13	2.50	0.46
1:G:25:LEU:O	1:G:29:ILE:HG23	2.15	0.46
1:G:267:PHE:HB3	1:G:268:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:THR:HG21	1:D:235:MET:HG2	1.96	0.46
1:E:131:VAL:HG12	1:E:131:VAL:O	2.15	0.46
1:F:191:ASP:HB3	1:F:271:ARG:HH11	1.80	0.46
1:G:44:ARG:C	1:G:46:TYR:N	2.69	0.46
1:G:191:ASP:HB3	1:G:271:ARG:HH11	1.79	0.46
1:G:240:THR:CG2	1:G:248:VAL:HG21	2.45	0.46
1:B:67:LEU:HD22	1:B:67:LEU:HA	1.61	0.46
1:E:106:ILE:HA	1:F:114:VAL:HG11	1.97	0.46
1:F:188:PHE:CE2	1:F:234:ILE:HG13	2.51	0.46
1:B:191:ASP:HB3	1:B:271:ARG:NH1	2.31	0.46
1:B:242:PRO:O	1:B:243:MET:HB2	2.16	0.46
1:C:254:TYR:OH	1:G:195:ASP:OD1	2.27	0.46
1:C:271:ARG:O	1:F:270:PRO:HD2	2.16	0.46
1:F:57:PRO:O	1:F:61:ILE:HG22	2.15	0.46
1:B:171:MET:HE2	1:B:173:THR:HG22	1.98	0.46
1:E:117:MET:HG2	1:E:149:LEU:HD13	1.98	0.45
1:E:193:ASP:O	1:E:197:ILE:HG12	2.15	0.45
1:F:38:ALA:HB1	1:F:72:VAL:HG11	1.98	0.45
1:G:137:ILE:HG23	1:G:169:ILE:HG13	1.98	0.45
1:A:27:ILE:O	1:A:30:ILE:HG22	2.16	0.45
1:D:249:GLU:O	1:D:253:ARG:HG3	2.16	0.45
1:E:162:HIS:ND1	1:E:162:HIS:N	2.64	0.45
1:F:189:PRO:HD2	1:F:192:GLU:HG3	1.99	0.45
1:B:137:ILE:HG23	1:B:169:ILE:HG13	1.96	0.45
1:D:64:LEU:HD12	1:E:125:PHE:CZ	2.51	0.45
1:D:136:THR:HG23	1:D:173:THR:HG23	1.98	0.45
1:E:169:ILE:O	1:E:169:ILE:HG22	2.15	0.45
1:B:212:ARG:HH11	1:B:212:ARG:HG3	1.76	0.45
1:D:38:ALA:HB1	1:D:72:VAL:HG11	1.98	0.45
1:D:169:ILE:O	1:D:169:ILE:HG22	2.17	0.45
1:E:89:ASN:ND2	1:F:26:LYS:HE3	2.31	0.45
1:A:89:ASN:ND2	1:D:26:LYS:HE3	2.32	0.45
1:A:180:MET:HE3	1:A:180:MET:HB2	1.86	0.45
1:B:150:ARG:O	1:B:150:ARG:HG2	2.16	0.45
1:C:158:SER:HB2	1:G:183:VAL:HG23	1.98	0.45
1:E:140:ILE:O	1:E:140:ILE:HG22	2.16	0.45
1:E:180:MET:HE3	1:E:180:MET:HB2	1.81	0.45
1:A:267:PHE:HB3	1:A:268:PRO:HD2	1.97	0.45
1:A:272:THR:O	1:D:274:VAL:HA	2.16	0.45
1:B:85:LEU:HD12	1:B:85:LEU:HA	1.63	0.45
1:B:254:TYR:CE2	1:B:258:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLU:O	1:C:253:ARG:HG3	2.16	0.45
1:A:176:THR:HA	1:A:180:MET:HE2	1.99	0.45
1:C:243:MET:C	1:C:245:LYS:H	2.20	0.45
1:D:243:MET:C	1:D:245:LYS:H	2.19	0.45
1:E:271:ARG:HE	1:E:271:ARG:HB3	1.42	0.45
1:F:162:HIS:ND1	1:F:162:HIS:N	2.65	0.45
1:D:95:LEU:HA	1:E:79:LEU:HD21	1.98	0.45
1:D:188:PHE:CE2	1:D:234:ILE:HG13	2.51	0.45
1:E:176:THR:HG22	1:E:180:MET:CE	2.46	0.45
1:F:188:PHE:CG	1:F:197:ILE:HD12	2.52	0.45
1:G:137:ILE:HD12	1:G:154:ILE:CD1	2.45	0.45
1:D:267:PHE:HB3	1:D:268:PRO:HD2	1.97	0.45
1:E:272:THR:O	1:F:274:VAL:HA	2.16	0.45
1:A:171:MET:HE2	1:A:173:THR:HG22	1.98	0.45
1:B:162:HIS:ND1	1:B:162:HIS:N	2.65	0.45
1:D:257:LYS:HD3	1:D:257:LYS:O	2.17	0.45
1:B:249:GLU:O	1:B:253:ARG:HG3	2.17	0.44
1:B:279:LYS:HG3	1:B:280:LYS:H	1.81	0.44
1:C:140:ILE:O	1:C:140:ILE:HG22	2.17	0.44
1:D:176:THR:HG22	1:D:180:MET:CE	2.46	0.44
1:E:171:MET:HE2	1:E:173:THR:HG22	2.00	0.44
1:E:171:MET:CE	1:E:173:THR:HG22	2.48	0.44
1:F:254:TYR:CE2	1:F:258:LYS:HD2	2.52	0.44
1:A:67:LEU:HD22	1:A:67:LEU:HA	1.72	0.44
1:A:103:SER:HA	1:B:101:ILE:HG12	2.00	0.44
1:E:116:ASP:O	1:E:119:SER:HB3	2.17	0.44
1:E:226:ASP:OD2	1:E:227:MET:N	2.50	0.44
1:F:133:ASP:OD1	1:F:133:ASP:N	2.39	0.44
1:G:102:GLY:O	1:G:106:ILE:HG12	2.17	0.44
1:A:83:SER:OG	1:B:90:ILE:HA	2.17	0.44
1:A:137:ILE:HD12	1:A:154:ILE:HD11	1.99	0.44
1:B:30:ILE:HB	1:G:88:PHE:CD1	2.51	0.44
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.80	0.44
1:D:67:LEU:HD22	1:D:67:LEU:HA	1.65	0.44
1:D:270:PRO:O	1:D:270:PRO:CD	2.65	0.44
1:D:279:LYS:HD2	1:D:279:LYS:HA	1.86	0.44
1:G:150:ARG:O	1:G:150:ARG:HG2	2.17	0.44
1:A:162:HIS:ND1	1:A:162:HIS:N	2.65	0.44
1:A:204:ILE:HD11	1:A:259:MET:HB2	1.99	0.44
1:C:190:ILE:O	1:F:257:LYS:NZ	2.42	0.44
1:C:245:LYS:HG2	1:C:246:TRP:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:HD2	1:D:192:GLU:HG3	1.99	0.44
1:E:133:ASP:O	1:E:144:VAL:HG13	2.18	0.44
1:F:279:LYS:HD2	1:F:279:LYS:HA	1.85	0.44
1:B:115:LYS:HB2	1:B:115:LYS:HE3	1.68	0.44
1:C:67:LEU:HA	1:C:67:LEU:HD22	1.58	0.44
1:C:117:MET:HG2	1:C:149:LEU:HD13	1.99	0.44
1:C:158:SER:HA	1:G:181:MET:HB3	1.99	0.44
1:D:242:PRO:O	1:D:243:MET:HB2	2.17	0.44
1:E:189:PRO:HD2	1:E:192:GLU:HG3	2.00	0.44
1:E:207:GLU:O	1:E:210:LYS:HB2	2.18	0.44
1:G:115:LYS:HB2	1:G:115:LYS:HE3	1.71	0.44
1:G:224:ILE:HG12	1:G:224:ILE:O	2.18	0.44
1:B:204:ILE:HD11	1:B:259:MET:HB2	2.00	0.44
1:E:120:GLY:HA3	1:E:166:ASN:HD22	1.83	0.44
1:G:117:MET:HG2	1:G:149:LEU:CD1	2.46	0.44
1:A:114:VAL:HG11	1:B:106:ILE:HA	1.99	0.44
1:A:217:GLU:HB3	1:A:239:LYS:HB2	2.00	0.44
1:C:183:VAL:HG23	1:F:158:SER:HB2	2.00	0.44
1:D:88:PHE:O	1:D:89:ASN:HB2	2.17	0.44
1:D:122:PHE:O	1:D:123:ILE:C	2.54	0.44
1:G:131:VAL:HG12	1:G:131:VAL:O	2.17	0.44
1:A:272:THR:HG22	1:D:272:THR:OG1	2.18	0.44
1:B:183:VAL:HG21	1:G:158:SER:HB2	2.00	0.44
1:B:279:LYS:HD2	1:B:279:LYS:HA	1.86	0.44
1:C:162:HIS:ND1	1:C:162:HIS:N	2.66	0.44
1:C:254:TYR:CE2	1:C:258:LYS:HG3	2.52	0.44
1:C:267:PHE:HB3	1:C:268:PRO:HD2	1.98	0.44
1:G:207:GLU:O	1:G:210:LYS:HB2	2.18	0.44
1:A:267:PHE:CD2	1:D:190:ILE:HD12	2.53	0.44
1:D:275:ILE:HG12	1:E:277:SER:HB3	2.00	0.44
1:F:171:MET:HE2	1:F:173:THR:HG22	2.00	0.44
1:G:171:MET:HE2	1:G:173:THR:HG22	2.00	0.44
1:G:235:MET:O	1:G:235:MET:HG3	2.16	0.44
1:A:26:LYS:HE3	1:B:89:ASN:ND2	2.33	0.43
1:A:245:LYS:HG2	1:A:246:TRP:N	2.32	0.43
1:B:188:PHE:CG	1:B:197:ILE:HD12	2.53	0.43
1:E:257:LYS:HE3	1:E:261:ASP:OD2	2.17	0.43
1:F:137:ILE:HG23	1:F:169:ILE:HG13	2.00	0.43
1:F:243:MET:C	1:F:245:LYS:H	2.22	0.43
1:G:162:HIS:ND1	1:G:162:HIS:N	2.66	0.43
1:A:131:VAL:HG12	1:A:131:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MET:HB3	1:F:158:SER:HA	2.00	0.43
1:C:222:LEU:HD12	1:C:223:GLY:H	1.83	0.43
1:C:269:TYR:O	1:C:270:PRO:C	2.55	0.43
1:D:150:ARG:O	1:D:150:ARG:HG2	2.18	0.43
1:E:267:PHE:HB3	1:E:268:PRO:HD2	1.99	0.43
1:G:88:PHE:O	1:G:89:ASN:HB2	2.17	0.43
1:C:183:VAL:HG21	1:F:158:SER:HB2	1.99	0.43
1:D:115:LYS:HE3	1:D:115:LYS:HB2	1.65	0.43
1:A:139:GLY:O	1:A:140:ILE:HD12	2.18	0.43
1:C:158:SER:HB2	1:G:183:VAL:HG21	2.00	0.43
1:F:172:VAL:O	1:F:172:VAL:HG22	2.17	0.43
1:G:85:LEU:HD12	1:G:85:LEU:HA	1.60	0.43
1:C:131:VAL:HG12	1:C:131:VAL:O	2.19	0.43
1:C:151:VAL:HG11	1:C:163:ILE:CG2	2.48	0.43
1:C:274:VAL:HA	1:F:272:THR:O	2.19	0.43
1:D:254:TYR:CE2	1:D:258:LYS:HG3	2.54	0.43
1:E:101:ILE:HG12	1:F:103:SER:HA	2.00	0.43
1:E:114:VAL:O	1:E:118:ILE:HG13	2.18	0.43
1:G:218:GLY:HA3	1:G:238:ALA:HA	2.01	0.43
1:D:171:MET:HE2	1:D:173:THR:HG22	2.00	0.43
1:F:267:PHE:HB3	1:F:268:PRO:HD2	2.01	0.43
1:G:279:LYS:HD2	1:G:279:LYS:HA	1.83	0.43
1:A:133:ASP:OD1	1:A:133:ASP:N	2.40	0.43
1:B:133:ASP:O	1:B:144:VAL:HG13	2.18	0.43
1:B:191:ASP:HB3	1:B:271:ARG:HH11	1.83	0.43
1:C:65:THR:HG22	1:C:66:SER:N	2.34	0.43
1:C:88:PHE:O	1:C:89:ASN:HB2	2.19	0.43
1:F:188:PHE:CE1	1:F:197:ILE:HG21	2.53	0.43
1:A:257:LYS:HG3	1:D:194:VAL:HG21	2.00	0.43
1:C:125:PHE:CZ	1:F:64:LEU:HD12	2.53	0.43
1:C:133:ASP:OD1	1:C:133:ASP:N	2.41	0.43
1:D:162:HIS:ND1	1:D:162:HIS:N	2.66	0.43
1:E:137:ILE:HD12	1:E:154:ILE:CD1	2.49	0.43
1:G:139:GLY:C	1:G:140:ILE:HD12	2.40	0.43
1:A:176:THR:HG22	1:A:180:MET:CE	2.48	0.43
1:B:245:LYS:HE3	1:B:249:GLU:OE2	2.19	0.43
1:E:178:ASP:O	1:E:179:SER:CB	2.66	0.43
1:B:224:ILE:HG12	1:B:224:ILE:O	2.19	0.42
1:D:171:MET:CE	1:D:173:THR:HG22	2.49	0.42
1:F:85:LEU:HD12	1:F:85:LEU:HA	1.73	0.42
1:G:189:PRO:HD2	1:G:192:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:PRO:HA	1:B:238:ALA:HB2	2.01	0.42
1:B:221:VAL:HG22	1:B:236:VAL:HG12	2.01	0.42
1:B:267:PHE:HB3	1:B:268:PRO:HD2	2.01	0.42
1:D:114:VAL:O	1:D:118:ILE:HG13	2.19	0.42
1:D:151:VAL:HG11	1:D:163:ILE:CG2	2.47	0.42
1:D:269:TYR:HD1	1:D:269:TYR:H	1.64	0.42
1:G:254:TYR:CE2	1:G:258:LYS:HD2	2.54	0.42
1:C:171:MET:HE2	1:C:173:THR:HG22	2.01	0.42
1:C:190:ILE:HD12	1:F:267:PHE:CD2	2.54	0.42
1:D:246:TRP:CD1	1:D:246:TRP:N	2.87	0.42
1:E:130:SER:O	1:E:133:ASP:OD1	2.37	0.42
1:A:257:LYS:HD3	1:A:257:LYS:O	2.19	0.42
1:B:85:LEU:HG	1:B:90:ILE:HG13	2.00	0.42
1:B:226:ASP:OD2	1:B:227:MET:N	2.52	0.42
1:D:226:ASP:OD2	1:D:227:MET:N	2.52	0.42
1:D:235:MET:O	1:D:235:MET:HG3	2.17	0.42
1:E:115:LYS:HB2	1:E:115:LYS:HE3	1.59	0.42
1:E:246:TRP:CD1	1:E:246:TRP:N	2.88	0.42
1:A:171:MET:CE	1:A:173:THR:HG22	2.50	0.42
1:B:26:LYS:HE3	1:G:89:ASN:HD21	1.84	0.42
1:B:180:MET:CE	1:B:243:MET:H	2.32	0.42
1:B:207:GLU:O	1:B:210:LYS:HB2	2.20	0.42
1:C:180:MET:HE3	1:C:180:MET:HB2	1.95	0.42
1:C:188:PHE:CG	1:C:197:ILE:HD12	2.55	0.42
1:G:212:ARG:HA	1:G:212:ARG:HD3	1.83	0.42
2:B:283:LMT:O3'	2:B:283:LMT:O2B	2.31	0.42
1:E:222:LEU:HD12	1:E:223:GLY:H	1.84	0.42
1:F:180:MET:HE3	1:F:180:MET:HB2	1.93	0.42
1:G:171:MET:CE	1:G:173:THR:HG22	2.50	0.42
1:B:177:LYS:C	1:B:179:SER:N	2.73	0.42
1:C:137:ILE:HG23	1:C:169:ILE:HG13	2.01	0.42
1:C:257:LYS:HD3	1:C:257:LYS:O	2.20	0.42
1:D:137:ILE:HG23	1:D:169:ILE:HG13	2.02	0.42
1:E:87:LEU:HD12	1:E:87:LEU:HA	1.83	0.42
1:D:275:ILE:CG2	1:E:279:LYS:HB3	2.49	0.42
1:E:197:ILE:HG12	1:E:197:ILE:H	1.61	0.42
1:A:224:ILE:HG12	1:A:224:ILE:O	2.19	0.42
1:E:158:SER:HA	1:F:181:MET:HB3	2.01	0.42
1:E:245:LYS:HG2	1:E:246:TRP:N	2.33	0.42
1:A:158:SER:HB2	1:D:183:VAL:CG2	2.50	0.42
1:D:85:LEU:HD12	1:D:85:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLY:HA3	1:D:238:ALA:HA	2.01	0.42
1:F:126:GLU:O	1:F:127:ASP:C	2.58	0.42
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.84	0.41
1:C:26:LYS:HE3	1:F:89:ASN:HD21	1.84	0.41
1:C:150:ARG:O	1:C:150:ARG:HG2	2.20	0.41
1:C:188:PHE:CE1	1:C:197:ILE:HG21	2.54	0.41
1:D:151:VAL:CG1	1:D:163:ILE:HG23	2.50	0.41
1:E:155:ARG:HH22	1:F:177:LYS:HB3	1.85	0.41
1:E:279:LYS:HD2	1:E:279:LYS:HA	1.83	0.41
1:F:44:ARG:C	1:F:46:TYR:N	2.72	0.41
1:F:204:ILE:HD11	1:F:259:MET:HB2	2.01	0.41
1:A:44:ARG:C	1:A:46:TYR:H	2.23	0.41
1:B:245:LYS:HG2	1:B:246:TRP:N	2.35	0.41
1:C:225:THR:HG21	1:C:235:MET:HG2	2.02	0.41
1:D:87:LEU:HD12	1:D:87:LEU:HA	1.84	0.41
1:D:175:LEU:O	1:D:180:MET:HE2	2.20	0.41
1:F:171:MET:CE	1:F:173:THR:HG22	2.50	0.41
1:A:58:GLN:HA	1:A:61:ILE:HG23	2.01	0.41
1:A:88:PHE:O	1:A:89:ASN:HB2	2.20	0.41
1:A:230:SER:HB2	1:A:271:ARG:HG2	2.01	0.41
1:B:279:LYS:CB	1:G:275:ILE:CG2	2.97	0.41
1:C:246:TRP:N	1:C:246:TRP:CD1	2.88	0.41
1:E:191:ASP:HB3	1:E:271:ARG:HH11	1.84	0.41
1:E:275:ILE:CG2	1:F:279:LYS:HB3	2.50	0.41
1:F:180:MET:CE	1:F:243:MET:H	2.33	0.41
1:G:151:VAL:HG11	1:G:163:ILE:CG2	2.49	0.41
1:A:100:GLY:HA2	1:A:103:SER:HB2	2.03	0.41
1:B:219:PRO:CA	1:B:238:ALA:HB2	2.50	0.41
1:F:219:PRO:HA	1:F:238:ALA:HB2	2.01	0.41
1:B:254:TYR:CE2	1:B:258:LYS:HD2	2.56	0.41
1:C:87:LEU:HA	1:C:87:LEU:HD12	1.79	0.41
1:C:155:ARG:HH22	1:G:177:LYS:HB3	1.85	0.41
1:C:254:TYR:CE2	1:C:258:LYS:HD2	2.55	0.41
1:F:67:LEU:HA	1:F:67:LEU:HD22	1.62	0.41
1:F:131:VAL:HG12	1:F:131:VAL:O	2.21	0.41
1:F:218:GLY:HA3	1:F:238:ALA:HA	2.02	0.41
1:G:180:MET:CE	1:G:243:MET:H	2.33	0.41
1:B:131:VAL:O	1:B:131:VAL:HG12	2.21	0.41
1:B:145:GLU:OE2	1:B:155:ARG:HD2	2.21	0.41
1:B:212:ARG:HA	1:B:212:ARG:HD3	1.88	0.41
1:C:175:LEU:O	1:C:180:MET:HE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ASP:O	1:C:179:SER:CB	2.68	0.41
1:E:242:PRO:O	1:E:243:MET:HB2	2.21	0.41
1:F:88:PHE:O	1:F:89:ASN:HB2	2.20	0.41
1:G:67:LEU:HD22	1:G:67:LEU:HA	1.65	0.41
1:C:212:ARG:HH11	1:C:212:ARG:HG3	1.79	0.41
1:E:95:LEU:HA	1:F:79:LEU:HD21	2.03	0.41
1:E:212:ARG:HA	1:E:212:ARG:HD3	1.86	0.41
1:F:87:LEU:HD12	1:F:87:LEU:HA	1.81	0.41
1:G:25:LEU:HD22	1:G:25:LEU:HA	1.91	0.41
1:G:188:PHE:CG	1:G:197:ILE:HD12	2.55	0.41
1:A:177:LYS:C	1:A:179:SER:N	2.74	0.41
1:A:226:ASP:OD2	1:A:227:MET:N	2.54	0.41
1:B:95:LEU:HA	1:B:95:LEU:HD23	1.94	0.41
1:D:137:ILE:HD12	1:D:154:ILE:CD1	2.50	0.41
1:E:190:ILE:C	1:E:192:GLU:N	2.73	0.41
1:A:188:PHE:CG	1:A:197:ILE:HD12	2.56	0.41
1:B:218:GLY:HA3	1:B:238:ALA:HA	2.02	0.41
1:B:219:PRO:CB	1:B:238:ALA:HB2	2.49	0.41
1:C:126:GLU:O	1:C:127:ASP:C	2.59	0.41
1:C:145:GLU:OE2	1:C:155:ARG:NH1	2.43	0.41
1:D:111:GLN:CG	1:D:112:ASN:N	2.84	0.41
1:D:219:PRO:HA	1:D:238:ALA:HB2	2.02	0.41
1:E:137:ILE:HG23	1:E:169:ILE:HG13	2.03	0.41
1:F:212:ARG:HA	1:F:212:ARG:HD3	1.89	0.41
1:A:181:MET:HE2	1:A:181:MET:HB2	2.01	0.41
1:C:101:ILE:HD13	1:G:106:ILE:HB	2.03	0.41
1:D:161:LEU:N	1:E:174:ASN:O	2.52	0.41
1:D:231:LYS:HD3	1:E:229:ASP:OD1	2.21	0.41
1:G:242:PRO:O	1:G:243:MET:CB	2.69	0.41
1:C:204:ILE:HD11	1:C:259:MET:HB2	2.03	0.40
1:C:269:TYR:C	1:C:270:PRO:O	2.55	0.40
1:D:191:ASP:HB3	1:D:271:ARG:NH1	2.36	0.40
1:B:243:MET:C	1:B:245:LYS:H	2.25	0.40
1:D:272:THR:O	1:E:274:VAL:HA	2.20	0.40
1:E:100:GLY:HA2	1:E:103:SER:HB2	2.03	0.40
1:A:254:TYR:CE2	1:A:258:LYS:HD2	2.55	0.40
1:B:44:ARG:C	1:B:46:TYR:H	2.24	0.40
1:C:177:LYS:HB3	1:F:155:ARG:HH22	1.87	0.40
1:C:229:ASP:OD1	1:F:231:LYS:HD3	2.22	0.40
1:F:177:LYS:C	1:F:179:SER:N	2.74	0.40
1:G:219:PRO:HA	1:G:238:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:SER:HB2	1:C:271:ARG:HG2	2.02	0.40
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.86	0.40
1:D:178:ASP:O	1:D:179:SER:CB	2.69	0.40
1:D:180:MET:HB2	1:D:180:MET:HE3	1.92	0.40
1:D:273:THR:OG1	1:D:273:THR:O	2.39	0.40
1:E:221:VAL:HG22	1:E:236:VAL:HG12	2.04	0.40
1:G:28:LEU:HD23	1:G:28:LEU:HA	1.91	0.40
1:A:189:PRO:HD2	1:A:192:GLU:HG3	2.03	0.40
1:C:278:GLU:HA	1:C:278:GLU:OE1	2.21	0.40
1:D:140:ILE:HG21	1:D:162:HIS:HD2	1.87	0.40
1:D:207:GLU:O	1:D:210:LYS:HB2	2.21	0.40
1:E:188:PHE:CG	1:E:197:ILE:HD12	2.56	0.40
1:G:246:TRP:CD1	1:G:246:TRP:N	2.87	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:GLN:OE1	1:E:46:TYR:OH[3_545]	1.91	0.29
1:E:278:GLU:OE1	1:G:212:ARG:NH1[4_545]	1.95	0.25
1:E:278:GLU:OE1	1:G:212:ARG:CZ[4_545]	2.07	0.13
1:F:212:ARG:NH1	2:B:283:LMT:O6B[3_555]	2.11	0.09
1:D:199:GLU:N	1:E:43:TYR:OH[3_545]	2.13	0.07
1:G:258:LYS:NZ	1:G:278:GLU:OE2[4_445]	2.17	0.03
1:A:55:GLN:NE2	1:F:212:ARG:O[3_545]	2.18	0.02
1:A:250:ARG:NH2	1:E:53:LYS:NZ[3_545]	2.18	0.02
1:F:51:LYS:O	1:G:43:TYR:OH[3_455]	2.18	0.02

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	262/282 (93%)	230 (88%)	19 (7%)	13 (5%)	2 18
1	B	260/282 (92%)	233 (90%)	16 (6%)	11 (4%)	3 22
1	C	260/282 (92%)	232 (89%)	15 (6%)	13 (5%)	2 18
1	D	261/282 (93%)	232 (89%)	16 (6%)	13 (5%)	2 18
1	E	260/282 (92%)	233 (90%)	15 (6%)	12 (5%)	2 20
1	F	260/282 (92%)	232 (89%)	16 (6%)	12 (5%)	2 20
1	G	260/282 (92%)	232 (89%)	16 (6%)	12 (5%)	2 20
All	All	1823/1974 (92%)	1624 (89%)	113 (6%)	86 (5%)	2 19

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL
1	A	178	ASP
1	A	218	GLY
1	B	131	VAL
1	B	178	ASP
1	C	131	VAL
1	C	178	ASP
1	D	131	VAL
1	D	177	LYS
1	D	178	ASP
1	D	218	GLY
1	E	131	VAL
1	E	177	LYS
1	E	178	ASP
1	E	191	ASP
1	F	131	VAL
1	F	178	ASP
1	G	131	VAL
1	G	178	ASP
1	A	17	ALA
1	A	177	LYS
1	A	179	SER
1	A	191	ASP
1	B	17	ALA
1	B	177	LYS
1	B	191	ASP
1	B	223	GLY
1	C	17	ALA
1	C	177	LYS

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Mol	Chain	Res	Type
1	C	179	SER
1	C	191	ASP
1	C	223	GLY
1	D	17	ALA
1	D	179	SER
1	D	191	ASP
1	D	223	GLY
1	E	17	ALA
1	E	179	SER
1	E	223	GLY
1	F	17	ALA
1	F	177	LYS
1	F	179	SER
1	F	191	ASP
1	F	223	GLY
1	G	17	ALA
1	G	177	LYS
1	G	179	SER
1	G	191	ASP
1	G	223	GLY
1	A	223	GLY
1	B	179	SER
1	G	243	MET
1	A	56	LEU
1	A	132	GLY
1	B	56	LEU
1	B	132	GLY
1	C	56	LEU
1	C	132	GLY
1	D	56	LEU
1	D	132	GLY
1	D	243	MET
1	E	56	LEU
1	E	132	GLY
1	E	243	MET
1	F	56	LEU
1	F	132	GLY
1	F	243	MET
1	G	56	LEU
1	G	132	GLY
1	A	48	LEU
1	A	243	MET

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Mol	Chain	Res	Type
1	B	243	MET
1	C	48	LEU
1	C	243	MET
1	D	280	LYS
1	E	280	LYS
1	F	48	LEU
1	A	280	LYS
1	B	280	LYS
1	C	45	PHE
1	C	280	LYS
1	D	48	LEU
1	E	48	LEU
1	F	280	LYS
1	G	48	LEU
1	G	280	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	235/250 (94%)	194 (83%)	41 (17%)	2 9
1	B	233/250 (93%)	193 (83%)	40 (17%)	2 10
1	C	233/250 (93%)	192 (82%)	41 (18%)	2 9
1	D	234/250 (94%)	191 (82%)	43 (18%)	1 7
1	E	233/250 (93%)	191 (82%)	42 (18%)	1 8
1	F	233/250 (93%)	192 (82%)	41 (18%)	2 9
1	G	233/250 (93%)	192 (82%)	41 (18%)	2 9
All	All	1634/1750 (93%)	1345 (82%)	289 (18%)	2 9

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	29	ILE
1	A	45	PHE
1	A	46	TYR
1	A	49	TYR
1	A	61	ILE
1	A	63	THR
1	A	65	THR
1	A	67	LEU
1	A	68	THR
1	A	85	LEU
1	A	87	LEU
1	A	95	LEU
1	A	127	ASP
1	A	133	ASP
1	A	141	SER
1	A	144	VAL
1	A	149	LEU
1	A	157	PHE
1	A	158	SER
1	A	162	HIS
1	A	171	MET
1	A	172	VAL
1	A	173	THR
1	A	179	SER
1	A	190	ILE
1	A	197	ILE
1	A	212	ARG
1	A	217	GLU
1	A	220	THR
1	A	224	ILE
1	A	232	LEU
1	A	235	MET
1	A	246	TRP
1	A	257	LYS
1	A	258	LYS
1	A	263	LYS
1	A	264	ASN
1	A	272	THR
1	A	276	LEU
1	B	21	LEU
1	B	25	LEU
1	B	29	ILE

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Mol	Chain	Res	Type
1	B	45	PHE
1	B	46	TYR
1	B	49	TYR
1	B	61	ILE
1	B	63	THR
1	B	65	THR
1	B	67	LEU
1	B	68	THR
1	B	85	LEU
1	B	87	LEU
1	B	95	LEU
1	B	127	ASP
1	B	133	ASP
1	B	149	LEU
1	B	157	PHE
1	B	158	SER
1	B	162	HIS
1	B	171	MET
1	B	172	VAL
1	B	173	THR
1	B	179	SER
1	B	190	ILE
1	B	197	ILE
1	B	212	ARG
1	B	220	THR
1	B	224	ILE
1	B	232	LEU
1	B	235	MET
1	B	244	GLN
1	B	246	TRP
1	B	257	LYS
1	B	258	LYS
1	B	260	PHE
1	B	263	LYS
1	B	264	ASN
1	B	272	THR
1	B	276	LEU
1	C	21	LEU
1	C	25	LEU
1	C	29	ILE
1	C	45	PHE
1	C	46	TYR

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Mol	Chain	Res	Type
1	C	61	ILE
1	C	63	THR
1	C	65	THR
1	C	67	LEU
1	C	68	THR
1	C	85	LEU
1	C	87	LEU
1	C	95	LEU
1	C	127	ASP
1	C	133	ASP
1	C	141	SER
1	C	144	VAL
1	C	149	LEU
1	C	157	PHE
1	C	158	SER
1	C	162	HIS
1	C	171	MET
1	C	172	VAL
1	C	173	THR
1	C	179	SER
1	C	190	ILE
1	C	197	ILE
1	C	212	ARG
1	C	220	THR
1	C	224	ILE
1	C	232	LEU
1	C	235	MET
1	C	244	GLN
1	C	246	TRP
1	C	258	LYS
1	C	260	PHE
1	C	263	LYS
1	C	264	ASN
1	C	271	ARG
1	C	272	THR
1	C	276	LEU
1	D	21	LEU
1	D	25	LEU
1	D	29	ILE
1	D	45	PHE
1	D	46	TYR
1	D	61	ILE

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Mol	Chain	Res	Type
1	D	63	THR
1	D	65	THR
1	D	67	LEU
1	D	68	THR
1	D	85	LEU
1	D	87	LEU
1	D	95	LEU
1	D	127	ASP
1	D	133	ASP
1	D	144	VAL
1	D	149	LEU
1	D	155	ARG
1	D	157	PHE
1	D	158	SER
1	D	162	HIS
1	D	171	MET
1	D	172	VAL
1	D	173	THR
1	D	179	SER
1	D	190	ILE
1	D	197	ILE
1	D	212	ARG
1	D	217	GLU
1	D	220	THR
1	D	224	ILE
1	D	232	LEU
1	D	235	MET
1	D	244	GLN
1	D	246	TRP
1	D	257	LYS
1	D	258	LYS
1	D	260	PHE
1	D	263	LYS
1	D	264	ASN
1	D	269	TYR
1	D	271	ARG
1	D	276	LEU
1	E	21	LEU
1	E	25	LEU
1	E	29	ILE
1	E	45	PHE
1	E	46	TYR

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Mol	Chain	Res	Type
1	E	49	TYR
1	E	61	ILE
1	E	63	THR
1	E	65	THR
1	E	67	LEU
1	E	68	THR
1	E	85	LEU
1	E	87	LEU
1	E	95	LEU
1	E	127	ASP
1	E	133	ASP
1	E	144	VAL
1	E	149	LEU
1	E	157	PHE
1	E	158	SER
1	E	162	HIS
1	E	171	MET
1	E	172	VAL
1	E	173	THR
1	E	179	SER
1	E	190	ILE
1	E	197	ILE
1	E	212	ARG
1	E	220	THR
1	E	224	ILE
1	E	232	LEU
1	E	235	MET
1	E	244	GLN
1	E	246	TRP
1	E	257	LYS
1	E	258	LYS
1	E	263	LYS
1	E	264	ASN
1	E	271	ARG
1	E	272	THR
1	E	274	VAL
1	E	276	LEU
1	F	21	LEU
1	F	25	LEU
1	F	29	ILE
1	F	45	PHE
1	F	46	TYR

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Mol	Chain	Res	Type
1	F	61	ILE
1	F	63	THR
1	F	65	THR
1	F	67	LEU
1	F	68	THR
1	F	85	LEU
1	F	87	LEU
1	F	95	LEU
1	F	127	ASP
1	F	133	ASP
1	F	144	VAL
1	F	149	LEU
1	F	157	PHE
1	F	158	SER
1	F	162	HIS
1	F	171	MET
1	F	172	VAL
1	F	173	THR
1	F	179	SER
1	F	190	ILE
1	F	197	ILE
1	F	212	ARG
1	F	220	THR
1	F	224	ILE
1	F	227	MET
1	F	232	LEU
1	F	235	MET
1	F	244	GLN
1	F	246	TRP
1	F	257	LYS
1	F	258	LYS
1	F	260	PHE
1	F	263	LYS
1	F	264	ASN
1	F	272	THR
1	F	276	LEU
1	G	21	LEU
1	G	25	LEU
1	G	29	ILE
1	G	45	PHE
1	G	46	TYR
1	G	61	ILE

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Mol	Chain	Res	Type
1	G	63	THR
1	G	65	THR
1	G	67	LEU
1	G	68	THR
1	G	85	LEU
1	G	87	LEU
1	G	95	LEU
1	G	127	ASP
1	G	133	ASP
1	G	136	THR
1	G	144	VAL
1	G	149	LEU
1	G	157	PHE
1	G	158	SER
1	G	162	HIS
1	G	171	MET
1	G	172	VAL
1	G	173	THR
1	G	179	SER
1	G	190	ILE
1	G	197	ILE
1	G	212	ARG
1	G	220	THR
1	G	224	ILE
1	G	232	LEU
1	G	235	MET
1	G	244	GLN
1	G	246	TRP
1	G	257	LYS
1	G	258	LYS
1	G	263	LYS
1	G	264	ASN
1	G	271	ARG
1	G	272	THR
1	G	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	ASN
1	D	89	ASN
1	E	89	ASN

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Mol	Chain	Res	Type
1	F	89	ASN
1	G	89	ASN
1	G	162	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	LMT	B	283	-	36,36,36	0.58	1 (2%)	47,47,47	1.00	5 (10%)
2	LMT	F	283	-	36,36,36	0.52	1 (2%)	47,47,47	1.19	4 (8%)

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	LMT	B	283	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	F	283	-	-	9/21/61/61	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	283	LMT	O1'-C1'	2.12	1.43	1.40
2	B	283	LMT	O1'-C1'	2.09	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	283	LMT	O1'-C1'-C2'	4.16	114.80	108.30
2	B	283	LMT	C3'-C4'-C5'	-2.39	105.44	110.93
2	B	283	LMT	O1B-C4'-C5'	2.34	115.86	109.45
2	B	283	LMT	O1B-C1B-C2B	2.29	114.03	108.10
2	F	283	LMT	C3B-C4B-C5B	-2.25	106.22	110.24
2	B	283	LMT	C3B-C4B-C5B	2.10	113.99	110.24
2	F	283	LMT	C4B-C3B-C2B	-2.08	107.19	110.82
2	F	283	LMT	O5B-C5B-C4B	-2.03	106.00	109.69
2	B	283	LMT	C1B-O5B-C5B	-2.00	109.75	113.69

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	283	LMT	C2'-C1'-O1'-C1
2	B	283	LMT	O5'-C1'-O1'-C1
2	F	283	LMT	C2-C1-O1'-C1'
2	B	283	LMT	O5B-C5B-C6B-O6B
2	F	283	LMT	O5'-C5'-C6'-O6'
2	B	283	LMT	C4B-C5B-C6B-O6B
2	F	283	LMT	C4'-C5'-C6'-O6'
2	F	283	LMT	O5B-C5B-C6B-O6B
2	B	283	LMT	C2-C1-O1'-C1'
2	B	283	LMT	C6-C7-C8-C9
2	B	283	LMT	C4-C5-C6-C7
2	B	283	LMT	C5-C6-C7-C8
2	F	283	LMT	C11-C10-C9-C8
2	F	283	LMT	C9-C10-C11-C12
2	B	283	LMT	C2-C3-C4-C5
2	F	283	LMT	C4-C5-C6-C7

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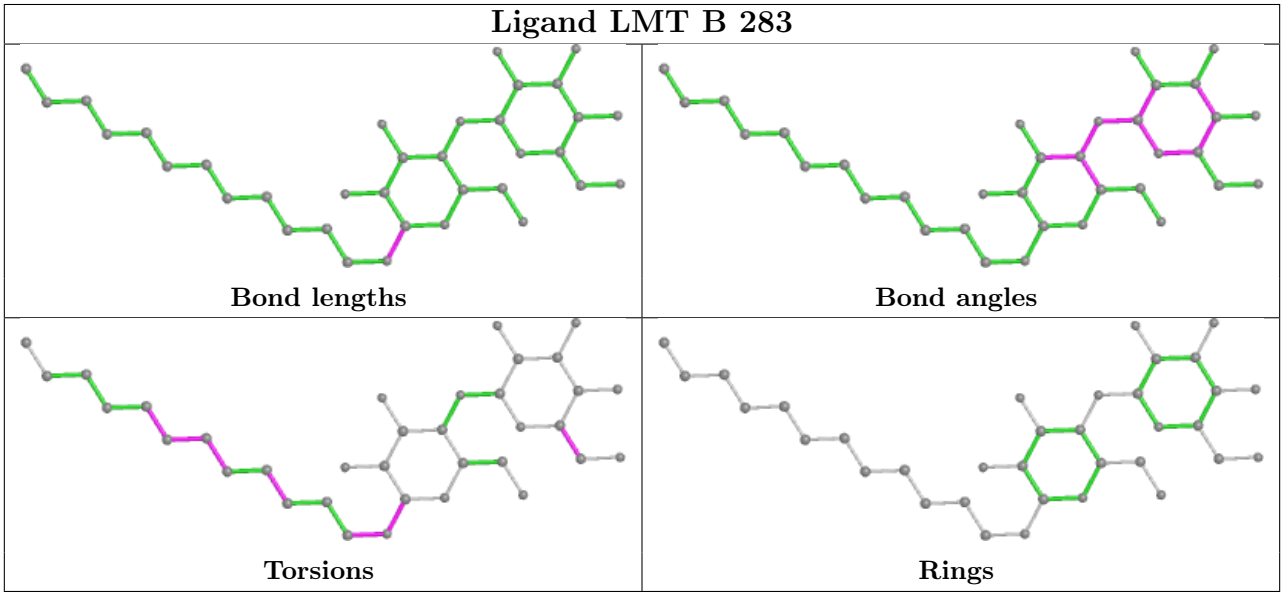
Mol	Chain	Res	Type	Atoms
2	F	283	LMT	C4B-C5B-C6B-O6B
2	F	283	LMT	C1-C2-C3-C4

There are no ring outliers.

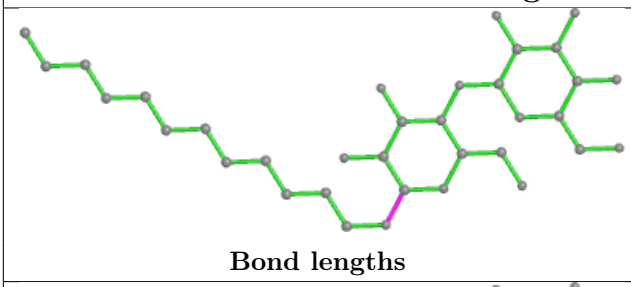
2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	283	LMT	3	1
2	F	283	LMT	10	0

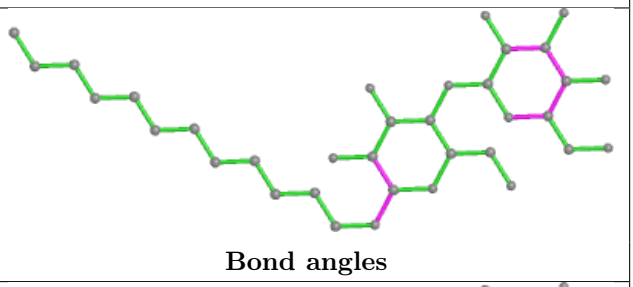
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



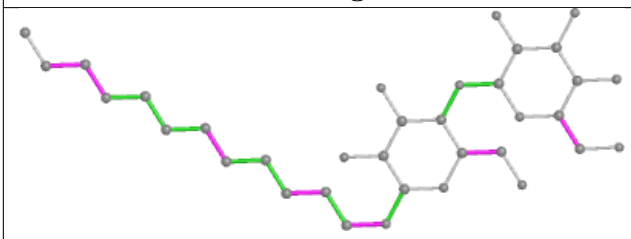
Ligand LMT F 283



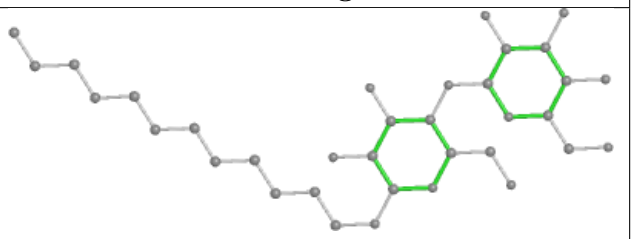
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	266/282 (94%)	0.38	23 (8%)	10	13	65, 120, 204, 296	0
1	B	264/282 (93%)	0.30	20 (7%)	13	16	62, 121, 206, 315	0
1	C	264/282 (93%)	0.35	20 (7%)	13	16	69, 124, 206, 324	0
1	D	265/282 (93%)	0.41	24 (9%)	9	11	62, 120, 231, 381	0
1	E	264/282 (93%)	0.39	24 (9%)	9	11	70, 126, 244, 426	0
1	F	264/282 (93%)	0.41	24 (9%)	9	11	62, 126, 231, 318	0
1	G	264/282 (93%)	0.22	18 (6%)	17	19	63, 129, 226, 322	0
All	All	1851/1974 (93%)	0.35	153 (8%)	11	14	62, 124, 225, 426	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	281	THR	24.9
1	C	178	ASP	12.8
1	E	279	LYS	9.7
1	G	277	SER	9.5
1	F	280	LYS	9.4
1	F	50	SER	8.9
1	D	281	THR	8.6
1	E	52	SER	8.6
1	E	50	SER	8.0
1	C	240	THR	7.7
1	A	281	THR	7.7
1	C	55	GLN	6.8
1	E	49	TYR	6.8
1	D	51	LYS	6.8
1	G	280	LYS	6.4
1	C	239	LYS	6.4
1	F	47	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	51	LYS	6.2
1	B	51	LYS	6.1
1	F	56	LEU	6.1
1	B	50	SER	6.0
1	A	280	LYS	5.9
1	C	238	ALA	5.9
1	F	49	TYR	5.8
1	F	55	GLN	5.7
1	F	51	LYS	5.6
1	G	281	THR	5.4
1	F	57	PRO	5.4
1	E	51	LYS	5.3
1	G	178	ASP	5.2
1	B	229	ASP	5.1
1	B	178	ASP	5.1
1	B	58	GLN	4.9
1	E	53	LYS	4.9
1	G	53	LYS	4.9
1	D	52	SER	4.8
1	D	264	ASN	4.6
1	C	49	TYR	4.6
1	C	281	THR	4.6
1	C	179	SER	4.6
1	A	229	ASP	4.5
1	C	56	LEU	4.4
1	G	279	LYS	4.3
1	F	279	LYS	4.2
1	A	138	ASN	4.2
1	C	48	LEU	4.2
1	G	278	GLU	4.1
1	D	13	TYR	4.1
1	E	256	VAL	4.0
1	F	278	GLU	3.9
1	G	52	SER	3.9
1	F	48	LEU	3.9
1	A	137	ILE	3.9
1	B	230	SER	3.8
1	F	191	ASP	3.8
1	C	175	LEU	3.7
1	G	49	TYR	3.6
1	G	50	SER	3.6
1	F	46	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	54	ILE	3.5
1	A	181	MET	3.5
1	F	17	ALA	3.4
1	D	56	LEU	3.3
1	E	47	LYS	3.3
1	A	191	ASP	3.2
1	E	278	GLU	3.2
1	G	55	GLN	3.2
1	C	218	GLY	3.2
1	G	54	ILE	3.2
1	D	45	PHE	3.2
1	C	174	ASN	3.1
1	D	47	LYS	3.1
1	E	125	PHE	3.1
1	D	49	TYR	3.0
1	D	50	SER	3.0
1	D	48	LEU	3.0
1	E	260	PHE	2.9
1	E	277	SER	2.9
1	D	226	ASP	2.9
1	E	55	GLN	2.9
1	B	211	SER	2.9
1	A	152	THR	2.8
1	B	212	ARG	2.8
1	E	46	TYR	2.8
1	E	164	ILE	2.8
1	G	170	LYS	2.8
1	B	48	LEU	2.8
1	F	58	GLN	2.8
1	F	45	PHE	2.8
1	A	244	GLN	2.7
1	A	209	LYS	2.7
1	C	51	LYS	2.7
1	A	45	PHE	2.7
1	C	44	ARG	2.6
1	A	182	ALA	2.6
1	B	59	ARG	2.6
1	A	49	TYR	2.5
1	C	241	GLN	2.5
1	A	150	ARG	2.5
1	B	52	SER	2.5
1	C	168	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	63	THR	2.5
1	G	134	TYR	2.5
1	D	273	THR	2.5
1	F	239	LYS	2.5
1	A	241	GLN	2.5
1	F	59	ARG	2.5
1	A	148	GLY	2.4
1	E	146	GLU	2.4
1	D	46	TYR	2.4
1	B	121	PHE	2.4
1	D	55	GLN	2.4
1	E	218	GLY	2.4
1	E	152	THR	2.4
1	E	137	ILE	2.4
1	A	164	ILE	2.4
1	D	129	PHE	2.3
1	C	209	LYS	2.3
1	F	178	ASP	2.3
1	D	125	PHE	2.3
1	B	244	GLN	2.3
1	D	262	GLN	2.3
1	E	212	ARG	2.3
1	C	52	SER	2.3
1	F	218	GLY	2.2
1	B	61	ILE	2.2
1	G	139	GLY	2.2
1	A	183	VAL	2.2
1	E	280	LYS	2.2
1	A	178	ASP	2.2
1	B	228	GLN	2.2
1	F	255	ARG	2.2
1	D	275	ILE	2.2
1	D	212	ARG	2.2
1	C	180	MET	2.2
1	D	263	LYS	2.2
1	A	87	LEU	2.1
1	F	171	MET	2.1
1	B	53	LYS	2.1
1	A	68	THR	2.1
1	B	44	ARG	2.1
1	B	210	LYS	2.1
1	E	129	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	170	LYS	2.1
1	A	163	ILE	2.1
1	G	48	LEU	2.1
1	G	199	GLU	2.1
1	D	53	LYS	2.1
1	B	49	TYR	2.1
1	E	169	ILE	2.1
1	B	55	GLN	2.0
1	E	224	ILE	2.0
1	D	58	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

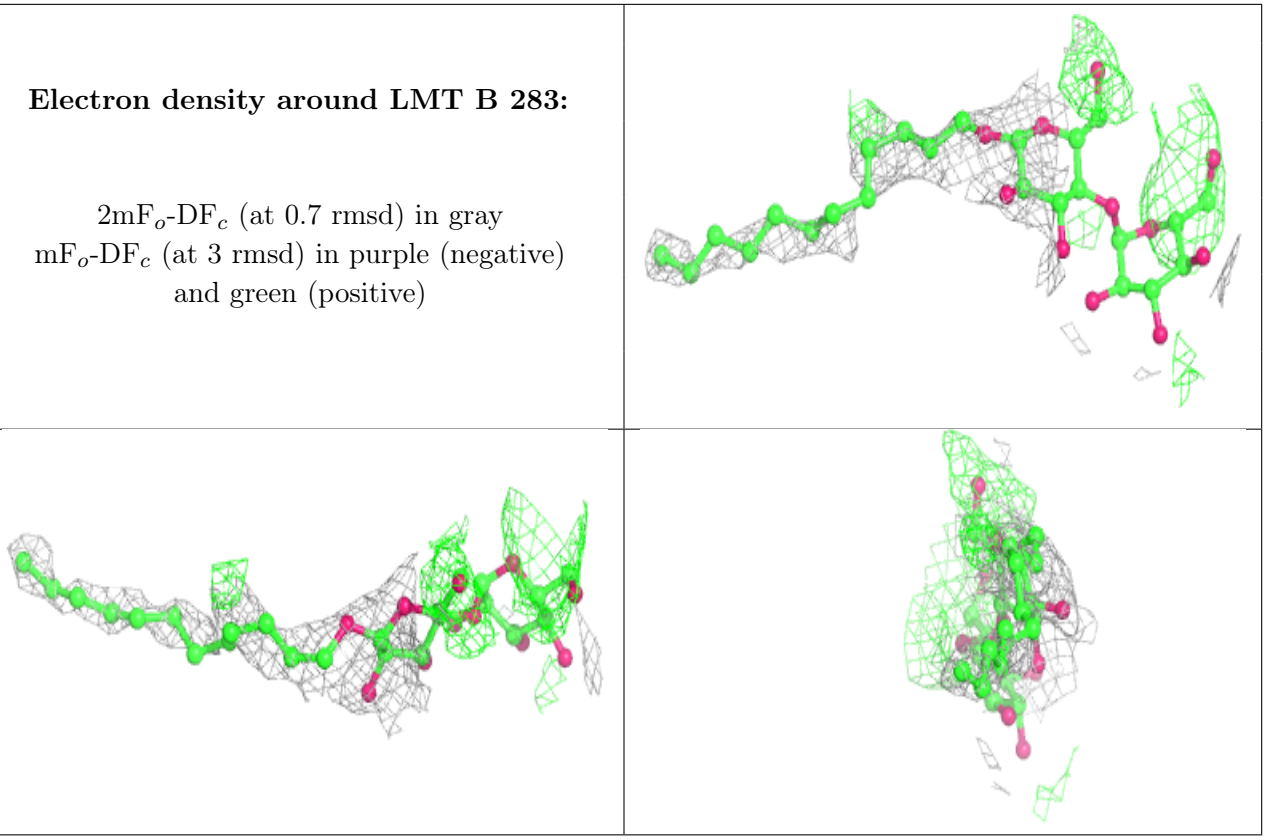
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	B	283	35/35	0.69	0.48	67,180,255,265	0
2	LMT	F	283	35/35	0.74	0.59	68,158,220,252	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.

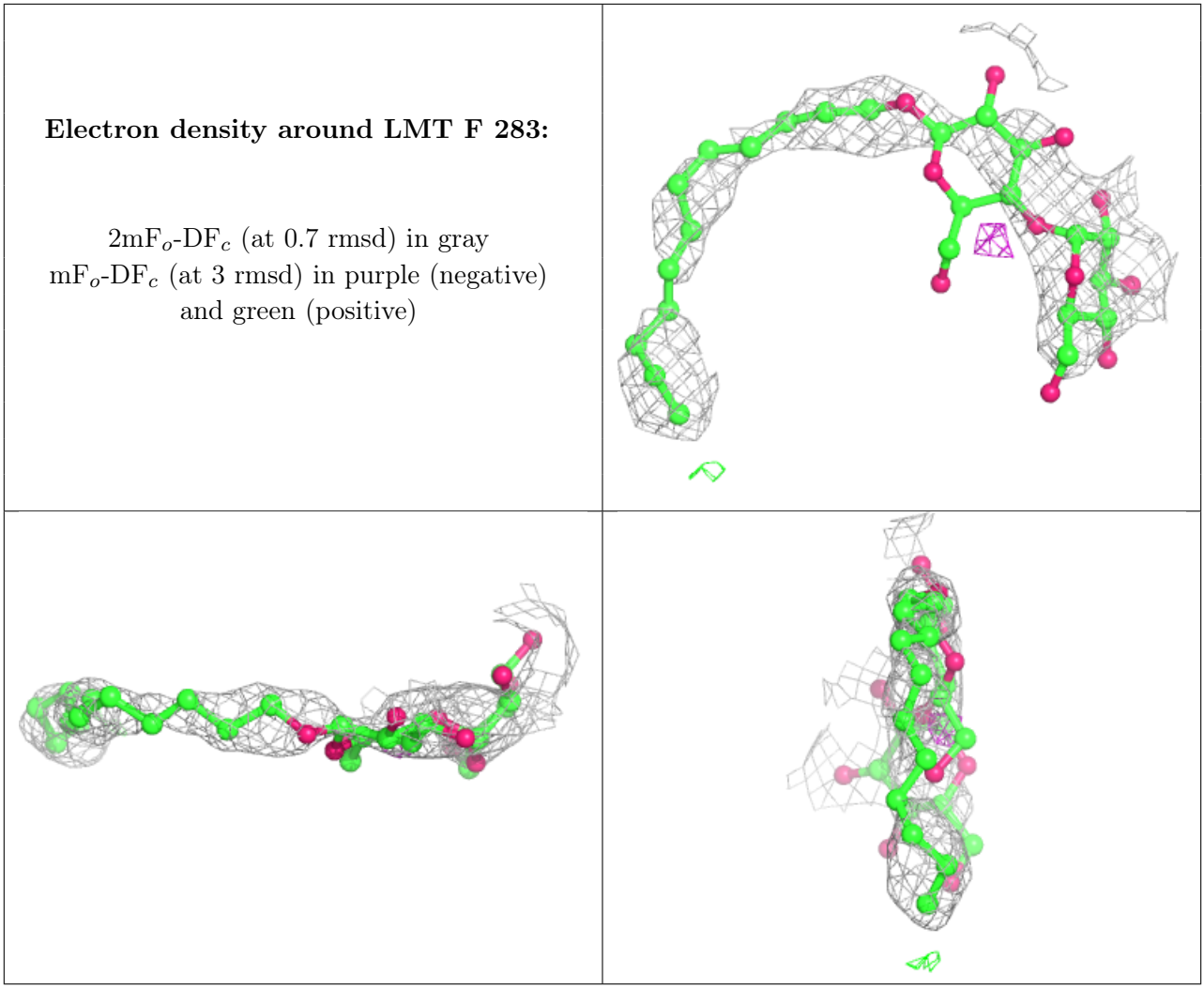
Electron density around LMT B 283:

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



Electron density around LMT F 283:

$2mF_o$-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.