Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 01:24 PM JST

PDB ID	:	5B0M
Title	:	Structure of MoeN5-Sso7d fusion protein in complex with beta-dodecyl maltoside
Authors	:	Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.
Deposited on	:	2015-11-02
Resolution	:	3.05 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:

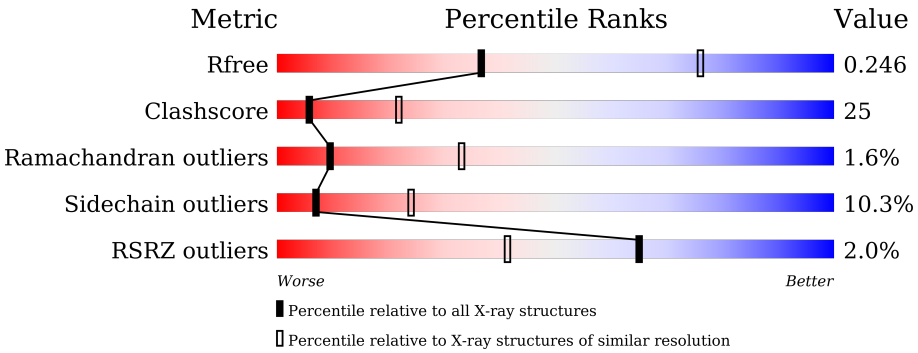
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.05 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	343	45% 28% 23%
1	B	343	50% 43%
1	C	343	41% 31% 23%
1	D	343	50% 41% 5%
1	E	343	44% 32% 21%
1	F	343	57% 35%

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Mol	Chain	Length	Quality of chain
1	G	343	
1	H	343	

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	G	902	-	-	-	X
2	LMT	H	903	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19074 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2010	1240	374	385	11			
1	B	334	Total	C	N	O	S	0	0	0
			2549	1582	466	487	14			
1	C	264	Total	C	N	O	S	0	0	0
			2010	1240	374	385	11			
1	D	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	E	270	Total	C	N	O	S	0	0	0
			2066	1274	388	393	11			
1	F	332	Total	C	N	O	S	0	0	0
			2534	1573	464	483	14			
1	G	267	Total	C	N	O	S	0	0	0
			2036	1256	379	390	11			
1	H	333	Total	C	N	O	S	0	0	0
			2542	1577	465	486	14			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010
E	-13	MET	-	expression tag	UNP A0A010
E	-12	ALA	-	expression tag	UNP A0A010
E	-11	HIS	-	expression tag	UNP A0A010
E	-10	HIS	-	expression tag	UNP A0A010
E	-9	HIS	-	expression tag	UNP A0A010
E	-8	HIS	-	expression tag	UNP A0A010
E	-7	HIS	-	expression tag	UNP A0A010
E	-6	HIS	-	expression tag	UNP A0A010
E	-5	VAL	-	expression tag	UNP A0A010
E	-4	ASP	-	expression tag	UNP A0A010
E	-3	ASP	-	expression tag	UNP A0A010
E	-2	ASP	-	expression tag	UNP A0A010
E	-1	ASP	-	expression tag	UNP A0A010
E	0	LYS	-	expression tag	UNP A0A010
E	261	ALA	-	linker	UNP A0A010
E	262	GLY	-	linker	UNP A0A010
E	263	ALA	-	linker	UNP A0A010
E	264	GLY	-	linker	UNP A0A010
E	265	ALA	-	linker	UNP A0A010
F	-13	MET	-	expression tag	UNP A0A010
F	-12	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP A0A010
F	-10	HIS	-	expression tag	UNP A0A010
F	-9	HIS	-	expression tag	UNP A0A010
F	-8	HIS	-	expression tag	UNP A0A010
F	-7	HIS	-	expression tag	UNP A0A010
F	-6	HIS	-	expression tag	UNP A0A010
F	-5	VAL	-	expression tag	UNP A0A010
F	-4	ASP	-	expression tag	UNP A0A010
F	-3	ASP	-	expression tag	UNP A0A010
F	-2	ASP	-	expression tag	UNP A0A010
F	-1	ASP	-	expression tag	UNP A0A010
F	0	LYS	-	expression tag	UNP A0A010
F	261	ALA	-	linker	UNP A0A010
F	262	GLY	-	linker	UNP A0A010
F	263	ALA	-	linker	UNP A0A010
F	264	GLY	-	linker	UNP A0A010
F	265	ALA	-	linker	UNP A0A010
G	-13	MET	-	expression tag	UNP A0A010
G	-12	ALA	-	expression tag	UNP A0A010
G	-11	HIS	-	expression tag	UNP A0A010
G	-10	HIS	-	expression tag	UNP A0A010
G	-9	HIS	-	expression tag	UNP A0A010
G	-8	HIS	-	expression tag	UNP A0A010
G	-7	HIS	-	expression tag	UNP A0A010
G	-6	HIS	-	expression tag	UNP A0A010
G	-5	VAL	-	expression tag	UNP A0A010
G	-4	ASP	-	expression tag	UNP A0A010
G	-3	ASP	-	expression tag	UNP A0A010
G	-2	ASP	-	expression tag	UNP A0A010
G	-1	ASP	-	expression tag	UNP A0A010
G	0	LYS	-	expression tag	UNP A0A010
G	261	ALA	-	linker	UNP A0A010
G	262	GLY	-	linker	UNP A0A010
G	263	ALA	-	linker	UNP A0A010
G	264	GLY	-	linker	UNP A0A010
G	265	ALA	-	linker	UNP A0A010
H	-13	MET	-	expression tag	UNP A0A010
H	-12	ALA	-	expression tag	UNP A0A010
H	-11	HIS	-	expression tag	UNP A0A010
H	-10	HIS	-	expression tag	UNP A0A010
H	-9	HIS	-	expression tag	UNP A0A010
H	-8	HIS	-	expression tag	UNP A0A010

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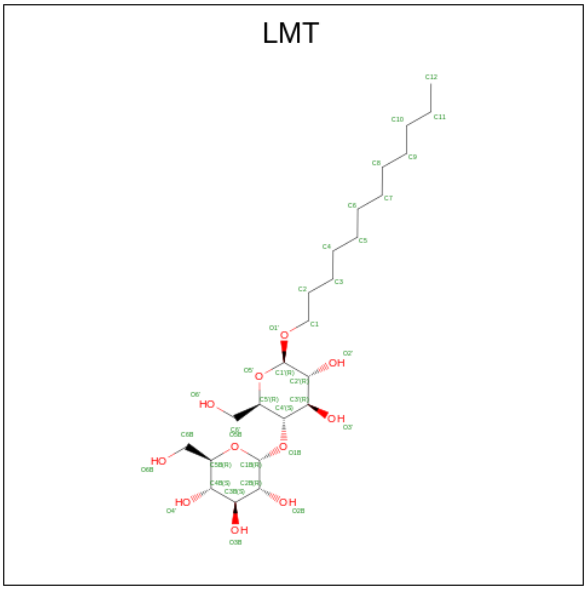
Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	HIS	-	expression tag	UNP A0A010
H	-6	HIS	-	expression tag	UNP A0A010
H	-5	VAL	-	expression tag	UNP A0A010
H	-4	ASP	-	expression tag	UNP A0A010
H	-3	ASP	-	expression tag	UNP A0A010
H	-2	ASP	-	expression tag	UNP A0A010
H	-1	ASP	-	expression tag	UNP A0A010
H	0	LYS	-	expression tag	UNP A0A010
H	261	ALA	-	linker	UNP A0A010
H	262	GLY	-	linker	UNP A0A010
H	263	ALA	-	linker	UNP A0A010
H	264	GLY	-	linker	UNP A0A010
H	265	ALA	-	linker	UNP A0A010

- 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	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		
2	G	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 35 24 11	0	0
2	H	1	Total C O 35 24 11	0	0
2	H	1	Total C O 35 24 11	0	0
2	H	1	Total C O 35 24 11	0	0

- Molecule 3 is water.

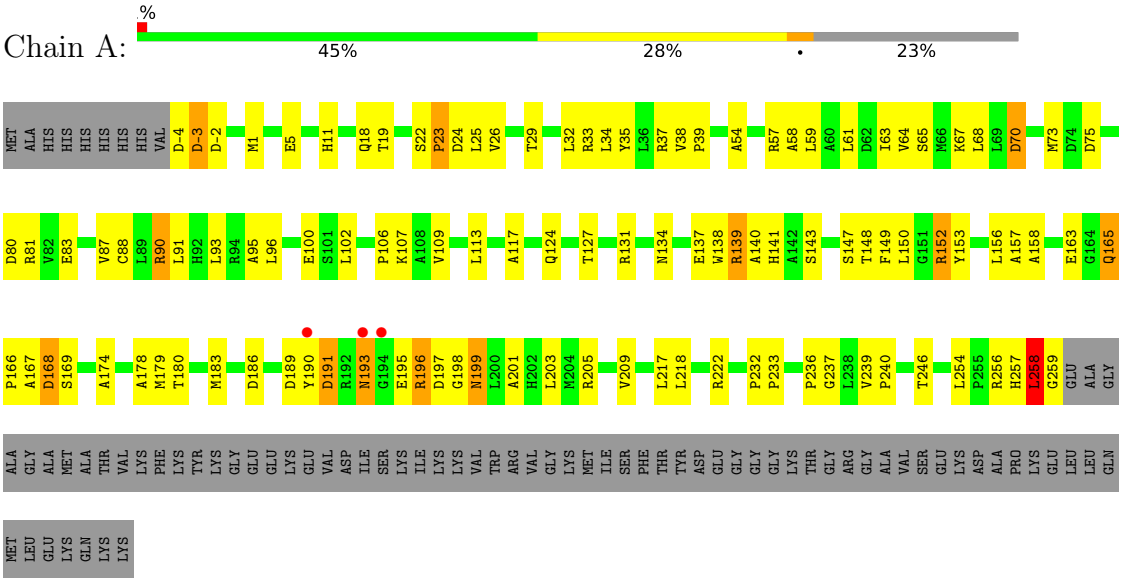
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	77	Total O 77 77	0	0
3	B	70	Total O 70 70	0	0
3	C	69	Total O 69 69	0	0
3	D	62	Total O 62 62	0	0
3	E	54	Total O 54 54	0	0
3	F	59	Total O 59 59	0	0
3	G	48	Total O 48 48	0	0
3	H	75	Total O 75 75	0	0

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.

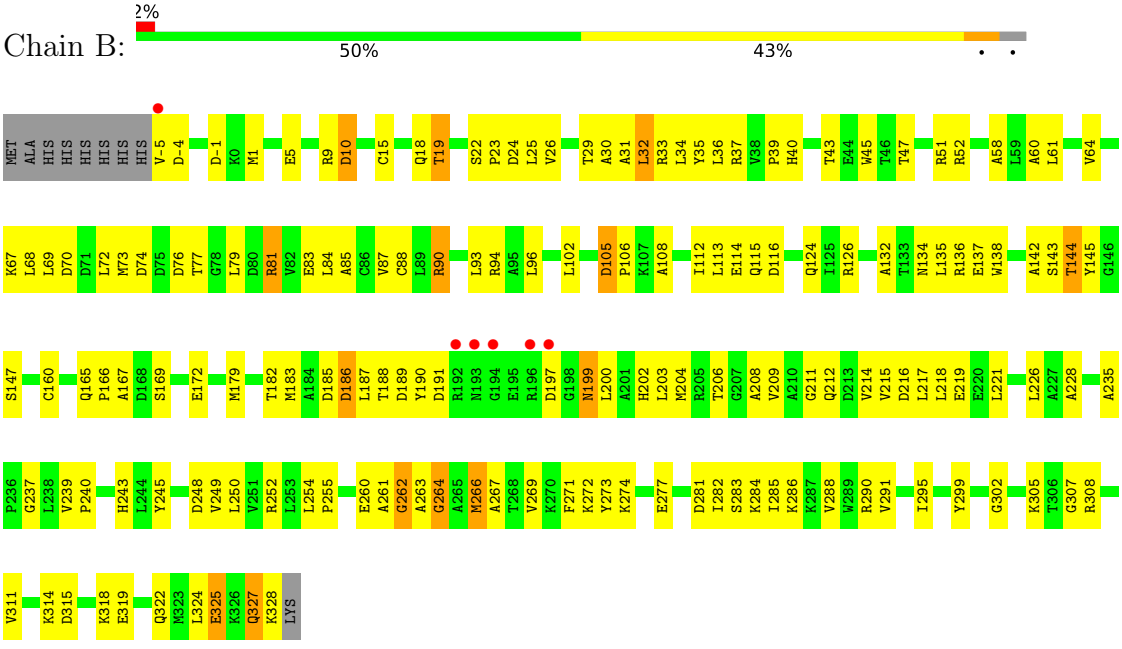
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain A:



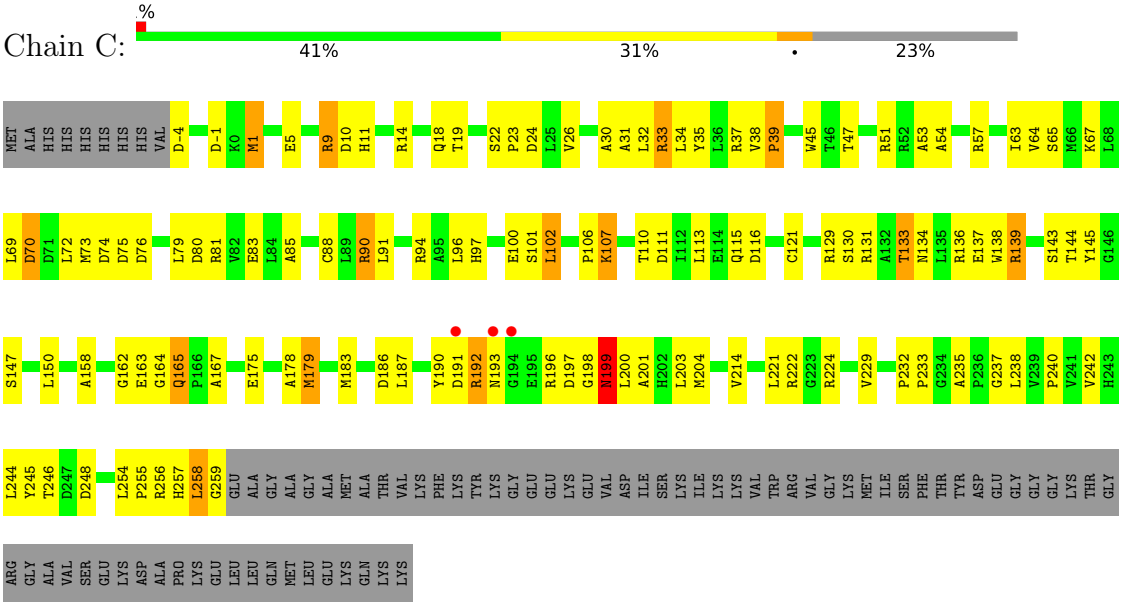
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain B:



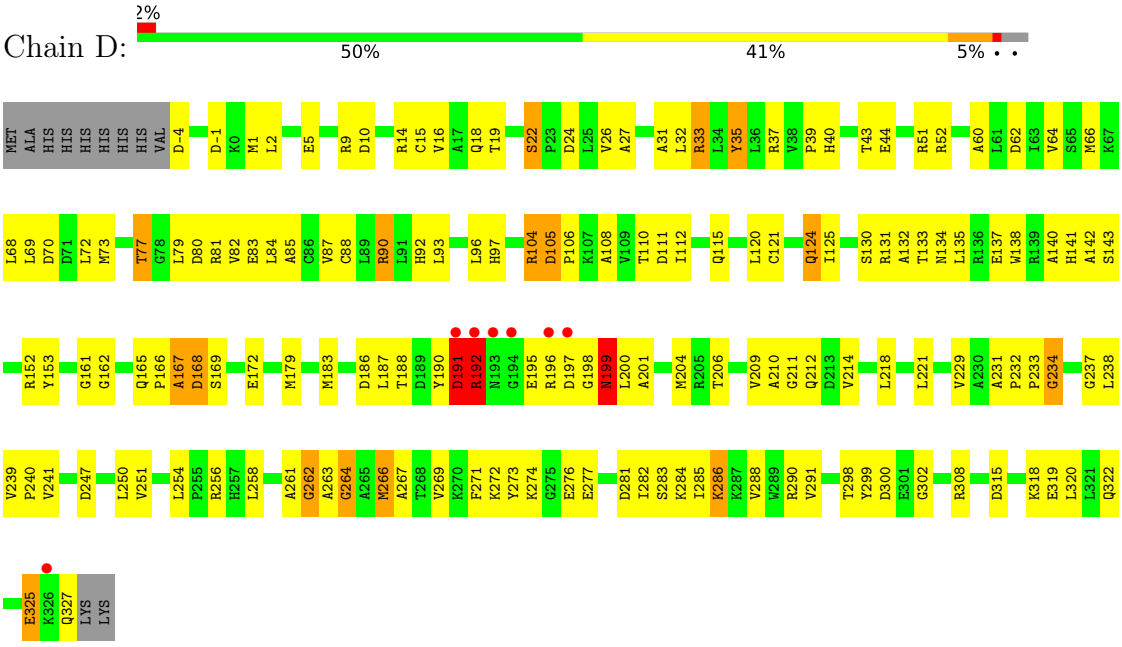
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain C:



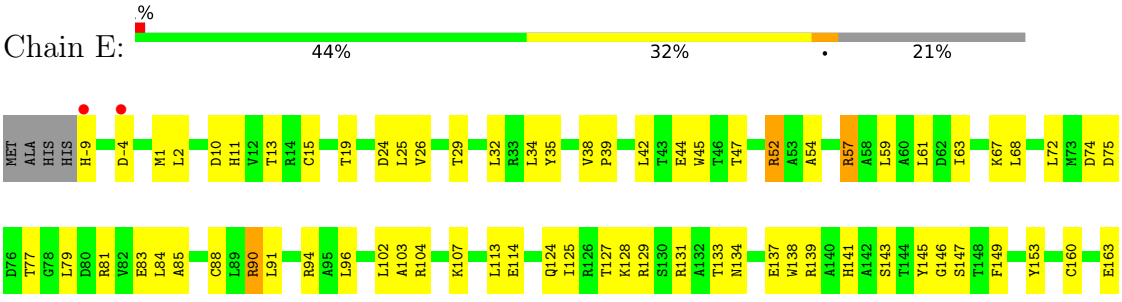
• Molecule 1: MoeN5,DNA-binding protein 7d

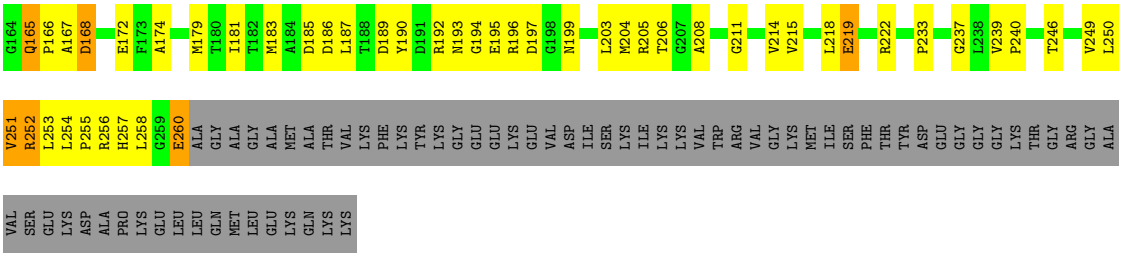
Chain D:



• Molecule 1: MoeN5,DNA-binding protein 7d

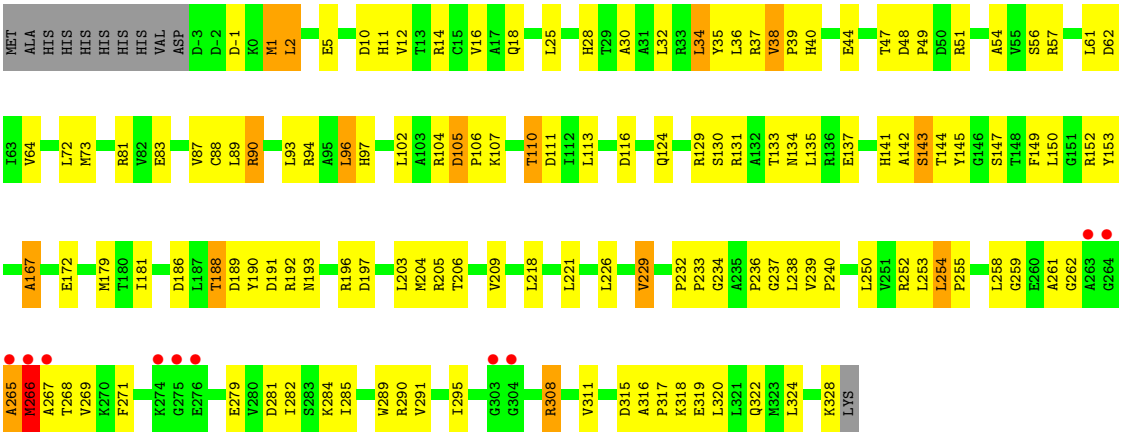
Chain E:





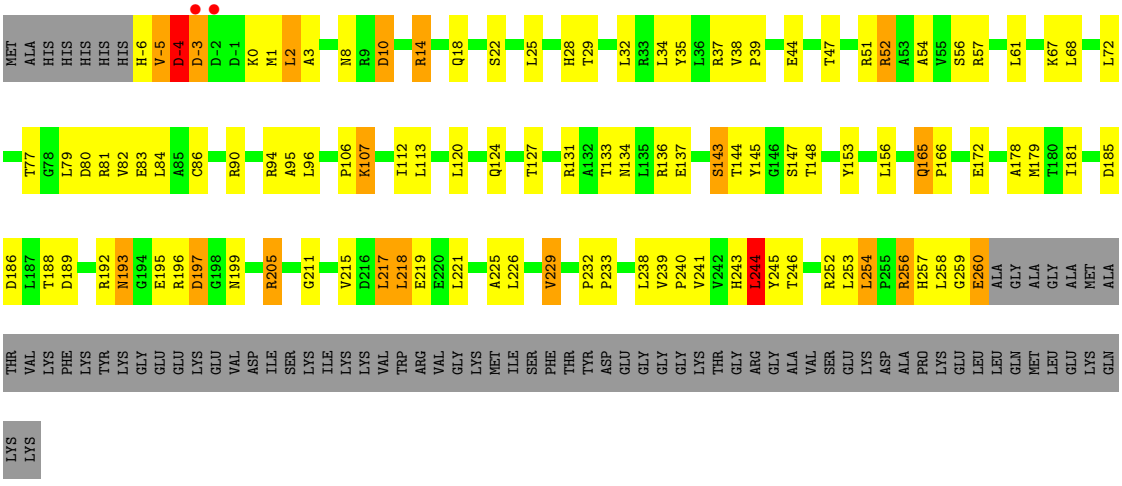
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain F:



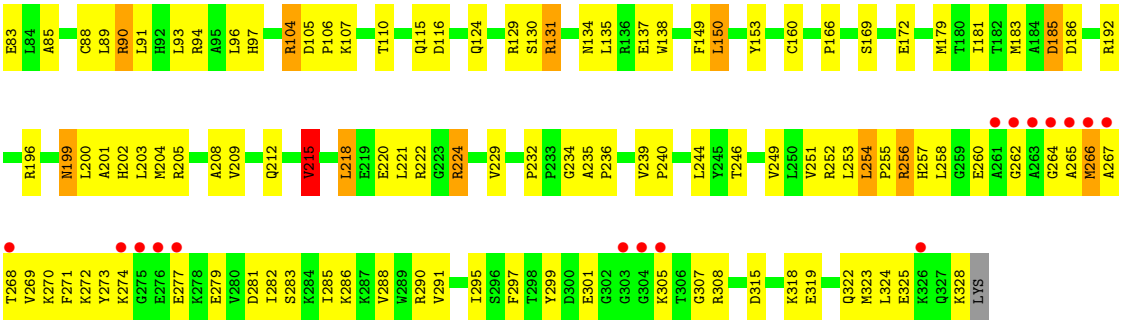
• Molecule 1: MoeN5,DNA-binding protein 7d

Chain G:



• Molecule 1: MoeN5,DNA-binding protein 7d

Chain H:


E83 L84 A85 C88 L89 R90 L91 H92 L93 R94 A95 L96 H97 R104 D105 P106 K107 T110 Q115 D116 Q124 R129 S130 R131 N134 L135 R136 E137 W138 F149 L150 Y153 C160 P166 S169 E172 M179 T180 I181 T182 M183 A184 D185 D186 R192
R196 N199 L200 A201 H202 L203 M204 R205 A208 V209 Q212 V215 L218 E219 E220 L221 R222 G223 R224 V229 P232 P233 G234 A235 P236 V239 P240 L244 Y245 T246 V249 L250 V251 R252 L253 L254 P255 R256 H257 L258 G259 E260 A261 G262 A263 G264 A265 M266 A267
T268 V269 K270 F271 K272 Y273 K274 G275 E276 E277 K278 E279 V280 D281 I282 S283 K284 I285 K286 K287 V288 W289 R290 V291 I295 S296 F297 T298 Y299 D300 E301 G302 G303 G304 K305 T306 G307 R308 D315 K318 E319 Q322 M323 L324 E325 K326 Q327 K328 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	143.06Å 206.13Å 218.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.05 24.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (25.00-3.05) 88.5 (24.92-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.177 , 0.249 0.171 , 0.246	Depositor DCC
R_{free} test set	2912 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19074	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4249e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.76	0/2042	0.88	0/2775
1	B	0.70	0/2588	0.87	0/3499
1	C	0.74	1/2042 (0.0%)	0.92	2/2775 (0.1%)
1	D	0.69	0/2572	0.86	0/3478
1	E	0.71	1/2102 (0.0%)	0.86	0/2857
1	F	0.70	0/2573	0.84	2/3478 (0.1%)
1	G	0.73	0/2069	0.91	2/2812 (0.1%)
1	H	0.70	0/2581	0.87	1/3489 (0.0%)
All	All	0.71	2/18569 (0.0%)	0.88	7/25163 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	121	CYS	CB-SG	-6.24	1.71	1.82
1	E	219	GLU	CG-CD	5.28	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	96	LEU	CA-CB-CG	7.58	132.73	115.30
1	G	244	LEU	CA-CB-CG	6.97	131.33	115.30
1	C	9	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	102	LEU	CA-CB-CG	6.20	129.55	115.30
1	F	62	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	215	VAL	CB-CA-C	-5.25	101.42	111.40
1	G	72	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	245	TYR	Sidechain
1	D	35	TYR	Sidechain
1	E	153	TYR	Sidechain
1	F	153	TYR	Sidechain
1	G	153	TYR	Sidechain
1	H	153	TYR	Sidechain

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	2010	0	1990	86	0
1	B	2549	0	2554	143	0
1	C	2010	0	1990	108	0
1	D	2533	0	2532	150	0
1	E	2066	0	2033	103	0
1	F	2534	0	2541	138	0
1	G	2036	0	2012	105	0
1	H	2542	0	2545	140	0
2	E	35	0	46	9	0
2	F	70	0	92	17	0
2	G	70	0	92	17	0
2	H	105	0	138	28	0
3	A	77	0	0	2	0
3	B	70	0	0	4	0
3	C	69	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	62	0	0	1	0
3	E	54	0	0	1	0
3	F	59	0	0	3	0
3	G	48	0	0	0	0
3	H	75	0	0	0	0
All	All	19074	0	18565	940	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 25.

All (940) 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:F:34:LEU:HG	2:F:902:LMT:H6D	1.18	1.18
1:B:77:THR:HB	1:B:79:LEU:HD12	1.28	1.07
1:H:67:LYS:NZ	2:H:902:LMT:H6'2	1.73	1.03
1:D:266:MET:HE2	1:D:267:ALA:H	1.21	1.02
2:F:902:LMT:H1B	2:F:902:LMT:H6E	1.40	1.01
1:G:245:TYR:HE1	2:G:902:LMT:H4O1	1.03	1.01
1:H:67:LYS:HZ3	2:H:902:LMT:H6'2	1.20	0.99
1:A:258:LEU:O	1:A:258:LEU:HG	1.63	0.98
1:C:1:MET:CE	1:C:37:ARG:HD2	1.94	0.98
1:D:124:GLN:HE21	1:D:124:GLN:HA	1.25	0.97
1:C:158:ALA:HA	1:C:165:GLN:HG2	1.45	0.97
1:E:134:ASN:ND2	1:E:137:GLU:HG3	1.79	0.97
1:G:229:VAL:HG11	1:G:238:LEU:HB2	1.44	0.96
1:C:14:ARG:HH22	2:G:902:LMT:H31	1.32	0.94
1:G:188:THR:HG21	2:G:902:LMT:H6E	1.48	0.93
1:F:72:LEU:O	1:F:81:ARG:NH1	2.00	0.93
1:E:25:LEU:HD22	1:E:83:GLU:HG2	1.47	0.93
1:G:10:ASP:HB3	1:G:14:ARG:NH2	1.82	0.92
1:C:131:ARG:HH22	1:C:196:ARG:NH1	1.67	0.91
1:E:104:ARG:HH21	1:E:104:ARG:HB2	1.35	0.91
1:G:10:ASP:HB3	1:G:14:ARG:HH22	1.30	0.90
1:G:-5:VAL:HG13	1:G:-3:ASP:HB2	1.53	0.90
1:H:38:VAL:HG12	1:H:39:PRO:HD3	1.55	0.89
1:A:236:PRO:O	1:A:239:VAL:HG23	1.72	0.88
1:C:131:ARG:HH22	1:C:196:ARG:HH12	1.22	0.88
1:G:107:LYS:O	1:G:107:LYS:HD3	1.74	0.87
1:E:38:VAL:HG12	1:E:39:PRO:HD3	1.56	0.87
1:D:80:ASP:HB3	1:D:83:GLU:HG3	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLN:HE21	1:B:124:GLN:HA	1.40	0.86
1:D:131:ARG:HH12	1:D:196:ARG:CD	1.87	0.86
2:H:902:LMT:H52	2:H:903:LMT:O3B	1.75	0.86
1:H:183:MET:HE1	1:H:218:LEU:HG	1.57	0.86
1:G:81:ARG:CD	1:H:81:ARG:HH12	1.89	0.85
1:D:237:GLY:O	1:D:240:PRO:HD2	1.77	0.85
1:D:179:MET:HG2	1:D:221:LEU:HD11	1.58	0.84
1:F:295:ILE:HD12	1:F:324:LEU:HD11	1.59	0.84
1:G:86:CYS:HA	2:H:901:LMT:H123	1.59	0.84
1:B:112:ILE:HA	1:B:115:GLN:NE2	1.93	0.84
1:B:37:ARG:HD2	3:B:420:HOH:O	1.78	0.83
1:F:254:LEU:HD22	1:F:258:LEU:HG	1.60	0.83
1:G:44:GLU:HG2	1:G:238:LEU:HG	1.59	0.82
1:C:1:MET:HE1	1:C:37:ARG:HD2	1.60	0.82
1:B:272:LYS:HE3	1:B:277:GLU:OE2	1.80	0.82
1:A:256:ARG:HA	1:F:130:SER:HB3	1.60	0.82
1:F:34:LEU:HG	2:F:902:LMT:C6'	2.06	0.82
1:C:31:ALA:O	1:C:33:ARG:HG3	1.80	0.81
1:D:33:ARG:NH1	1:D:33:ARG:HB3	1.94	0.81
1:A:1:MET:SD	1:A:37:ARG:HD2	2.20	0.81
1:G:29:THR:HA	1:G:32:LEU:HD12	1.64	0.80
1:C:113:LEU:HB3	1:D:93:LEU:HD22	1.62	0.80
1:B:179:MET:HE2	1:B:221:LEU:HD11	1.63	0.80
1:G:120:LEU:HD12	1:G:148:THR:HG22	1.64	0.80
1:F:267:ALA:HB1	1:F:282:ILE:HG13	1.62	0.79
1:A:22:SER:HB2	1:A:23:PRO:HD2	1.63	0.79
1:H:224:ARG:H	1:H:224:ARG:HD2	1.47	0.79
1:C:14:ARG:NH2	2:G:902:LMT:H31	1.97	0.79
1:E:205:ARG:HG2	1:E:260:GLU:HG3	1.63	0.79
1:A:75:ASP:HB2	1:A:81:ARG:HH12	1.49	0.78
2:F:902:LMT:H5'	3:F:1010:HOH:O	1.83	0.78
1:C:237:GLY:O	1:C:240:PRO:HD2	1.83	0.78
1:G:229:VAL:CG1	1:G:238:LEU:HB2	2.12	0.78
1:F:237:GLY:O	1:F:240:PRO:HD2	1.84	0.78
1:A:131:ARG:NH2	1:A:196:ARG:NH1	2.31	0.77
1:F:12:VAL:HG22	1:F:61:LEU:HD23	1.66	0.77
1:G:217:LEU:HD12	1:G:217:LEU:O	1.84	0.77
1:C:9:ARG:HD3	1:C:30:ALA:HB1	1.67	0.77
1:E:81:ARG:HD2	1:F:81:ARG:NH1	2.00	0.76
1:H:104:ARG:CZ	1:H:104:ARG:HB3	2.15	0.76
1:E:107:LYS:NZ	1:F:97:HIS:ND1	2.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLU:HG3	1:D:195:GLU:O	1.86	0.76
1:C:139:ARG:HD3	1:C:179:MET:HE1	1.67	0.76
1:C:96:LEU:HD11	1:D:96:LEU:HD11	1.66	0.76
1:G:51:ARG:HH21	1:G:51:ARG:HG3	1.50	0.76
1:H:183:MET:CE	1:H:218:LEU:HG	2.16	0.75
1:F:266:MET:O	1:F:266:MET:HG3	1.86	0.75
2:F:902:LMT:H6E	2:F:902:LMT:C1B	2.16	0.75
1:D:131:ARG:HH12	1:D:196:ARG:HD3	1.48	0.75
1:G:256:ARG:HG3	1:G:256:ARG:HH11	1.52	0.75
1:F:124:GLN:HA	1:F:124:GLN:OE1	1.85	0.75
1:G:218:LEU:CD2	1:G:246:THR:HG23	2.17	0.74
1:B:32:LEU:HB3	1:B:35:TYR:HD2	1.52	0.74
1:D:267:ALA:HB2	1:D:319:GLU:OE2	1.88	0.74
1:G:226:LEU:O	1:G:229:VAL:HG23	1.87	0.74
1:A:22:SER:O	1:A:26:VAL:HG23	1.87	0.73
1:F:308:ARG:HG2	1:F:308:ARG:HH11	1.54	0.73
1:F:267:ALA:HB1	1:F:282:ILE:CG1	2.18	0.73
1:H:272:LYS:HE3	1:H:277:GLU:OE2	1.88	0.73
2:F:901:LMT:H4'	2:F:901:LMT:O2B	1.88	0.73
1:G:211:GLY:O	1:G:215:VAL:HG23	1.88	0.73
1:B:134:ASN:OD1	1:B:136:ARG:HB3	1.89	0.73
1:D:272:LYS:HE3	1:D:277:GLU:OE2	1.89	0.72
1:E:205:ARG:HA	1:E:260:GLU:HB2	1.71	0.72
1:H:199:ASN:O	1:H:203:LEU:HD12	1.89	0.72
1:B:134:ASN:ND2	1:B:137:GLU:HG3	2.04	0.72
1:F:131:ARG:HG3	1:F:131:ARG:HH11	1.52	0.72
1:A:196:ARG:HD3	1:A:197:ASP:O	1.89	0.72
1:D:131:ARG:HH12	1:D:196:ARG:HD2	1.54	0.72
1:E:25:LEU:HD22	1:E:83:GLU:CG	2.18	0.71
1:G:112:ILE:HD12	1:G:156:LEU:HD23	1.72	0.71
1:C:38:VAL:HG13	1:C:39:PRO:HD3	1.71	0.71
1:E:183:MET:HE3	1:E:214:VAL:HG13	1.72	0.71
1:C:35:TYR:HB3	1:C:63:ILE:HG21	1.72	0.71
1:D:192:ARG:HH11	1:D:192:ARG:HB3	1.54	0.71
1:D:266:MET:CE	1:D:267:ALA:H	2.00	0.71
1:B:22:SER:O	1:B:26:VAL:HG23	1.90	0.71
1:C:22:SER:HB3	1:C:83:GLU:OE2	1.89	0.71
1:G:-5:VAL:CG1	1:G:-3:ASP:HB2	2.20	0.70
1:B:237:GLY:O	1:B:240:PRO:HD2	1.89	0.70
1:F:10:ASP:HB3	1:F:14:ARG:NH2	2.06	0.70
1:D:266:MET:HE2	1:D:267:ALA:N	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1010:HOH:O	1:F:107:LYS:HG2	1.91	0.70
1:G:22:SER:N	1:G:83:GLU:OE2	2.24	0.70
1:D:179:MET:HG2	1:D:221:LEU:CD1	2.22	0.70
1:F:252:ARG:HH11	1:F:252:ARG:HG2	1.57	0.70
1:H:220:GLU:O	1:H:224:ARG:HD2	1.90	0.70
1:D:124:GLN:HA	1:D:124:GLN:NE2	2.05	0.69
1:A:138:TRP:CH2	1:A:183:MET:HG2	2.26	0.69
1:G:81:ARG:CG	1:H:81:ARG:HH12	2.04	0.69
1:H:244:LEU:HD11	2:H:903:LMT:H42	1.74	0.69
1:A:190:TYR:O	1:A:191:ASP:HB2	1.93	0.69
1:F:134:ASN:ND2	1:F:137:GLU:HG3	2.07	0.69
1:H:218:LEU:HD23	1:H:246:THR:HG23	1.73	0.69
1:C:158:ALA:CA	1:C:165:GLN:HG2	2.21	0.69
1:G:188:THR:CG2	2:G:902:LMT:H6E	2.21	0.69
1:B:245:TYR:O	1:B:249:VAL:HG23	1.93	0.68
1:F:1:MET:HE3	1:F:2:LEU:HD23	1.75	0.68
1:F:34:LEU:CG	2:F:902:LMT:H6D	2.11	0.68
1:H:-2:ASP:O	1:H:2:LEU:HB2	1.94	0.68
1:C:179:MET:HG2	1:C:221:LEU:HD11	1.75	0.68
1:E:113:LEU:HB3	1:F:93:LEU:HD22	1.74	0.68
1:A:107:LYS:O	1:A:107:LYS:HD3	1.93	0.67
1:B:25:LEU:O	1:B:29:THR:HG23	1.95	0.67
1:C:5:GLU:OE1	1:C:37:ARG:HD3	1.94	0.67
1:D:1:MET:SD	1:D:37:ARG:HD3	2.34	0.67
1:C:198:GLY:O	1:C:201:ALA:N	2.27	0.67
1:D:31:ALA:O	1:D:33:ARG:HG2	1.95	0.67
2:F:901:LMT:H5B	2:F:901:LMT:O3'	1.94	0.67
1:G:205:ARG:HH11	1:G:205:ARG:HG2	1.59	0.67
1:G:96:LEU:HD11	1:H:96:LEU:HD11	1.77	0.67
1:E:81:ARG:HD2	1:F:81:ARG:HH12	1.60	0.67
1:E:68:LEU:HD22	1:E:84:LEU:CD2	2.25	0.66
1:A:222:ARG:HB2	1:A:246:THR:HG21	1.76	0.66
1:B:250:LEU:HD23	1:B:254:LEU:HD12	1.78	0.66
1:A:113:LEU:HB3	1:B:93:LEU:HD22	1.78	0.66
1:G:29:THR:HA	1:G:32:LEU:CD1	2.24	0.66
1:H:183:MET:HE1	1:H:218:LEU:CG	2.25	0.66
1:C:133:THR:HG23	1:C:137:GLU:OE1	1.96	0.65
1:C:232:PRO:HA	1:C:233:PRO:C	2.16	0.65
1:B:5:GLU:OE1	1:B:37:ARG:HD3	1.97	0.65
1:C:74:ASP:HB3	1:C:76:ASP:OD2	1.96	0.65
1:D:108:ALA:O	1:D:112:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ASN:HD21	1:F:137:GLU:HG3	1.62	0.65
1:G:106:PRO:HB2	1:H:106:PRO:HB2	1.78	0.65
1:B:77:THR:HB	1:B:79:LEU:CD1	2.15	0.65
1:D:33:ARG:HH11	1:D:33:ARG:CB	2.09	0.65
1:E:134:ASN:HD21	1:E:137:GLU:HG3	1.61	0.65
1:F:259:GLY:HA2	1:F:322:GLN:OE1	1.96	0.65
1:F:204:MET:HE3	1:F:254:LEU:HD21	1.78	0.65
1:F:267:ALA:HB2	1:F:319:GLU:CD	2.17	0.65
1:B:1:MET:HG2	1:B:40:HIS:CD2	2.32	0.65
1:C:139:ARG:HD3	1:C:179:MET:CE	2.27	0.65
1:F:38:VAL:HG12	1:F:39:PRO:HD3	1.79	0.64
1:A:22:SER:HB3	1:A:83:GLU:OE2	1.96	0.64
1:B:203:LEU:HB3	1:B:209:VAL:HG23	1.79	0.64
1:A:258:LEU:O	1:A:258:LEU:CG	2.43	0.64
1:A:113:LEU:O	1:A:152:ARG:NH1	2.31	0.64
1:C:51:ARG:HH21	1:C:162:GLY:CA	2.10	0.64
1:E:124:GLN:HE22	2:E:901:LMT:H71	1.61	0.64
2:E:901:LMT:H122	1:F:89:LEU:HD23	1.80	0.64
1:G:127:THR:HG21	1:G:145:TYR:HD2	1.60	0.64
1:H:252:ARG:NH1	1:H:253:LEU:HD21	2.13	0.64
1:D:192:ARG:HB3	1:D:192:ARG:NH1	2.12	0.64
1:B:60:ALA:O	1:B:64:VAL:HG23	1.98	0.63
1:H:221:LEU:HA	1:H:224:ARG:HD3	1.80	0.63
1:D:318:LYS:O	1:D:322:GLN:HG3	1.99	0.63
1:H:324:LEU:O	1:H:328:LYS:HG2	1.99	0.63
1:B:-4:ASP:O	1:B:-1:ASP:HB2	1.99	0.63
1:D:273:TYR:O	1:D:274:LYS:HB2	1.99	0.63
1:G:81:ARG:CD	1:H:81:ARG:NH1	2.62	0.63
1:G:178:ALA:O	1:G:181:ILE:HB	1.98	0.63
1:F:318:LYS:O	1:F:322:GLN:HG3	1.98	0.63
1:B:40:HIS:CE1	1:B:52:ARG:NH2	2.67	0.63
1:C:10:ASP:OD2	2:G:902:LMT:H22	1.98	0.62
1:H:124:GLN:HA	1:H:124:GLN:OE1	1.99	0.62
1:B:77:THR:CB	1:B:79:LEU:HD12	2.17	0.62
1:H:72:LEU:O	1:H:81:ARG:NH2	2.32	0.62
1:C:187:LEU:HD21	1:C:204:MET:CE	2.29	0.62
1:C:229:VAL:HG11	1:C:238:LEU:HB2	1.81	0.62
1:G:68:LEU:HD22	1:G:84:LEU:CD2	2.29	0.62
1:H:295:ILE:HD12	1:H:324:LEU:HD11	1.81	0.62
1:A:75:ASP:HB2	1:A:81:ARG:NH1	2.14	0.62
1:A:139:ARG:HD3	1:A:179:MET:CE	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:MET:CE	1:F:254:LEU:HD21	2.29	0.62
1:A:143:SER:O	1:A:147:SER:HB2	1.99	0.62
1:B:134:ASN:HD21	1:B:137:GLU:HG3	1.65	0.62
1:C:19:THR:OG1	1:C:90:ARG:HG3	2.00	0.62
1:C:35:TYR:CE2	1:C:67:LYS:HG3	2.34	0.62
1:C:111:ASP:O	1:C:115:GLN:HB2	2.00	0.62
1:A:158:ALA:HA	1:A:165:GLN:HG2	1.81	0.62
1:C:131:ARG:NH2	1:C:196:ARG:HH12	1.95	0.62
1:E:131:ARG:HD2	1:E:197:ASP:OD2	1.99	0.62
1:E:96:LEU:HD11	1:F:96:LEU:HD11	1.80	0.61
1:G:134:ASN:OD1	1:G:137:GLU:HG3	1.99	0.61
1:G:218:LEU:HD21	1:G:246:THR:HG23	1.81	0.61
1:H:115:GLN:HG3	1:H:116:ASP:N	2.14	0.61
1:E:104:ARG:HB2	1:E:104:ARG:NH2	2.10	0.61
1:C:257:HIS:O	1:C:258:LEU:C	2.39	0.61
1:E:194:GLY:HA2	1:E:196:ARG:HH22	1.63	0.61
1:G:218:LEU:HD22	1:G:246:THR:HG23	1.82	0.61
1:H:25:LEU:HD22	1:H:83:GLU:HG2	1.82	0.61
1:H:267:ALA:HB2	1:H:319:GLU:OE2	1.99	0.61
1:G:38:VAL:N	1:G:39:PRO:CD	2.63	0.61
1:B:85:ALA:O	1:B:88:CYS:HB3	2.01	0.61
1:C:11:HIS:CD2	1:C:57:ARG:HD2	2.35	0.61
1:C:54:ALA:HB1	1:C:102:LEU:HD21	1.82	0.61
1:F:90:ARG:C	1:F:90:ARG:HD3	2.21	0.61
1:B:197:ASP:HB2	3:B:422:HOH:O	1.99	0.61
1:C:131:ARG:NH2	1:C:196:ARG:NH1	2.44	0.61
1:G:239:VAL:HB	1:G:240:PRO:HD3	1.83	0.61
1:D:33:ARG:HB3	1:D:33:ARG:HH11	1.64	0.60
1:B:124:GLN:HA	1:B:124:GLN:NE2	2.12	0.60
2:F:902:LMT:H1B	2:F:902:LMT:C6'	2.24	0.60
1:A:134:ASN:OD1	1:A:137:GLU:HG3	2.00	0.60
1:D:258:LEU:HD13	1:D:262:GLY:O	2.02	0.60
1:H:-4:ASP:C	1:H:-2:ASP:H	2.04	0.60
1:D:212:GLN:N	1:D:263:ALA:HB1	2.16	0.60
1:D:212:GLN:CA	1:D:263:ALA:HB1	2.32	0.60
1:G:51:ARG:HG3	1:G:51:ARG:NH2	2.16	0.60
2:H:901:LMT:H6E	2:H:901:LMT:C5B	2.31	0.60
1:C:147:SER:HB3	1:C:175:GLU:HG2	1.83	0.60
1:E:251:VAL:HG12	1:E:252:ARG:N	2.16	0.60
1:E:127:THR:HG21	1:E:145:TYR:HD2	1.65	0.60
1:B:15:CYS:O	1:B:19:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:SER:O	1:B:147:SER:HB2	2.00	0.60
1:C:35:TYR:HA	1:C:38:VAL:HG12	1.84	0.60
1:D:24:ASP:O	1:D:27:ALA:HB3	2.02	0.60
1:D:263:ALA:O	1:D:264:GLY:O	2.20	0.60
1:D:121:CYS:O	1:D:125:ILE:HG13	2.02	0.60
1:B:166:PRO:HB2	1:B:169:SER:HB2	1.82	0.59
1:G:252:ARG:NH2	1:G:253:LEU:HD21	2.16	0.59
1:E:205:ARG:HA	1:E:260:GLU:CB	2.32	0.59
1:H:318:LYS:O	1:H:322:GLN:HG3	2.02	0.59
1:B:22:SER:HB2	1:B:23:PRO:HD2	1.83	0.59
1:G:107:LYS:NZ	1:H:97:HIS:ND1	2.50	0.59
1:D:232:PRO:HA	1:D:233:PRO:C	2.22	0.59
1:G:254:LEU:HD22	1:G:258:LEU:HD13	1.84	0.59
1:E:13:THR:HB	1:E:26:VAL:HG13	1.84	0.59
1:F:205:ARG:HA	1:F:261:ALA:CB	2.33	0.59
1:F:267:ALA:O	1:F:282:ILE:HG12	2.03	0.59
1:G:232:PRO:HA	1:G:233:PRO:C	2.21	0.59
1:D:33:ARG:NH1	1:D:33:ARG:CB	2.65	0.59
1:F:11:HIS:CD2	1:F:57:ARG:HB2	2.38	0.59
1:H:25:LEU:HD22	1:H:83:GLU:CG	2.32	0.59
1:C:214:VAL:HG11	1:C:254:LEU:HD21	1.83	0.59
1:E:45:TRP:HB2	1:E:165:GLN:NE2	2.17	0.59
1:E:206:THR:HG23	1:E:208:ALA:H	1.68	0.59
1:C:192:ARG:HG2	1:C:193:ASN:ND2	2.17	0.59
1:C:45:TRP:CE2	1:C:235:ALA:HB2	2.38	0.59
1:C:32:LEU:CD1	1:C:64:VAL:HG13	2.33	0.58
2:F:902:LMT:C6'	2:F:902:LMT:C1B	2.81	0.58
1:A:32:LEU:HD22	1:A:67:LYS:HG2	1.85	0.58
1:D:250:LEU:HD23	1:D:254:LEU:HD12	1.84	0.58
1:H:104:ARG:CZ	1:H:104:ARG:CB	2.81	0.58
1:F:12:VAL:O	1:F:16:VAL:HG23	2.02	0.58
1:H:134:ASN:ND2	1:H:137:GLU:HG3	2.18	0.58
1:B:318:LYS:O	1:B:322:GLN:HG3	2.03	0.58
1:G:34:LEU:HB2	2:G:902:LMT:H6'2	1.84	0.58
1:H:229:VAL:HG13	1:H:235:ALA:O	2.03	0.58
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.34	0.58
1:B:212:GLN:CA	1:B:263:ALA:HB1	2.34	0.58
1:E:219:GLU:CD	1:E:222:ARG:HE	2.06	0.58
1:H:212:GLN:H	1:H:264:GLY:HA3	1.69	0.58
1:A:258:LEU:HA	3:A:420:HOH:O	2.04	0.58
1:G:77:THR:HB	1:G:79:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ASP:OD1	1:G:82:VAL:HB	2.04	0.58
1:H:203:LEU:HB3	1:H:208:ALA:HB3	1.84	0.58
1:D:22:SER:O	1:D:26:VAL:HG23	2.03	0.57
1:G:205:ARG:HG2	1:G:205:ARG:NH1	2.19	0.57
1:E:1:MET:HE3	1:E:2:LEU:HG	1.86	0.57
1:H:52:ARG:HG3	1:H:52:ARG:HH11	1.68	0.57
1:B:58:ALA:O	1:B:61:LEU:HB2	2.04	0.57
1:C:197:ASP:HA	3:C:403:HOH:O	2.03	0.57
1:D:14:ARG:NH1	1:F:191:ASP:HB3	2.19	0.57
1:H:260:GLU:C	1:H:262:GLY:H	2.04	0.57
1:H:222:ARG:HB2	1:H:246:THR:HG21	1.87	0.57
2:H:902:LMT:C5B	2:H:902:LMT:H4'	2.34	0.57
1:F:167:ALA:HB3	3:F:1025:HOH:O	2.04	0.57
1:H:138:TRP:CD2	1:H:200:LEU:HD13	2.39	0.57
1:D:266:MET:HG3	1:D:267:ALA:N	2.20	0.57
1:G:81:ARG:HD3	1:H:81:ARG:NH1	2.19	0.57
1:B:132:ALA:HB1	1:B:137:GLU:HB2	1.86	0.57
1:D:285:ILE:HD13	1:D:320:LEU:HD13	1.87	0.57
1:F:135:LEU:HB2	1:F:209:VAL:HG22	1.85	0.57
1:E:38:VAL:CG1	1:E:39:PRO:HD3	2.31	0.57
1:F:206:THR:HG22	1:F:206:THR:O	2.05	0.57
1:F:268:THR:HG22	1:F:281:ASP:OD1	2.05	0.57
1:G:35:TYR:CE2	1:G:67:LYS:HG3	2.40	0.57
1:A:139:ARG:HD3	1:A:179:MET:HE3	1.87	0.56
1:B:183:MET:HE1	1:B:214:VAL:HG13	1.87	0.56
1:D:131:ARG:NH1	1:D:196:ARG:HH11	2.03	0.56
1:D:190:TYR:O	1:D:191:ASP:HB2	2.04	0.56
1:E:90:ARG:NH1	1:E:94:ARG:HB2	2.20	0.56
2:F:901:LMT:H22	2:F:902:LMT:H82	1.87	0.56
1:E:203:LEU:HA	1:E:206:THR:HG22	1.85	0.56
1:F:32:LEU:HD12	1:F:64:VAL:HG13	1.88	0.56
1:H:1:MET:CE	2:H:903:LMT:H91	2.36	0.56
2:H:901:LMT:H6E	2:H:901:LMT:H5B	1.88	0.56
1:H:67:LYS:HZ1	2:H:902:LMT:H6'2	1.64	0.56
1:A:237:GLY:O	1:A:240:PRO:HD2	2.06	0.56
1:D:135:LEU:HB2	1:D:209:VAL:HG22	1.87	0.56
1:B:90:ARG:NH1	1:B:94:ARG:HB2	2.21	0.56
1:E:190:TYR:CD1	1:E:257:HIS:HE1	2.23	0.56
1:D:83:GLU:O	1:D:87:VAL:HG23	2.06	0.56
1:D:124:GLN:HE21	1:D:124:GLN:CA	2.02	0.56
1:C:80:ASP:HB3	1:C:83:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ARG:HG2	1:H:81:ARG:HH12	1.69	0.55
1:G:143:SER:O	1:G:147:SER:HB2	2.05	0.55
1:A:25:LEU:CD2	1:A:87:VAL:HG21	2.37	0.55
1:B:204:MET:CE	1:B:214:VAL:HG21	2.36	0.55
1:D:90:ARG:HD3	1:D:90:ARG:C	2.26	0.55
1:D:232:PRO:HA	1:D:234:GLY:N	2.21	0.55
1:H:1:MET:SD	1:H:37:ARG:HD3	2.47	0.55
1:B:204:MET:HE1	1:B:214:VAL:HG21	1.88	0.55
1:C:134:ASN:HD21	1:C:136:ARG:NH1	2.05	0.55
1:G:86:CYS:SG	2:H:901:LMT:H112	2.46	0.55
2:H:902:LMT:H4'	2:H:902:LMT:H5B	1.87	0.55
1:F:271:PHE:HB3	1:F:311:VAL:CG1	2.37	0.55
1:E:203:LEU:O	1:E:206:THR:HG22	2.07	0.55
1:G:217:LEU:HD12	1:G:217:LEU:C	2.27	0.55
1:A:90:ARG:C	1:A:90:ARG:HD3	2.27	0.55
1:B:308:ARG:HH11	1:B:308:ARG:HG2	1.72	0.55
1:C:32:LEU:HD12	1:C:64:VAL:HG13	1.89	0.55
1:D:43:THR:HB	1:D:52:ARG:HG3	1.88	0.55
1:E:72:LEU:O	1:F:81:ARG:NH2	2.40	0.55
1:E:239:VAL:HB	1:E:240:PRO:HD3	1.89	0.55
1:G:226:LEU:HD11	1:G:243:HIS:NE2	2.21	0.55
1:H:38:VAL:CG1	1:H:39:PRO:HD3	2.34	0.55
1:H:268:THR:HB	1:H:279:GLU:HG3	1.89	0.55
1:A:19:THR:OG1	1:A:90:ARG:HG3	2.07	0.55
1:A:33:ARG:NH2	1:E:77:THR:HB	2.22	0.55
1:H:308:ARG:HG2	1:H:308:ARG:HH11	1.71	0.55
1:C:38:VAL:CG1	1:C:39:PRO:HD3	2.37	0.54
1:D:40:HIS:CE1	1:D:52:ARG:NH2	2.76	0.54
1:D:204:MET:HE2	1:D:214:VAL:HG21	1.87	0.54
1:E:237:GLY:O	1:E:240:PRO:HD2	2.07	0.54
1:G:10:ASP:O	1:G:14:ARG:HB2	2.06	0.54
1:G:113:LEU:HB3	1:H:93:LEU:HD22	1.87	0.54
1:A:25:LEU:HD21	1:A:87:VAL:HG21	1.89	0.54
1:A:198:GLY:O	1:A:201:ALA:N	2.40	0.54
1:F:269:VAL:O	1:F:279:GLU:HA	2.06	0.54
1:G:38:VAL:N	1:G:39:PRO:HD3	2.23	0.54
1:H:149:PHE:CZ	2:H:901:LMT:H42	2.42	0.54
1:E:183:MET:CE	1:E:214:VAL:HG13	2.38	0.54
1:F:229:VAL:HG21	1:F:238:LEU:HB2	1.90	0.54
1:G:0:LYS:O	1:G:3:ALA:HB3	2.08	0.54
1:G:81:ARG:HD3	1:H:81:ARG:HH12	1.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:VAL:HG21	1:D:285:ILE:HD11	1.88	0.54
1:E:127:THR:HG21	1:E:145:TYR:CD2	2.43	0.54
1:F:239:VAL:N	1:F:240:PRO:CD	2.71	0.54
1:H:203:LEU:HD12	1:H:203:LEU:H	1.72	0.54
1:E:54:ALA:HB1	1:E:102:LEU:HD11	1.89	0.54
1:F:236:PRO:O	1:F:239:VAL:HG23	2.07	0.54
1:D:14:ARG:HH12	1:F:191:ASP:CB	2.19	0.54
1:D:247:ASP:O	1:D:251:VAL:HG23	2.08	0.54
1:E:44:GLU:OE2	1:E:52:ARG:NH2	2.40	0.54
1:H:90:ARG:NH1	1:H:94:ARG:HB2	2.23	0.54
1:D:271:PHE:HZ	1:D:299:TYR:CE2	2.26	0.54
1:G:34:LEU:HD13	2:G:902:LMT:H4B	1.89	0.54
1:H:67:LYS:NZ	2:H:902:LMT:C6B	2.60	0.54
1:B:285:ILE:HG22	1:B:285:ILE:O	2.08	0.54
1:E:107:LYS:O	1:E:107:LYS:HD3	2.08	0.54
1:B:179:MET:CE	1:B:217:LEU:HD11	2.38	0.53
1:B:212:GLN:HA	1:B:263:ALA:HB1	1.89	0.53
1:F:32:LEU:CD1	1:F:64:VAL:HG13	2.37	0.53
1:F:104:ARG:HG3	1:F:105:ASP:N	2.22	0.53
1:H:138:TRP:CH2	1:H:183:MET:HG2	2.43	0.53
1:C:187:LEU:HD21	1:C:204:MET:HE3	1.89	0.53
1:D:16:VAL:HG22	1:D:87:VAL:HG11	1.89	0.53
1:D:298:THR:HG22	1:D:308:ARG:HG2	1.91	0.53
1:A:149:PHE:O	1:A:152:ARG:HG3	2.08	0.53
1:B:138:TRP:CH2	1:B:183:MET:HG2	2.43	0.53
1:C:-4:ASP:O	1:C:-1:ASP:HB2	2.07	0.53
1:F:90:ARG:HD3	1:F:90:ARG:O	2.07	0.53
1:F:265:ALA:C	1:F:267:ALA:H	2.12	0.53
1:H:8:ASN:O	1:H:12:VAL:HG23	2.08	0.53
1:H:185:ASP:OD1	2:H:902:LMT:H62	2.09	0.53
1:H:85:ALA:O	1:H:88:CYS:HB3	2.09	0.53
1:B:136:ARG:HD3	3:B:426:HOH:O	2.08	0.53
1:C:196:ARG:HG3	1:C:196:ARG:HH11	1.73	0.53
1:D:192:ARG:HH11	1:D:192:ARG:CB	2.21	0.53
1:E:61:LEU:HD22	1:E:91:LEU:HD23	1.89	0.53
1:E:187:LEU:HD21	1:E:204:MET:CE	2.39	0.53
1:E:190:TYR:O	1:E:194:GLY:HA2	2.09	0.53
1:H:5:GLU:OE1	1:H:37:ARG:HB2	2.09	0.53
1:D:166:PRO:HB2	1:D:169:SER:HB2	1.89	0.53
1:F:308:ARG:HH11	1:F:308:ARG:CG	2.21	0.53
2:F:901:LMT:O6'	2:F:902:LMT:H61	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:THR:CA	1:G:32:LEU:HD12	2.37	0.53
1:H:150:LEU:HD13	2:H:902:LMT:H122	1.91	0.53
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.90	0.53
1:F:189:ASP:OD1	1:F:192:ARG:HD3	2.09	0.53
1:D:198:GLY:O	1:D:199:ASN:C	2.47	0.53
1:F:1:MET:CE	1:F:2:LEU:HD23	2.38	0.53
1:B:19:THR:HG21	1:B:90:ARG:HD2	1.91	0.52
1:D:266:MET:HE3	1:D:266:MET:HA	1.91	0.52
1:G:166:PRO:HD3	1:G:233:PRO:HD2	1.90	0.52
1:H:104:ARG:CG	1:H:105:ASP:N	2.72	0.52
1:A:75:ASP:HB3	1:B:81:ARG:NH2	2.25	0.52
1:B:179:MET:HE2	1:B:221:LEU:HD21	1.90	0.52
1:B:172:GLU:HG3	1:B:228:ALA:HB2	1.89	0.52
1:C:75:ASP:HB2	1:C:81:ARG:HH12	1.74	0.52
1:D:1:MET:SD	1:D:37:ARG:CD	2.96	0.52
1:A:11:HIS:CG	1:A:57:ARG:HD2	2.44	0.52
1:B:72:LEU:HD13	1:B:84:LEU:HB3	1.91	0.52
1:C:54:ALA:CB	1:C:102:LEU:HD21	2.39	0.52
1:C:81:ARG:NH2	1:D:72:LEU:O	2.38	0.52
1:D:134:ASN:ND2	1:D:137:GLU:HG3	2.25	0.52
1:E:218:LEU:HD11	1:E:249:VAL:CG1	2.39	0.52
1:B:299:TYR:CE1	1:B:307:GLY:HA3	2.45	0.52
1:E:187:LEU:HD21	1:E:204:MET:HE3	1.91	0.52
1:F:290:ARG:HG2	1:F:291:VAL:N	2.24	0.52
1:A:80:ASP:HB3	1:A:83:GLU:HG3	1.92	0.52
1:B:51:ARG:NH2	1:B:160:CYS:O	2.43	0.52
1:C:190:TYR:O	1:C:191:ASP:HB2	2.09	0.52
1:F:188:THR:HG22	1:F:189:ASP:N	2.24	0.52
1:E:251:VAL:CG1	1:E:252:ARG:N	2.71	0.52
1:A:100:GLU:HG3	1:A:109:VAL:HG21	1.92	0.51
1:B:202:HIS:O	1:B:206:THR:HG22	2.10	0.51
1:C:65:SER:HB2	1:C:91:LEU:HB2	1.91	0.51
1:A:54:ALA:HB1	1:A:102:LEU:HD11	1.92	0.51
1:B:203:LEU:HA	1:B:206:THR:CG2	2.39	0.51
1:D:198:GLY:O	1:D:201:ALA:N	2.43	0.51
1:F:252:ARG:HG2	1:F:252:ARG:NH1	2.24	0.51
1:G:-4:ASP:O	1:G:1:MET:HE3	2.10	0.51
2:G:901:LMT:H121	1:H:89:LEU:HD22	1.91	0.51
1:H:299:TYR:HE1	1:H:301:GLU:HB2	1.75	0.51
1:D:131:ARG:HE	1:D:199:ASN:ND2	2.09	0.51
1:E:25:LEU:HD13	1:E:79:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:HB2	1:F:40:HIS:CD2	2.45	0.51
1:F:289:TRP:CB	1:F:328:LYS:HE2	2.39	0.51
1:E:11:HIS:CE1	1:E:57:ARG:HD2	2.45	0.51
1:G:54:ALA:HA	1:G:57:ARG:NH2	2.26	0.51
1:A:58:ALA:HA	1:A:61:LEU:HD12	1.91	0.51
1:B:263:ALA:O	1:B:264:GLY:O	2.28	0.51
1:B:206:THR:HG23	1:B:208:ALA:H	1.76	0.51
1:D:-4:ASP:O	1:D:-1:ASP:HB2	2.11	0.51
1:D:138:TRP:NE1	1:D:200:LEU:HB2	2.25	0.51
1:A:65:SER:HB2	1:A:91:LEU:HB2	1.91	0.51
1:B:126:ARG:HG3	1:B:126:ARG:HH11	1.76	0.51
1:D:60:ALA:O	1:D:64:VAL:HG23	2.10	0.51
1:D:256:ARG:NH1	1:E:129:ARG:HD2	2.25	0.51
1:E:45:TRP:HB2	1:E:165:GLN:HE21	1.75	0.51
1:A:205:ARG:NH1	1:F:131:ARG:HG2	2.24	0.51
1:A:256:ARG:CA	1:F:130:SER:HB3	2.39	0.51
1:B:1:MET:HG2	1:B:40:HIS:HD2	1.76	0.51
1:B:203:LEU:HB3	1:B:209:VAL:CG2	2.41	0.51
1:B:254:LEU:CB	1:B:255:PRO:HD3	2.41	0.51
1:B:295:ILE:HD12	1:B:324:LEU:HD11	1.93	0.51
1:C:150:LEU:HD23	1:C:178:ALA:HB2	1.93	0.51
1:F:285:ILE:CD1	1:F:320:LEU:HD13	2.41	0.51
1:H:10:ASP:OD2	1:H:14:ARG:NH2	2.44	0.51
1:H:1:MET:HE1	2:H:903:LMT:H91	1.93	0.51
1:H:251:VAL:O	1:H:255:PRO:HG2	2.11	0.50
1:C:259:GLY:HA2	1:H:131:ARG:HH12	1.76	0.50
1:E:134:ASN:HD22	1:E:137:GLU:HG3	1.72	0.50
1:F:205:ARG:HA	1:F:261:ALA:HB2	1.93	0.50
1:A:152:ARG:O	1:A:156:LEU:HG	2.12	0.50
1:B:226:LEU:HD11	1:B:243:HIS:CE1	2.46	0.50
1:D:-4:ASP:HA	1:D:-1:ASP:OD2	2.12	0.50
1:D:35:TYR:O	1:D:39:PRO:HD3	2.12	0.50
2:E:901:LMT:H122	1:F:89:LEU:CD2	2.40	0.50
1:A:25:LEU:O	1:A:29:THR:HG23	2.12	0.50
1:A:166:PRO:O	1:A:169:SER:N	2.40	0.50
1:G:1:MET:SD	1:G:2:LEU:HD23	2.51	0.50
1:G:8:ASN:OD1	1:G:57:ARG:HA	2.11	0.50
1:G:131:ARG:HD2	1:G:197:ASP:OD1	2.11	0.50
1:B:45:TRP:CD1	1:B:166:PRO:HG3	2.46	0.50
1:B:261:ALA:O	1:B:262:GLY:O	2.30	0.50
1:E:-4:ASP:OD2	1:E:1:MET:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ARG:CG	1:F:105:ASP:N	2.74	0.50
1:F:252:ARG:HH12	1:F:253:LEU:HD21	1.76	0.50
1:G:-5:VAL:C	1:G:-3:ASP:H	2.14	0.50
1:G:189:ASP:OD1	1:G:192:ARG:NH1	2.43	0.50
2:H:902:LMT:H31	2:H:903:LMT:O3B	2.12	0.50
1:F:34:LEU:HD11	1:F:181:ILE:HD13	1.92	0.50
1:G:34:LEU:HD13	2:G:902:LMT:H6'2	1.94	0.50
1:B:31:ALA:O	1:B:33:ARG:N	2.45	0.50
1:C:256:ARG:HD3	1:H:129:ARG:HB3	1.94	0.50
1:F:254:LEU:N	1:F:255:PRO:CD	2.75	0.50
1:B:239:VAL:HB	1:B:240:PRO:CD	2.41	0.50
1:B:271:PHE:HB3	1:B:311:VAL:CG1	2.42	0.50
1:B:19:THR:O	1:B:19:THR:OG1	2.27	0.50
1:C:258:LEU:O	1:C:258:LEU:HD22	2.11	0.50
1:D:286:LYS:HE3	1:D:299:TYR:C	2.32	0.50
1:E:59:LEU:O	1:E:63:ILE:HG13	2.11	0.50
1:D:16:VAL:HG22	1:D:87:VAL:CG1	2.42	0.49
1:D:281:ASP:C	1:D:283:SER:N	2.65	0.49
1:F:44:GLU:HG2	1:F:238:LEU:HG	1.93	0.49
1:D:190:TYR:O	1:D:191:ASP:CB	2.60	0.49
1:F:16:VAL:HG13	1:F:87:VAL:HG11	1.95	0.49
1:G:188:THR:CB	2:G:902:LMT:H6E	2.41	0.49
1:H:72:LEU:HD12	1:H:81:ARG:HH21	1.76	0.49
1:B:186:ASP:OD2	1:B:200:LEU:N	2.37	0.49
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.47	0.49
1:F:25:LEU:HB2	1:F:83:GLU:OE2	2.12	0.49
1:H:32:LEU:HB3	1:H:35:TYR:HD2	1.76	0.49
1:C:144:THR:OG1	1:C:145:TYR:N	2.45	0.49
1:G:256:ARG:HH11	1:G:256:ARG:CG	2.22	0.49
1:A:131:ARG:HH22	1:A:196:ARG:NH1	2.08	0.49
1:B:182:THR:O	1:B:182:THR:HG22	2.11	0.49
1:C:258:LEU:C	1:C:258:LEU:HD22	2.33	0.49
2:E:901:LMT:O2B	2:E:901:LMT:H6E	2.13	0.49
1:C:107:LYS:NZ	1:D:97:HIS:ND1	2.61	0.49
1:H:1:MET:O	1:H:4:ALA:N	2.45	0.49
1:A:203:LEU:HB3	1:A:209:VAL:HG23	1.94	0.49
1:C:179:MET:HG2	1:C:221:LEU:CD1	2.41	0.49
1:H:254:LEU:HD22	1:H:258:LEU:HG	1.95	0.49
1:B:203:LEU:HA	1:B:206:THR:HG22	1.94	0.49
1:D:131:ARG:NH1	1:D:196:ARG:HD2	2.27	0.49
1:H:201:ALA:O	1:H:204:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:MET:HE2	1:B:267:ALA:O	2.12	0.48
1:D:161:GLY:O	1:D:165:GLN:NE2	2.41	0.48
1:D:288:VAL:HG12	1:D:327:GLN:HE22	1.78	0.48
1:D:288:VAL:HG13	1:D:288:VAL:O	2.13	0.48
1:B:33:ARG:NH1	1:H:79:LEU:HG	2.28	0.48
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.95	0.48
1:C:222:ARG:HB2	1:C:246:THR:HG21	1.96	0.48
1:H:257:HIS:H	1:H:257:HIS:CD2	2.29	0.48
1:C:67:LYS:O	1:C:67:LYS:HD3	2.12	0.48
1:D:92:HIS:CE1	1:D:96:LEU:HG	2.48	0.48
1:E:61:LEU:HD22	1:E:91:LEU:CD2	2.44	0.48
1:H:19:THR:O	1:H:19:THR:HG22	2.12	0.48
1:H:150:LEU:HD13	2:H:902:LMT:C12	2.43	0.48
1:H:212:GLN:O	1:H:215:VAL:HG23	2.12	0.48
1:A:232:PRO:HA	1:A:233:PRO:C	2.33	0.48
1:C:75:ASP:HB2	1:C:81:ARG:NH1	2.29	0.48
1:F:48:ASP:C	1:F:48:ASP:OD1	2.51	0.48
1:D:70:ASP:O	1:D:73:MET:HB2	2.14	0.48
1:F:1:MET:HG3	1:F:2:LEU:N	2.28	0.48
1:G:133:THR:OG1	1:G:137:GLU:OE1	2.32	0.48
1:H:196:ARG:HD2	1:H:202:HIS:ND1	2.28	0.48
1:D:231:ALA:O	1:D:234:GLY:HA2	2.14	0.48
1:E:25:LEU:HB2	1:E:83:GLU:OE2	2.14	0.48
1:G:195:GLU:O	1:G:196:ARG:HG2	2.13	0.48
1:H:-2:ASP:OD2	2:H:903:LMT:H52	2.14	0.48
1:H:179:MET:HG2	1:H:221:LEU:CD1	2.44	0.48
1:H:244:LEU:HD11	2:H:903:LMT:H22	1.95	0.48
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.96	0.48
1:C:53:ALA:O	1:C:57:ARG:HG2	2.12	0.48
1:A:198:GLY:O	1:A:199:ASN:C	2.51	0.48
2:F:902:LMT:H2'	2:F:902:LMT:H11	1.62	0.48
1:H:32:LEU:HD22	1:H:35:TYR:CD2	2.49	0.48
1:C:51:ARG:HH21	1:C:162:GLY:HA2	1.77	0.48
1:E:143:SER:HA	1:E:147:SER:HB2	1.95	0.48
1:F:48:ASP:OD1	1:F:49:PRO:HD2	2.14	0.48
1:A:61:LEU:HB2	1:A:95:ALA:HB2	1.96	0.48
1:B:199:ASN:O	1:B:203:LEU:HG	2.14	0.48
1:B:212:GLN:OE1	1:B:264:GLY:CA	2.62	0.48
1:E:138:TRP:CH2	1:E:183:MET:HG2	2.49	0.48
1:H:51:ARG:NH2	1:H:160:CYS:O	2.46	0.48
1:H:179:MET:HB3	1:H:221:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HD3	1:F:129:ARG:HB3	1.96	0.47
1:E:131:ARG:HD2	1:E:197:ASP:HB3	1.96	0.47
1:F:105:ASP:CG	1:F:106:PRO:HD2	2.34	0.47
1:B:35:TYR:O	1:B:39:PRO:HD3	2.14	0.47
1:B:239:VAL:N	1:B:240:PRO:HD2	2.29	0.47
1:C:244:LEU:HD12	3:C:406:HOH:O	2.15	0.47
1:D:165:GLN:O	1:D:167:ALA:N	2.42	0.47
1:E:203:LEU:HA	1:E:206:THR:CG2	2.44	0.47
1:F:142:ALA:HA	1:F:145:TYR:CE2	2.49	0.47
1:F:285:ILE:HD12	1:F:320:LEU:HD13	1.96	0.47
1:G:238:LEU:HA	1:G:241:VAL:CG2	2.43	0.47
1:B:74:ASP:HB3	1:B:76:ASP:OD2	2.14	0.47
1:F:289:TRP:HB2	1:F:328:LYS:CE	2.44	0.47
1:G:254:LEU:O	1:G:258:LEU:HB2	2.14	0.47
1:B:288:VAL:HG12	1:B:327:GLN:HE22	1.79	0.47
1:D:90:ARG:HD3	1:D:90:ARG:O	2.14	0.47
1:F:51:ARG:NH2	1:F:102:LEU:HB3	2.29	0.47
1:H:134:ASN:HD21	1:H:137:GLU:HG3	1.79	0.47
1:B:70:ASP:HA	1:B:73:MET:HG2	1.97	0.47
1:B:290:ARG:HG2	1:B:291:VAL:N	2.30	0.47
1:E:139:ARG:NE	1:E:179:MET:HE1	2.29	0.47
1:E:258:LEU:HD23	1:E:258:LEU:HA	1.68	0.47
1:F:189:ASP:HA	1:F:192:ARG:HB3	1.96	0.47
1:B:273:TYR:O	1:B:274:LYS:HB2	2.15	0.47
1:D:44:GLU:HG2	1:D:238:LEU:HG	1.97	0.47
2:F:901:LMT:O2B	2:F:901:LMT:C4'	2.59	0.47
1:H:290:ARG:HG2	1:H:291:VAL:N	2.30	0.47
1:A:22:SER:CB	1:A:23:PRO:HD2	2.40	0.47
1:B:45:TRP:HB2	1:B:165:GLN:HE22	1.79	0.47
1:B:179:MET:HE2	1:B:221:LEU:CD1	2.42	0.47
1:B:212:GLN:HB2	1:B:263:ALA:HB1	1.97	0.47
1:D:5:GLU:OE2	1:D:9:ARG:NH2	2.48	0.47
1:D:167:ALA:HB3	1:D:168:ASP:OD2	2.14	0.47
1:D:290:ARG:HG2	1:D:291:VAL:N	2.29	0.47
1:E:74:ASP:OD2	1:E:128:LYS:NZ	2.44	0.47
1:B:32:LEU:O	1:B:36:LEU:HD12	2.15	0.47
1:C:11:HIS:CG	1:C:57:ARG:HD2	2.49	0.47
1:E:11:HIS:O	1:E:15:CYS:HB2	2.14	0.47
1:H:67:LYS:HZ1	2:H:902:LMT:C6B	2.25	0.47
1:H:93:LEU:HD23	1:H:93:LEU:HA	1.77	0.47
1:C:199:ASN:O	1:C:203:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:HD1	1:A:63:ILE:CG2	2.28	0.47
1:C:259:GLY:HA2	1:H:131:ARG:NH1	2.30	0.47
1:E:187:LEU:CD2	1:E:204:MET:HE3	2.45	0.47
1:G:14:ARG:HH11	1:G:14:ARG:HG3	1.80	0.47
1:B:212:GLN:HA	1:B:263:ALA:CB	2.45	0.46
1:B:269:VAL:HG23	1:B:282:ILE:CD1	2.45	0.46
1:C:85:ALA:O	1:C:88:CYS:HB3	2.15	0.46
1:D:111:ASP:O	1:D:115:GLN:HG2	2.15	0.46
1:E:85:ALA:O	1:E:88:CYS:HB3	2.15	0.46
2:H:902:LMT:H41	2:H:902:LMT:H71	1.71	0.46
1:A:64:VAL:O	1:A:68:LEU:HG	2.15	0.46
1:A:70:ASP:O	1:A:73:MET:HG2	2.15	0.46
1:A:257:HIS:O	1:A:259:GLY:N	2.49	0.46
1:B:267:ALA:HB2	1:B:319:GLU:OE2	2.14	0.46
1:F:25:LEU:O	1:F:28:HIS:HB3	2.15	0.46
1:F:316:ALA:HA	1:F:317:PRO:HD3	1.79	0.46
1:H:224:ARG:HD2	1:H:224:ARG:N	2.22	0.46
1:A:124:GLN:HA	1:A:124:GLN:OE1	2.15	0.46
1:E:133:THR:OG1	1:E:137:GLU:OE1	2.32	0.46
1:H:288:VAL:HG22	1:H:324:LEU:HD21	1.97	0.46
1:C:1:MET:SD	1:C:37:ARG:HD2	2.55	0.46
1:D:286:LYS:HE3	1:D:300:ASP:N	2.30	0.46
1:H:67:LYS:HZ1	2:H:902:LMT:C5B	2.26	0.46
1:A:106:PRO:O	1:A:109:VAL:HG23	2.15	0.46
1:B:134:ASN:HD21	1:B:137:GLU:CG	2.27	0.46
1:B:190:TYR:HE2	3:B:402:HOH:O	1.98	0.46
1:F:295:ILE:CD1	1:F:324:LEU:HD11	2.38	0.46
1:H:252:ARG:CZ	1:H:253:LEU:HD21	2.45	0.46
1:C:22:SER:HB2	1:C:23:PRO:CD	2.46	0.46
1:G:120:LEU:HD12	1:G:148:THR:CG2	2.41	0.46
1:C:96:LEU:HD11	1:D:96:LEU:CD1	2.40	0.46
1:F:190:TYR:CZ	1:F:196:ARG:CZ	2.98	0.46
1:H:239:VAL:N	1:H:240:PRO:HD2	2.31	0.46
1:H:288:VAL:HA	1:H:297:PHE:HA	1.98	0.46
1:F:131:ARG:HD3	1:F:197:ASP:OD1	2.16	0.46
1:C:147:SER:O	1:C:175:GLU:HG3	2.16	0.46
1:D:14:ARG:HH12	1:F:191:ASP:HB2	1.80	0.46
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.80	0.46
1:D:231:ALA:O	1:D:234:GLY:CA	2.64	0.46
1:D:281:ASP:C	1:D:283:SER:H	2.18	0.46
1:F:104:ARG:CG	1:F:105:ASP:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:PRO:HA	1:F:233:PRO:C	2.35	0.46
1:B:211:GLY:O	1:B:215:VAL:HG23	2.16	0.46
1:C:73:MET:SD	1:D:82:VAL:HG22	2.56	0.46
1:E:203:LEU:CA	1:E:206:THR:HG22	2.46	0.46
1:D:132:ALA:HB2	1:D:141:HIS:CD2	2.51	0.45
1:H:255:PRO:O	1:H:256:ARG:C	2.54	0.45
1:B:81:ARG:HE	1:B:81:ARG:HB2	1.34	0.45
1:B:212:GLN:CB	1:B:263:ALA:HB1	2.47	0.45
1:E:29:THR:HA	1:E:32:LEU:HD12	1.98	0.45
1:F:105:ASP:OD1	1:F:105:ASP:C	2.54	0.45
1:F:133:THR:N	1:F:137:GLU:OE1	2.41	0.45
1:G:258:LEU:HD12	1:G:258:LEU:HA	1.60	0.45
1:H:15:CYS:O	1:H:18:GLN:HG2	2.16	0.45
1:H:282:ILE:HG22	1:H:323:MET:SD	2.55	0.45
1:C:100:GLU:OE2	1:D:110:THR:OG1	2.21	0.45
1:D:68:LEU:HD22	1:D:84:LEU:HD23	1.98	0.45
1:E:113:LEU:HB3	1:F:93:LEU:CD2	2.45	0.45
2:H:901:LMT:H121	2:H:901:LMT:H92	1.83	0.45
1:A:148:THR:O	1:A:152:ARG:HG2	2.16	0.45
1:A:174:ALA:O	1:A:178:ALA:HB2	2.17	0.45
1:E:32:LEU:HD22	1:E:35:TYR:CD2	2.52	0.45
1:F:232:PRO:HA	1:F:234:GLY:N	2.32	0.45
1:A:5:GLU:OE1	1:A:37:ARG:HD3	2.17	0.45
1:B:322:GLN:O	1:B:325:GLU:HB2	2.16	0.45
1:C:35:TYR:HB3	1:C:63:ILE:CG2	2.44	0.45
1:D:51:ARG:HH21	1:D:162:GLY:CA	2.29	0.45
1:D:124:GLN:NE2	1:D:124:GLN:CA	2.74	0.45
1:H:105:ASP:OD2	1:H:105:ASP:C	2.54	0.45
1:H:135:LEU:O	1:H:135:LEU:HD12	2.15	0.45
1:F:116:ASP:OD1	1:F:152:ARG:NH1	2.45	0.45
1:B:183:MET:O	1:B:187:LEU:HG	2.16	0.45
1:E:125:ILE:HD13	1:F:83:GLU:HA	1.97	0.45
1:B:212:GLN:O	1:B:212:GLN:HG3	2.17	0.45
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.98	0.45
1:A:153:TYR:CD1	1:A:156:LEU:HD12	2.52	0.45
1:D:187:LEU:HD21	1:D:204:MET:HE3	1.99	0.45
1:A:113:LEU:O	1:A:117:ALA:HB2	2.17	0.45
1:B:35:TYR:CE2	1:B:67:LYS:HG3	2.52	0.45
1:A:90:ARG:HD3	1:A:90:ARG:O	2.18	0.44
1:D:134:ASN:HD21	1:D:137:GLU:HG3	1.81	0.44
1:E:34:LEU:HD21	1:E:181:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LEU:CD2	1:E:174:ALA:HB2	2.47	0.44
1:E:214:VAL:O	1:E:218:LEU:HB2	2.17	0.44
1:B:108:ALA:O	1:B:112:ILE:HG13	2.17	0.44
1:B:142:ALA:HA	1:B:145:TYR:CE2	2.52	0.44
1:B:188:THR:HG22	1:B:190:TYR:CE1	2.52	0.44
1:D:231:ALA:O	1:D:234:GLY:N	2.50	0.44
1:F:149:PHE:CE2	2:F:901:LMT:H42	2.52	0.44
1:H:-4:ASP:O	1:H:-1:ASP:HB2	2.17	0.44
2:H:902:LMT:H11	2:H:902:LMT:H2'	1.70	0.44
1:A:22:SER:HB2	1:A:23:PRO:CD	2.40	0.44
1:C:57:ARG:HH12	2:G:902:LMT:H111	1.82	0.44
1:E:85:ALA:HB2	1:F:73:MET:HB3	1.99	0.44
1:E:114:GLU:OE1	1:F:94:ARG:HA	2.17	0.44
1:F:35:TYR:OH	2:F:901:LMT:H21	2.16	0.44
1:F:254:LEU:N	1:F:255:PRO:HD3	2.32	0.44
1:G:144:THR:HA	1:G:148:THR:HB	1.98	0.44
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.84	0.44
1:D:120:LEU:HD22	1:D:152:ARG:NE	2.32	0.44
1:F:226:LEU:HD23	1:F:226:LEU:HA	1.76	0.44
1:H:48:ASP:OD1	1:H:48:ASP:C	2.56	0.44
1:H:229:VAL:CG1	1:H:235:ALA:O	2.64	0.44
1:H:271:PHE:HZ	1:H:299:TYR:CE2	2.35	0.44
1:A:33:ARG:HH21	1:E:77:THR:HB	1.81	0.44
1:A:93:LEU:HD13	1:B:113:LEU:O	2.17	0.44
1:E:189:ASP:HA	1:E:192:ARG:HB2	1.99	0.44
1:H:52:ARG:HG3	1:H:52:ARG:NH1	2.33	0.44
1:D:322:GLN:O	1:D:325:GLU:HB2	2.17	0.44
1:F:11:HIS:CD2	1:F:57:ARG:HG3	2.53	0.44
1:F:203:LEU:HD23	1:F:203:LEU:HA	1.78	0.44
1:H:179:MET:HG2	1:H:221:LEU:HD11	2.00	0.44
1:H:299:TYR:CE1	1:H:307:GLY:HA3	2.53	0.44
1:B:190:TYR:O	1:B:191:ASP:HB2	2.17	0.44
1:D:267:ALA:O	1:D:282:ILE:HG12	2.18	0.44
1:F:143:SER:O	1:F:147:SER:HB2	2.17	0.44
1:H:61:LEU:HD22	1:H:91:LEU:HD22	2.00	0.44
1:D:32:LEU:HB3	1:D:35:TYR:HD2	1.83	0.44
1:E:25:LEU:CD2	1:E:83:GLU:CG	2.94	0.44
2:E:901:LMT:H32	2:E:901:LMT:H62	1.75	0.44
2:G:901:LMT:H121	1:H:89:LEU:CD2	2.48	0.44
1:H:281:ASP:C	1:H:283:SER:H	2.21	0.44
1:D:33:ARG:HG2	1:D:33:ARG:H	1.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:PHE:CZ	1:D:299:TYR:HE2	2.36	0.43
1:D:272:LYS:HE2	1:D:272:LYS:HB3	1.85	0.43
1:E:127:THR:HG23	1:E:141:HIS:CG	2.53	0.43
1:F:150:LEU:HD12	1:F:150:LEU:HA	1.73	0.43
1:F:206:THR:O	1:F:206:THR:CG2	2.65	0.43
1:H:72:LEU:CD2	1:H:85:ALA:HA	2.47	0.43
1:B:-5:VAL:O	1:B:-1:ASP:OD2	2.35	0.43
1:G:61:LEU:HB2	1:G:95:ALA:HB2	2.00	0.43
1:H:236:PRO:O	1:H:239:VAL:HG23	2.18	0.43
1:B:10:ASP:OD2	1:H:192:ARG:HD2	2.18	0.43
1:B:51:ARG:HH22	1:B:102:LEU:HB3	1.83	0.43
1:B:105:ASP:O	1:B:106:PRO:C	2.54	0.43
1:B:182:THR:O	1:B:182:THR:CG2	2.65	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.84	0.43
1:C:51:ARG:NH2	1:C:162:GLY:HA2	2.33	0.43
1:C:143:SER:HA	1:C:147:SER:HB2	2.00	0.43
1:C:256:ARG:HA	1:H:130:SER:HB3	2.00	0.43
1:D:188:THR:HG21	1:D:190:TYR:CZ	2.52	0.43
1:D:288:VAL:HG12	1:D:327:GLN:NE2	2.33	0.43
1:F:105:ASP:OD1	1:F:107:LYS:N	2.51	0.43
1:H:285:ILE:O	1:H:285:ILE:HG22	2.17	0.43
1:B:248:ASP:OD2	1:B:252:ARG:NH2	2.42	0.43
1:C:9:ARG:HD3	1:C:30:ALA:CB	2.44	0.43
1:H:232:PRO:HA	1:H:234:GLY:N	2.32	0.43
1:H:299:TYR:CE1	1:H:301:GLU:HB2	2.51	0.43
1:B:216:ASP:O	1:B:219:GLU:HB2	2.18	0.43
1:C:106:PRO:HB2	1:D:106:PRO:HB2	1.99	0.43
1:D:14:ARG:NH1	1:F:191:ASP:CB	2.81	0.43
1:B:212:GLN:O	1:B:216:ASP:OD1	2.37	0.43
1:D:72:LEU:HD13	1:D:84:LEU:HB3	1.99	0.43
1:D:85:ALA:O	1:D:88:CYS:HB3	2.18	0.43
1:E:168:ASP:OD2	1:E:168:ASP:N	2.52	0.43
1:G:217:LEU:HD12	1:G:221:LEU:HG	2.00	0.43
1:H:260:GLU:C	1:H:262:GLY:N	2.72	0.43
1:B:45:TRP:CE2	1:B:235:ALA:HB2	2.53	0.43
1:B:260:GLU:HG2	1:G:136:ARG:NH2	2.33	0.43
1:E:183:MET:HE2	1:E:183:MET:HB3	1.86	0.43
1:G:120:LEU:CD2	2:G:901:LMT:H123	2.49	0.43
1:G:81:ARG:HE	1:G:81:ARG:HB2	1.57	0.43
1:G:84:LEU:HD23	1:G:84:LEU:HA	1.68	0.43
1:B:188:THR:HG21	1:B:190:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:CD	1:C:30:ALA:HB1	2.45	0.43
1:D:104:ARG:CG	1:D:105:ASP:N	2.82	0.43
1:D:105:ASP:OD1	1:D:105:ASP:C	2.57	0.43
1:H:72:LEU:CD1	1:H:81:ARG:HH21	2.31	0.43
1:H:94:ARG:O	1:H:97:HIS:HB3	2.19	0.43
1:H:270:LYS:NZ	1:H:279:GLU:OE2	2.52	0.43
1:C:57:ARG:NH1	2:G:902:LMT:H111	2.34	0.43
1:E:67:LYS:HD3	1:E:67:LYS:O	2.18	0.43
1:G:217:LEU:O	1:G:221:LEU:HG	2.19	0.43
1:H:269:VAL:O	1:H:279:GLU:HA	2.19	0.43
1:C:33:ARG:NH2	1:G:28:HIS:ND1	2.67	0.42
1:C:158:ALA:CB	1:C:165:GLN:HG2	2.48	0.42
1:D:1:MET:HB2	3:D:420:HOH:O	2.18	0.42
1:D:19:THR:OG1	1:D:90:ARG:HG3	2.20	0.42
1:E:75:ASP:HB2	1:F:81:ARG:HD2	2.00	0.42
1:E:103:ALA:HA	1:E:160:CYS:HA	2.02	0.42
1:E:203:LEU:C	1:E:206:THR:HG22	2.39	0.42
1:B:19:THR:CG2	1:B:90:ARG:HD2	2.49	0.42
1:B:32:LEU:HB3	1:B:35:TYR:CD2	2.42	0.42
1:D:77:THR:C	1:D:79:LEU:N	2.69	0.42
1:F:179:MET:HG2	1:F:221:LEU:HD11	2.00	0.42
1:G:256:ARG:HG3	1:G:257:HIS:CE1	2.54	0.42
1:E:124:GLN:NE2	2:E:901:LMT:H71	2.31	0.42
1:E:125:ILE:CD1	1:F:83:GLU:HA	2.49	0.42
1:F:11:HIS:CE1	1:F:57:ARG:NH1	2.88	0.42
2:F:901:LMT:H6D	3:F:1006:HOH:O	2.18	0.42
1:H:166:PRO:HB2	1:H:169:SER:HB2	2.01	0.42
1:B:166:PRO:O	1:B:169:SER:N	2.49	0.42
1:E:253:LEU:CD2	1:E:256:ARG:HH21	2.33	0.42
1:H:205:ARG:HG2	1:H:260:GLU:HG3	2.01	0.42
1:H:254:LEU:O	1:H:255:PRO:C	2.57	0.42
1:C:196:ARG:HH11	1:C:196:ARG:CG	2.33	0.42
1:D:261:ALA:O	1:D:262:GLY:O	2.37	0.42
1:G:256:ARG:CG	1:G:256:ARG:NH1	2.81	0.42
1:H:61:LEU:HD23	1:H:61:LEU:HA	1.79	0.42
1:D:212:GLN:HB2	1:D:264:GLY:H	1.85	0.42
1:D:285:ILE:O	1:D:285:ILE:HG22	2.20	0.42
1:F:5:GLU:OE1	1:F:37:ARG:NE	2.52	0.42
1:F:48:ASP:OD1	1:F:49:PRO:CD	2.68	0.42
1:F:54:ALA:O	1:F:57:ARG:HG2	2.20	0.42
1:A:59:LEU:HD11	1:A:157:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.87	0.42
1:B:39:PRO:O	1:B:43:THR:HG23	2.20	0.42
1:B:135:LEU:HB2	1:B:209:VAL:HG13	2.00	0.42
1:B:138:TRP:NE1	1:B:200:LEU:HB2	2.34	0.42
1:C:26:VAL:HG11	1:G:193:ASN:HB2	2.01	0.42
1:C:33:ARG:HH11	1:C:33:ARG:HB3	1.85	0.42
1:C:200:LEU:HG	1:C:204:MET:HE2	2.02	0.42
1:G:68:LEU:HD22	1:G:84:LEU:HD22	2.02	0.42
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.85	0.42
1:C:198:GLY:O	1:C:200:LEU:N	2.53	0.42
1:C:238:LEU:O	1:C:242:VAL:HG23	2.20	0.42
1:D:135:LEU:HA	1:D:135:LEU:HD12	1.63	0.42
1:D:308:ARG:HG2	1:D:308:ARG:HH11	1.85	0.42
1:E:149:PHE:CD2	2:E:901:LMT:H61	2.54	0.42
1:F:131:ARG:HG3	1:F:131:ARG:NH1	2.26	0.42
1:H:1:MET:CG	1:H:2:LEU:N	2.81	0.42
1:A:165:GLN:HE21	1:A:165:GLN:HB2	1.40	0.42
1:B:215:VAL:HG22	1:B:254:LEU:HD11	2.02	0.42
1:D:22:SER:H	1:D:22:SER:HG	1.35	0.42
1:D:168:ASP:OD2	1:D:168:ASP:N	2.29	0.42
1:E:1:MET:SD	1:E:1:MET:C	2.98	0.42
1:F:267:ALA:HB1	1:F:282:ILE:HG12	1.96	0.42
1:G:86:CYS:SG	2:H:901:LMT:C11	3.08	0.42
1:G:225:ALA:O	1:G:229:VAL:HG22	2.19	0.42
1:H:281:ASP:C	1:H:283:SER:N	2.73	0.42
1:A:127:THR:HG23	1:A:141:HIS:HB3	2.02	0.42
1:A:131:ARG:HH21	1:A:196:ARG:NH1	2.13	0.42
1:B:9:ARG:NH2	1:B:30:ALA:O	2.53	0.42
1:B:124:GLN:NE2	1:B:145:TYR:HB3	2.35	0.42
1:E:96:LEU:HB3	1:F:110:THR:HG22	2.02	0.42
1:A:96:LEU:HD11	1:B:96:LEU:HD11	2.00	0.41
1:B:70:ASP:O	1:B:73:MET:N	2.49	0.41
1:B:179:MET:CE	1:B:221:LEU:HD21	2.50	0.41
1:B:267:ALA:O	1:B:282:ILE:HG12	2.20	0.41
1:D:281:ASP:O	1:D:283:SER:N	2.53	0.41
1:E:149:PHE:CE1	2:E:901:LMT:H81	2.55	0.41
1:F:51:ARG:HH22	1:F:102:LEU:HB3	1.86	0.41
1:H:218:LEU:HD21	1:H:249:VAL:HB	2.01	0.41
1:A:-4:ASP:OD2	1:A:-3:ASP:N	2.53	0.41
1:B:282:ILE:HG21	1:B:319:GLU:O	2.20	0.41
1:F:205:ARG:HA	1:F:261:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:HH11	1:A:131:ARG:HB3	1.85	0.41
1:B:212:GLN:OE1	1:B:264:GLY:N	2.53	0.41
1:B:250:LEU:HD23	1:B:254:LEU:CD1	2.49	0.41
1:D:212:GLN:HA	1:D:263:ALA:HB1	2.02	0.41
1:E:250:LEU:O	1:E:255:PRO:HD3	2.20	0.41
1:F:-1:ASP:O	1:F:2:LEU:N	2.53	0.41
1:F:38:VAL:N	1:F:39:PRO:CD	2.83	0.41
1:G:34:LEU:CD1	2:G:902:LMT:H6'2	2.50	0.41
1:C:70:ASP:C	1:C:72:LEU:N	2.73	0.41
1:D:239:VAL:N	1:D:240:PRO:HD2	2.35	0.41
1:F:308:ARG:CG	1:F:308:ARG:NH1	2.81	0.41
1:G:195:GLU:C	1:G:196:ARG:HG2	2.41	0.41
1:H:135:LEU:HB2	1:H:209:VAL:HG22	2.03	0.41
1:D:66:MET:HG3	1:D:153:TYR:OH	2.20	0.41
1:G:37:ARG:O	1:G:37:ARG:HG2	2.20	0.41
1:H:48:ASP:OD1	1:H:49:PRO:N	2.53	0.41
1:H:273:TYR:O	1:H:274:LYS:HB2	2.21	0.41
1:B:204:MET:HE3	1:B:204:MET:HB2	1.74	0.41
1:C:94:ARG:NH2	1:C:97:HIS:CD2	2.89	0.41
1:F:196:ARG:HG2	1:F:196:ARG:HH11	1.86	0.41
1:H:9:ARG:NH2	1:H:33:ARG:HG2	2.36	0.41
1:D:134:ASN:OD1	1:D:137:GLU:HG3	2.20	0.41
1:E:195:GLU:HG2	1:E:199:ASN:HB2	2.02	0.41
1:G:240:PRO:O	1:G:244:LEU:HB2	2.21	0.41
1:A:87:VAL:O	1:A:88:CYS:C	2.59	0.41
1:A:140:ALA:O	1:A:143:SER:HB3	2.20	0.41
1:B:281:ASP:C	1:B:283:SER:N	2.72	0.41
1:C:163:GLU:CD	1:C:164:GLY:H	2.21	0.41
1:D:77:THR:C	1:D:79:LEU:H	2.23	0.41
1:F:250:LEU:HD23	1:F:250:LEU:HA	1.93	0.41
1:F:285:ILE:HD13	1:F:320:LEU:CD1	2.51	0.41
1:H:32:LEU:HD22	1:H:35:TYR:HD2	1.85	0.41
1:A:150:LEU:HD23	1:A:178:ALA:HB2	2.02	0.41
1:B:144:THR:OG1	1:B:145:TYR:N	2.53	0.41
1:C:69:LEU:O	1:C:72:LEU:HB3	2.19	0.41
1:C:81:ARG:HH22	1:D:81:ARG:HD2	1.86	0.41
1:D:51:ARG:HH21	1:D:162:GLY:N	2.18	0.41
1:D:132:ALA:HB2	1:D:141:HIS:HD2	1.85	0.41
1:D:183:MET:CE	1:D:218:LEU:HG	2.51	0.41
1:E:218:LEU:HD11	1:E:249:VAL:HG11	2.03	0.41
1:F:32:LEU:O	1:F:36:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:GLU:H	1:G:260:GLU:HG2	1.26	0.41
1:A:217:LEU:O	1:A:218:LEU:C	2.58	0.41
1:B:69:LEU:HB2	1:B:88:CYS:SG	2.60	0.41
1:C:131:ARG:HH22	1:C:196:ARG:CZ	2.30	0.41
1:D:84:LEU:O	1:D:85:ALA:C	2.57	0.41
1:F:239:VAL:N	1:F:240:PRO:HD3	2.36	0.41
1:F:268:THR:HB	1:F:279:GLU:HG3	2.03	0.41
1:F:289:TRP:HB3	1:F:328:LYS:HE2	2.03	0.41
1:G:68:LEU:HD22	1:G:84:LEU:HD21	1.99	0.41
1:H:104:ARG:CB	1:H:104:ARG:NH1	2.84	0.41
1:A:35:TYR:CD2	3:A:436:HOH:O	2.72	0.40
1:B:83:GLU:O	1:B:87:VAL:HG23	2.21	0.40
1:B:114:GLU:O	1:B:115:GLN:C	2.59	0.40
1:C:34:LEU:HD12	1:C:34:LEU:O	2.21	0.40
1:C:90:ARG:HD3	1:C:90:ARG:C	2.41	0.40
1:C:150:LEU:CD2	1:C:178:ALA:HB2	2.51	0.40
1:C:254:LEU:N	1:C:255:PRO:CD	2.84	0.40
1:D:62:ASP:OD2	1:D:153:TYR:CE1	2.74	0.40
1:F:87:VAL:O	1:F:88:CYS:C	2.58	0.40
1:G:-5:VAL:HG13	1:G:-3:ASP:H	1.86	0.40
1:H:90:ARG:HD3	1:H:90:ARG:C	2.42	0.40
1:D:210:ALA:O	1:D:211:GLY:C	2.59	0.40
1:E:34:LEU:HD12	1:E:34:LEU:HA	1.85	0.40
1:E:38:VAL:CG1	1:E:39:PRO:CD	3.00	0.40
1:E:166:PRO:HD3	1:E:233:PRO:HD2	2.03	0.40
1:E:211:GLY:O	1:E:215:VAL:HG23	2.22	0.40
1:A:1:MET:SD	1:A:37:ARG:CD	3.02	0.40
1:A:168:ASP:OD1	1:A:168:ASP:N	2.54	0.40
1:A:189:ASP:HA	1:A:195:GLU:OE1	2.21	0.40
1:B:203:LEU:CA	1:B:206:THR:HG22	2.50	0.40
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.83	0.40
1:D:140:ALA:O	1:D:143:SER:HB2	2.21	0.40
1:D:238:LEU:O	1:D:241:VAL:HB	2.21	0.40
1:D:276:GLU:HB3	1:D:277:GLU:H	1.68	0.40
1:E:61:LEU:CD2	1:E:91:LEU:CD2	2.99	0.40
1:F:113:LEU:HD23	1:F:113:LEU:HA	1.79	0.40
1:H:33:ARG:HH22	1:H:37:ARG:NH1	2.19	0.40
1:H:185:ASP:OD2	2:H:902:LMT:H32	2.21	0.40
1:B:-4:ASP:HA	1:B:-1:ASP:OD2	2.22	0.40
1:D:69:LEU:O	1:D:72:LEU:HB3	2.22	0.40
1:D:141:HIS:O	1:D:142:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:901:LMT:O5'	2:E:901:LMT:H21	2.21	0.40
1:F:267:ALA:HB2	1:F:319:GLU:OE2	2.21	0.40
1:G:25:LEU:HD22	1:G:83:GLU:HB3	2.03	0.40
1:G:165:GLN:HE21	1:G:165:GLN:HB2	1.67	0.40
1:G:226:LEU:HD11	1:G:243:HIS:HE2	1.84	0.40
1:D:2:LEU:HD11	1:F:30:ALA:HB1	2.04	0.40
1:D:254:LEU:HD23	1:D:254:LEU:HA	1.78	0.40
1:E:203:LEU:HA	1:E:203:LEU:HD23	1.85	0.40
1:G:124:GLN:HG2	2:G:901:LMT:H111	2.04	0.40
1:G:226:LEU:C	1:G:229:VAL:HG23	2.40	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	262/343 (76%)	239 (91%)	19 (7%)	4 (2%)	10 35
1	B	332/343 (97%)	300 (90%)	25 (8%)	7 (2%)	7 26
1	C	262/343 (76%)	241 (92%)	18 (7%)	3 (1%)	14 42
1	D	330/343 (96%)	296 (90%)	25 (8%)	9 (3%)	5 21
1	E	268/343 (78%)	251 (94%)	15 (6%)	2 (1%)	22 52
1	F	330/343 (96%)	297 (90%)	29 (9%)	4 (1%)	13 40
1	G	265/343 (77%)	247 (93%)	15 (6%)	3 (1%)	14 42
1	H	331/343 (96%)	298 (90%)	28 (8%)	5 (2%)	10 35
All	All	2380/2744 (87%)	2169 (91%)	174 (7%)	37 (2%)	9 33

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ALA
1	B	32	LEU
1	B	167	ALA
1	C	167	ALA
1	D	167	ALA
1	F	167	ALA
1	F	265	ALA
1	G	-4	ASP
1	H	265	ALA
1	B	262	GLY
1	B	264	GLY
1	C	199	ASN
1	D	192	ARG
1	D	262	GLY
1	D	264	GLY
1	E	167	ALA
1	H	256	ARG
1	H	266	MET
1	A	191	ASP
1	A	258	LEU
1	B	286	LYS
1	B	327	GLN
1	C	192	ARG
1	D	191	ASP
1	D	199	ASN
1	G	52	ARG
1	D	286	LYS
1	F	266	MET
1	H	286	LYS
1	A	193	ASN
1	G	259	GLY
1	H	-3	ASP
1	B	302	GLY
1	F	262	GLY
1	D	234	GLY
1	E	146	GLY
1	D	302	GLY

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	207/270 (77%)	187 (90%)	20 (10%)	8 27
1	B	262/270 (97%)	240 (92%)	22 (8%)	11 34
1	C	207/270 (77%)	183 (88%)	24 (12%)	5 19
1	D	260/270 (96%)	235 (90%)	25 (10%)	8 27
1	E	213/270 (79%)	193 (91%)	20 (9%)	8 28
1	F	260/270 (96%)	235 (90%)	25 (10%)	8 27
1	G	210/270 (78%)	178 (85%)	32 (15%)	3 10
1	H	261/270 (97%)	236 (90%)	25 (10%)	8 27
All	All	1880/2160 (87%)	1687 (90%)	193 (10%)	7 24

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ASP
1	A	-2	ASP
1	A	18	GLN
1	A	23	PRO
1	A	24	ASP
1	A	34	LEU
1	A	70	ASP
1	A	90	ARG
1	A	139	ARG
1	A	152	ARG
1	A	163	GLU
1	A	165	GLN
1	A	168	ASP
1	A	180	THR
1	A	186	ASP
1	A	193	ASN
1	A	196	ARG
1	A	199	ASN
1	A	254	LEU
1	A	258	LEU
1	B	10	ASP
1	B	18	GLN
1	B	19	THR
1	B	24	ASP

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Mol	Chain	Res	Type
1	B	34	LEU
1	B	47	THR
1	B	81	ARG
1	B	90	ARG
1	B	105	ASP
1	B	116	ASP
1	B	144	THR
1	B	185	ASP
1	B	186	ASP
1	B	189	ASP
1	B	199	ASN
1	B	266	MET
1	B	284	LYS
1	B	305	LYS
1	B	314	LYS
1	B	315	ASP
1	B	325	GLU
1	B	328	LYS
1	C	1	MET
1	C	18	GLN
1	C	24	ASP
1	C	33	ARG
1	C	39	PRO
1	C	47	THR
1	C	70	ASP
1	C	79	LEU
1	C	90	ARG
1	C	101	SER
1	C	107	LYS
1	C	110	THR
1	C	116	ASP
1	C	129	ARG
1	C	130	SER
1	C	133	THR
1	C	139	ARG
1	C	165	GLN
1	C	179	MET
1	C	186	ASP
1	C	199	ASN
1	C	224	ARG
1	C	248	ASP
1	C	258	LEU

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Mol	Chain	Res	Type
1	D	10	ASP
1	D	15	CYS
1	D	18	GLN
1	D	22	SER
1	D	33	ARG
1	D	77	THR
1	D	90	ARG
1	D	104	ARG
1	D	105	ASP
1	D	124	GLN
1	D	130	SER
1	D	133	THR
1	D	168	ASP
1	D	172	GLU
1	D	186	ASP
1	D	191	ASP
1	D	192	ARG
1	D	197	ASP
1	D	199	ASN
1	D	206	THR
1	D	229	VAL
1	D	266	MET
1	D	284	LYS
1	D	315	ASP
1	D	325	GLU
1	E	-9	HIS
1	E	10	ASP
1	E	19	THR
1	E	24	ASP
1	E	47	THR
1	E	52	ARG
1	E	57	ARG
1	E	90	ARG
1	E	163	GLU
1	E	165	GLN
1	E	168	ASP
1	E	172	GLU
1	E	185	ASP
1	E	186	ASP
1	E	193	ASN
1	E	246	THR
1	E	251	VAL

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Mol	Chain	Res	Type
1	E	252	ARG
1	E	254	LEU
1	E	260	GLU
1	F	1	MET
1	F	2	LEU
1	F	18	GLN
1	F	34	LEU
1	F	38	VAL
1	F	47	THR
1	F	56	SER
1	F	90	ARG
1	F	105	ASP
1	F	110	THR
1	F	111	ASP
1	F	141	HIS
1	F	143	SER
1	F	144	THR
1	F	172	GLU
1	F	186	ASP
1	F	188	THR
1	F	193	ASN
1	F	218	LEU
1	F	229	VAL
1	F	254	LEU
1	F	266	MET
1	F	284	LYS
1	F	308	ARG
1	F	315	ASP
1	G	-6	HIS
1	G	-5	VAL
1	G	-4	ASP
1	G	-3	ASP
1	G	2	LEU
1	G	10	ASP
1	G	14	ARG
1	G	18	GLN
1	G	47	THR
1	G	52	ARG
1	G	56	SER
1	G	90	ARG
1	G	94	ARG
1	G	107	LYS

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Mol	Chain	Res	Type
1	G	143	SER
1	G	165	GLN
1	G	172	GLU
1	G	179	MET
1	G	185	ASP
1	G	186	ASP
1	G	193	ASN
1	G	197	ASP
1	G	199	ASN
1	G	205	ARG
1	G	217	LEU
1	G	218	LEU
1	G	219	GLU
1	G	229	VAL
1	G	244	LEU
1	G	254	LEU
1	G	256	ARG
1	G	260	GLU
1	H	2	LEU
1	H	18	GLN
1	H	38	VAL
1	H	39	PRO
1	H	47	THR
1	H	52	ARG
1	H	90	ARG
1	H	104	ARG
1	H	107	LYS
1	H	110	THR
1	H	131	ARG
1	H	150	LEU
1	H	172	GLU
1	H	181	ILE
1	H	185	ASP
1	H	186	ASP
1	H	199	ASN
1	H	215	VAL
1	H	218	LEU
1	H	224	ARG
1	H	254	LEU
1	H	266	MET
1	H	305	LYS
1	H	315	ASP

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Mol	Chain	Res	Type
1	H	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	199	ASN
1	B	18	GLN
1	B	40	HIS
1	B	115	GLN
1	B	124	GLN
1	B	165	GLN
1	B	199	ASN
1	C	97	HIS
1	C	165	GLN
1	C	193	ASN
1	C	199	ASN
1	D	18	GLN
1	D	124	GLN
1	D	141	HIS
1	D	199	ASN
1	E	124	GLN
1	E	193	ASN
1	F	18	GLN
1	F	40	HIS
1	F	119	HIS
1	G	141	HIS
1	G	165	GLN
1	G	193	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	F	901	-	36,36,36	0.98	2 (5%)	47,47,47	0.90	2 (4%)
2	LMT	G	901	-	36,36,36	0.94	2 (5%)	47,47,47	1.13	5 (10%)
2	LMT	H	902	-	36,36,36	1.02	1 (2%)	47,47,47	0.82	1 (2%)
2	LMT	G	902	-	36,36,36	1.05	1 (2%)	47,47,47	0.75	1 (2%)
2	LMT	H	903	-	36,36,36	1.17	3 (8%)	47,47,47	0.74	2 (4%)
2	LMT	E	901	-	36,36,36	0.87	2 (5%)	47,47,47	0.94	1 (2%)
2	LMT	F	902	-	36,36,36	1.09	3 (8%)	47,47,47	1.01	3 (6%)
2	LMT	H	901	-	36,36,36	0.78	1 (2%)	47,47,47	0.59	1 (2%)

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	F	901	-	-	11/21/61/61	0/2/2/2
2	LMT	G	901	-	-	13/21/61/61	0/2/2/2
2	LMT	H	902	-	-	15/21/61/61	0/2/2/2
2	LMT	G	902	-	-	13/21/61/61	0/2/2/2
2	LMT	H	903	-	-	10/21/61/61	0/2/2/2
2	LMT	E	901	-	-	12/21/61/61	0/2/2/2
2	LMT	F	902	-	-	15/21/61/61	0/2/2/2
2	LMT	H	901	-	-	11/21/61/61	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	902	LMT	O1'-C1	4.38	1.55	1.43
2	F	902	LMT	O1'-C1	4.37	1.55	1.43
2	H	902	LMT	O1'-C1	4.28	1.54	1.43
2	H	903	LMT	O1'-C1	4.19	1.54	1.43
2	F	901	LMT	O1'-C1	3.98	1.54	1.43
2	H	901	LMT	O1'-C1	3.76	1.53	1.43
2	E	901	LMT	O1'-C1	3.70	1.53	1.43
2	G	901	LMT	O1'-C1	2.95	1.51	1.43
2	G	901	LMT	C4B-C3B	2.42	1.58	1.52
2	H	903	LMT	C1B-C2B	2.12	1.58	1.52
2	F	902	LMT	C1B-C2B	2.12	1.58	1.52
2	F	902	LMT	O5B-C1B	2.11	1.47	1.41
2	H	903	LMT	O5B-C1B	2.10	1.47	1.41
2	F	901	LMT	C3'-C4'	2.07	1.57	1.52
2	E	901	LMT	O5B-C1B	2.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	901	LMT	C3B-C4B-C5B	3.97	117.31	110.24
2	F	902	LMT	C1B-C2B-C3B	3.65	117.60	110.00
2	E	901	LMT	C1B-C2B-C3B	3.16	116.57	110.00
2	G	901	LMT	O5B-C1B-C2B	-2.96	104.08	110.35
2	F	902	LMT	O1'-C1'-C2'	2.74	112.58	108.30
2	F	901	LMT	C1B-O1B-C4'	2.63	124.48	117.96
2	G	901	LMT	O5B-C5B-C4B	2.49	114.22	109.69
2	G	902	LMT	O1B-C4'-C3'	2.39	113.63	107.28
2	H	903	LMT	C1B-C2B-C3B	2.37	114.93	110.00
2	F	901	LMT	O1B-C1B-C2B	2.26	113.95	108.10
2	H	902	LMT	O5B-C1B-C2B	2.20	115.00	110.35
2	H	903	LMT	O1B-C1B-C2B	2.17	113.72	108.10
2	F	902	LMT	O1B-C4'-C3'	2.14	112.97	107.28
2	G	901	LMT	C4B-C3B-C2B	2.03	114.37	110.82
2	G	901	LMT	C1B-O1B-C4'	2.02	122.95	117.96
2	H	901	LMT	C1-O1'-C1'	-2.02	110.50	113.84

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	901	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
2	E	901	LMT	O5'-C1'-O1'-C1
2	F	901	LMT	C2B-C1B-O1B-C4'
2	F	901	LMT	C2-C1-O1'-C1'
2	F	902	LMT	C2'-C1'-O1'-C1
2	F	902	LMT	C2-C1-O1'-C1'
2	G	902	LMT	C2'-C1'-O1'-C1
2	G	902	LMT	O5'-C1'-O1'-C1
2	H	901	LMT	C2'-C1'-O1'-C1
2	H	901	LMT	O5'-C1'-O1'-C1
2	H	902	LMT	O5B-C1B-O1B-C4'
2	H	903	LMT	C4B-C5B-C6B-O6B
2	G	901	LMT	O5B-C1B-O1B-C4'
2	H	903	LMT	O5B-C5B-C6B-O6B
2	H	901	LMT	C4B-C5B-C6B-O6B
2	G	902	LMT	C5'-C4'-O1B-C1B
2	G	901	LMT	O5B-C5B-C6B-O6B
2	F	902	LMT	O5B-C5B-C6B-O6B
2	H	901	LMT	O5B-C5B-C6B-O6B
2	E	901	LMT	C3'-C4'-O1B-C1B
2	H	902	LMT	C4-C5-C6-C7
2	H	902	LMT	O5'-C5'-C6'-O6'
2	F	902	LMT	O5'-C5'-C6'-O6'
2	G	901	LMT	C4B-C5B-C6B-O6B
2	G	901	LMT	C2B-C1B-O1B-C4'
2	H	902	LMT	C4'-C5'-C6'-O6'
2	F	902	LMT	C4'-C5'-C6'-O6'
2	F	902	LMT	C3'-C4'-O1B-C1B
2	H	901	LMT	C4'-C5'-C6'-O6'
2	H	902	LMT	O1'-C1-C2-C3
2	E	901	LMT	C3-C4-C5-C6
2	G	901	LMT	O1'-C1-C2-C3
2	G	902	LMT	O5B-C5B-C6B-O6B
2	F	902	LMT	C7-C8-C9-C10
2	H	903	LMT	C4-C5-C6-C7
2	F	901	LMT	C4-C5-C6-C7
2	H	903	LMT	C5-C6-C7-C8
2	F	902	LMT	C6-C7-C8-C9
2	H	902	LMT	C2-C3-C4-C5
2	F	902	LMT	O1'-C1-C2-C3
2	H	902	LMT	C11-C10-C9-C8
2	H	903	LMT	C6-C7-C8-C9
2	F	902	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
2	H	902	LMT	C6-C7-C8-C9
2	H	902	LMT	C7-C8-C9-C10
2	E	901	LMT	C11-C10-C9-C8
2	E	901	LMT	C1-C2-C3-C4
2	G	902	LMT	C1-C2-C3-C4
2	E	901	LMT	C5-C6-C7-C8
2	H	901	LMT	O5'-C5'-C6'-O6'
2	H	901	LMT	C1-C2-C3-C4
2	H	902	LMT	C3-C4-C5-C6
2	G	901	LMT	C1-C2-C3-C4
2	G	901	LMT	C5-C6-C7-C8
2	G	902	LMT	C5-C6-C7-C8
2	H	901	LMT	C7-C8-C9-C10
2	H	903	LMT	C1-C2-C3-C4
2	G	902	LMT	C11-C10-C9-C8
2	F	901	LMT	C1-C2-C3-C4
2	H	903	LMT	C7-C8-C9-C10
2	F	901	LMT	C6-C7-C8-C9
2	H	902	LMT	C4B-C5B-C6B-O6B
2	F	901	LMT	C2-C3-C4-C5
2	F	902	LMT	C5-C6-C7-C8
2	E	901	LMT	C6-C7-C8-C9
2	F	901	LMT	C9-C10-C11-C12
2	E	901	LMT	C5'-C4'-O1B-C1B
2	G	902	LMT	C7-C8-C9-C10
2	H	902	LMT	C2'-C1'-O1'-C1
2	F	901	LMT	C11-C10-C9-C8
2	G	902	LMT	C4'-C5'-C6'-O6'
2	F	902	LMT	C9-C10-C11-C12
2	H	903	LMT	C2-C3-C4-C5
2	F	902	LMT	C4B-C5B-C6B-O6B
2	G	902	LMT	C3'-C4'-O1B-C1B
2	E	901	LMT	C2-C1-O1'-C1'
2	G	901	LMT	C2-C1-O1'-C1'
2	H	903	LMT	O1'-C1-C2-C3
2	H	902	LMT	C9-C10-C11-C12
2	F	901	LMT	C7-C8-C9-C10
2	H	902	LMT	O5B-C5B-C6B-O6B
2	H	902	LMT	C2-C1-O1'-C1'
2	G	901	LMT	C9-C10-C11-C12
2	H	903	LMT	C3-C4-C5-C6
2	E	901	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	F	902	LMT	C3-C4-C5-C6
2	F	901	LMT	C5'-C4'-O1B-C1B
2	G	901	LMT	O5'-C1'-O1'-C1
2	G	902	LMT	O5'-C5'-C6'-O6'
2	H	901	LMT	C11-C10-C9-C8
2	G	901	LMT	C2'-C1'-O1'-C1
2	E	901	LMT	C2-C3-C4-C5
2	G	901	LMT	C11-C10-C9-C8
2	G	901	LMT	C7-C8-C9-C10
2	F	901	LMT	C3'-C4'-O1B-C1B
2	F	902	LMT	C11-C10-C9-C8
2	H	901	LMT	C9-C10-C11-C12
2	G	902	LMT	C4B-C5B-C6B-O6B
2	G	902	LMT	C6-C7-C8-C9
2	H	901	LMT	C3-C4-C5-C6

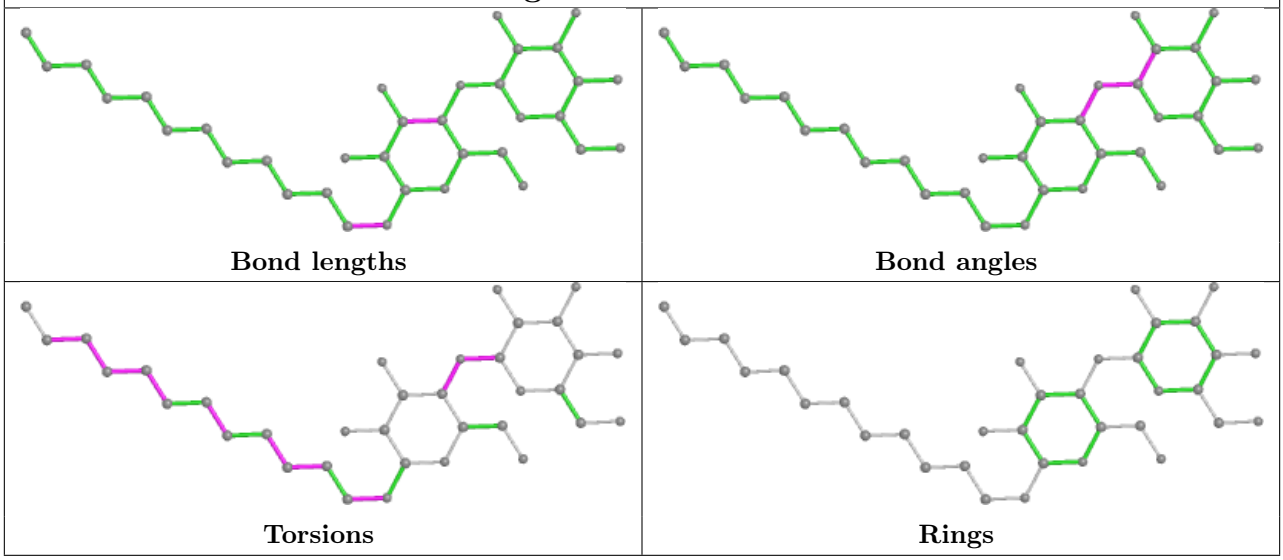
There are no ring outliers.

8 monomers are involved in 71 short contacts:

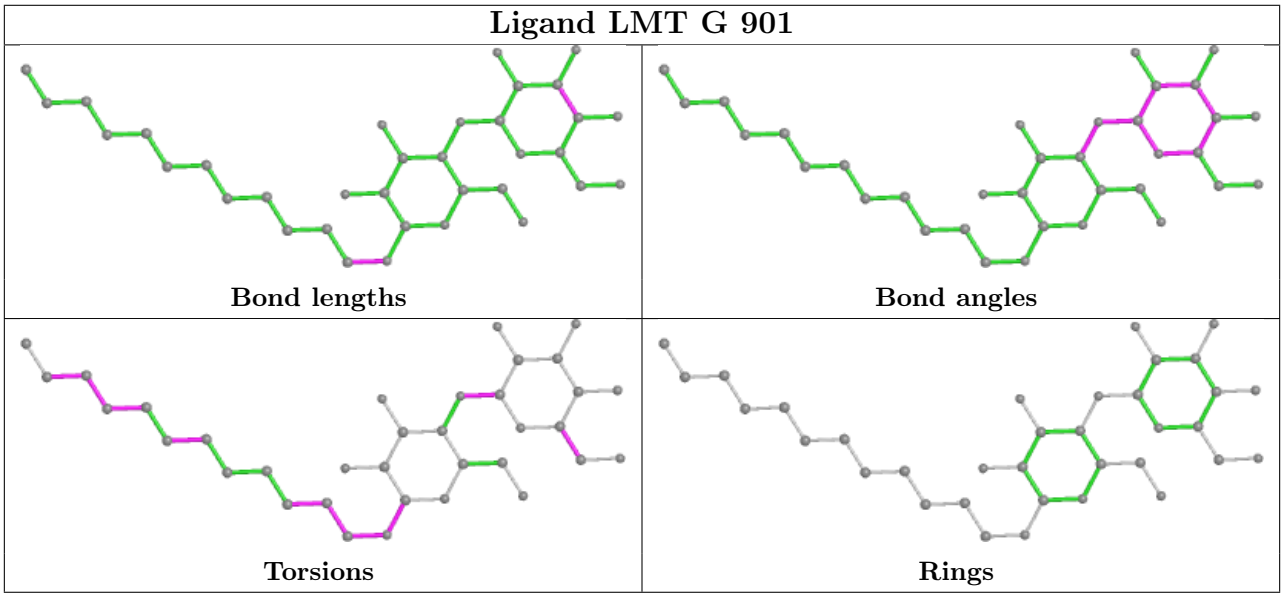
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	LMT	8	0
2	G	901	LMT	4	0
2	H	902	LMT	16	0
2	G	902	LMT	13	0
2	H	903	LMT	7	0
2	E	901	LMT	9	0
2	F	902	LMT	11	0
2	H	901	LMT	7	0

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.

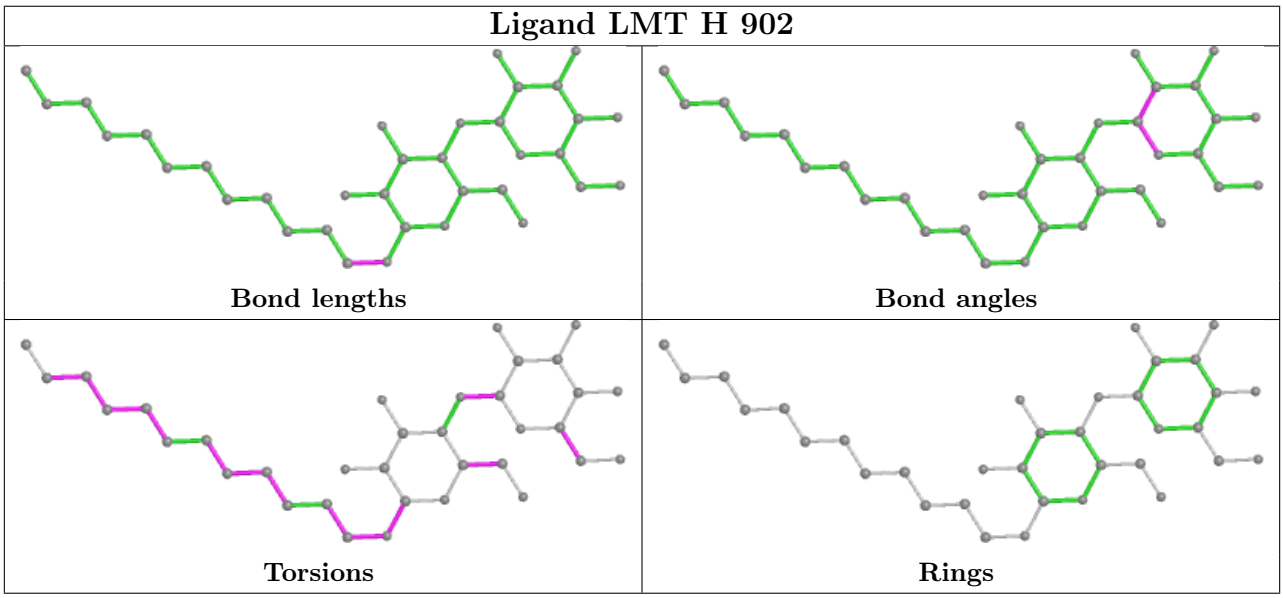
Ligand LMT F 901



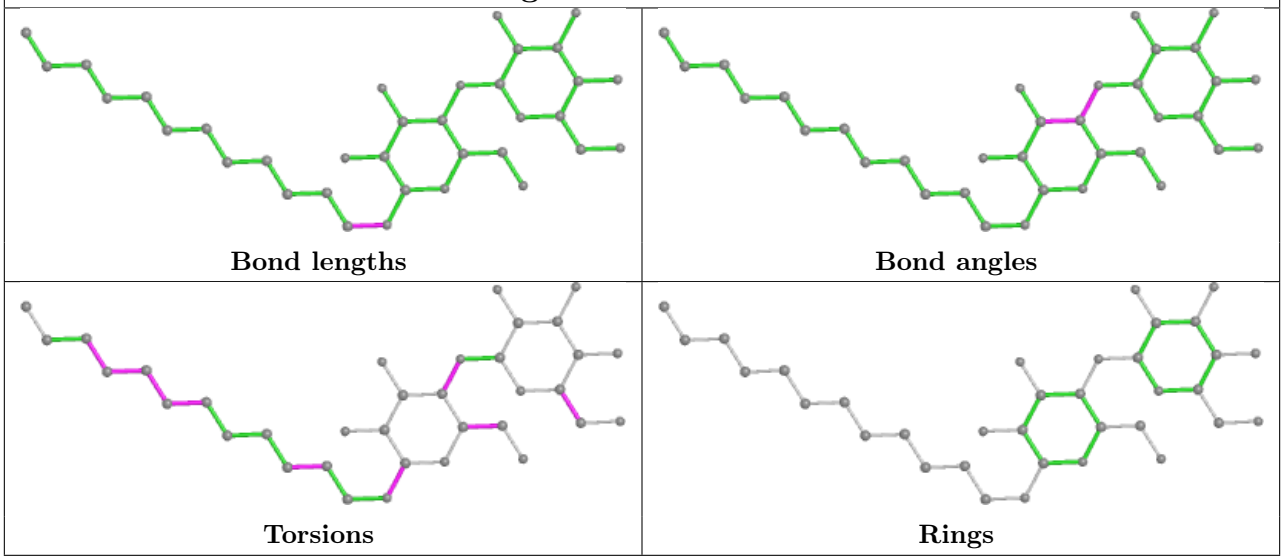
Ligand LMT G 901



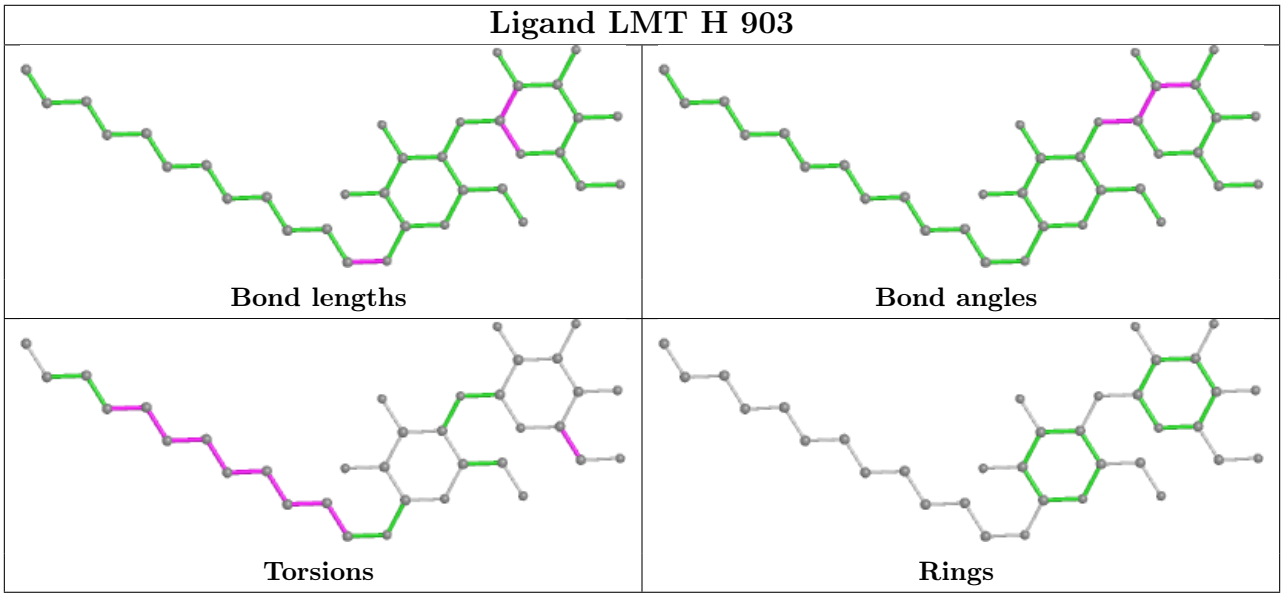
Ligand LMT H 902



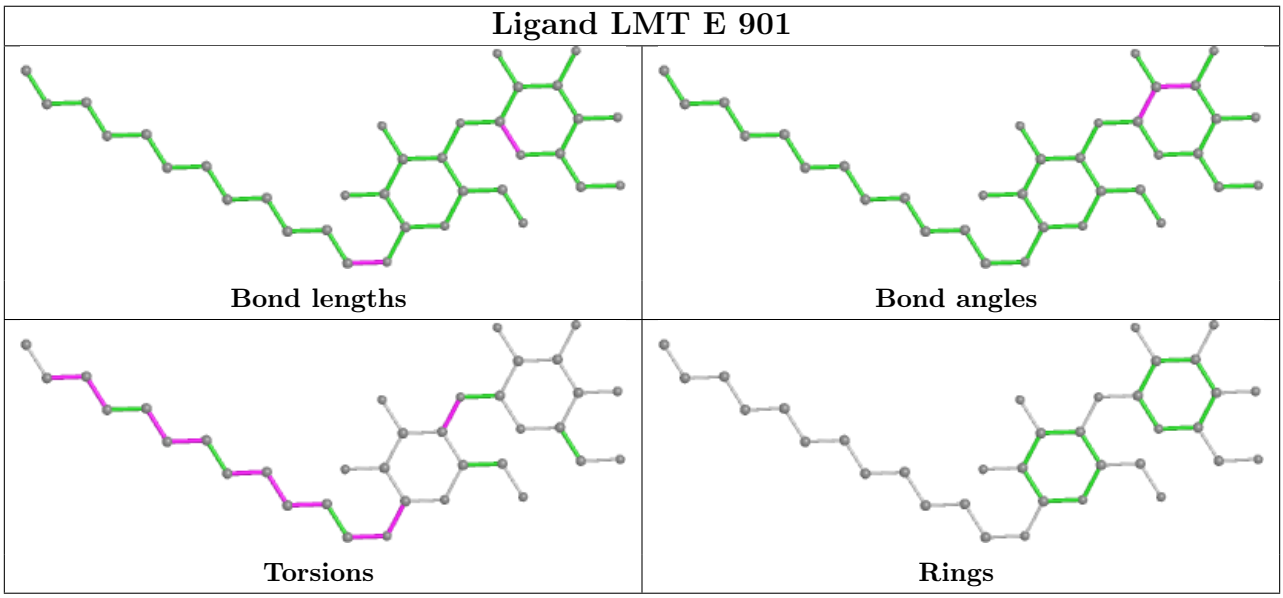
Ligand LMT G 902



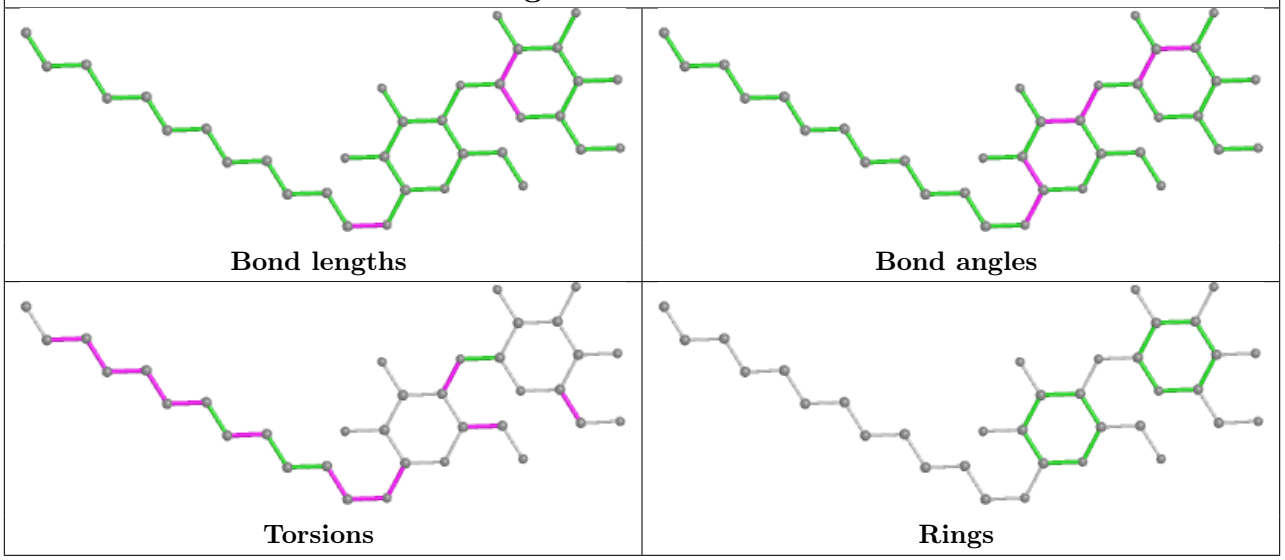
Ligand LMT H 903



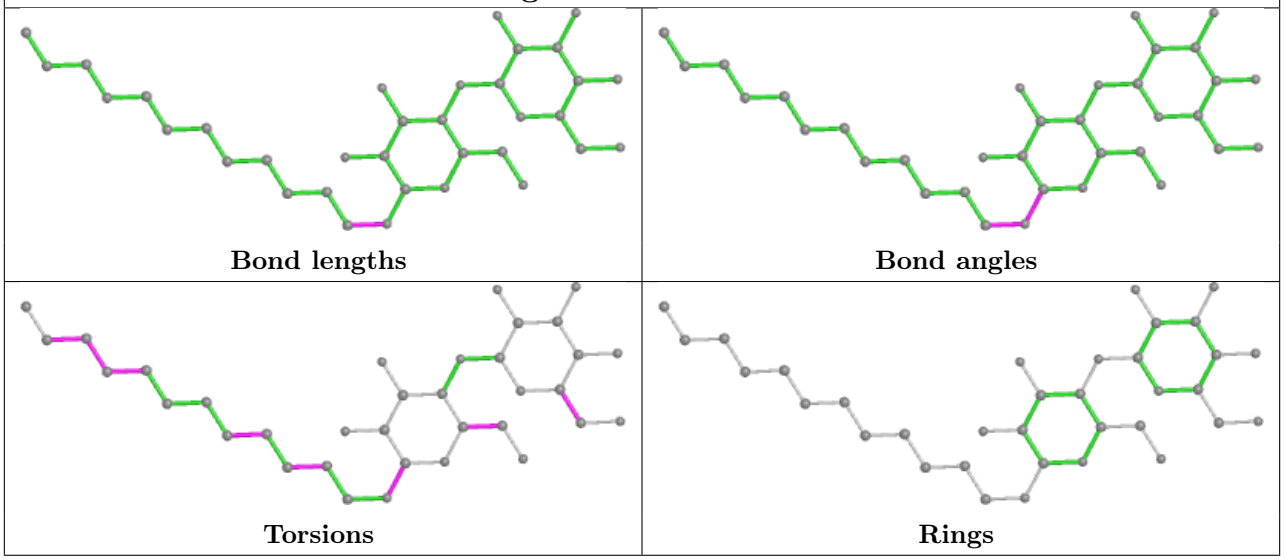
Ligand LMT E 901



Ligand LMT F 902



Ligand LMT H 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	264/343 (76%)	-0.69	3 (1%)	80	60	30, 45, 76, 122	0
1	B	334/343 (97%)	-0.49	6 (1%)	68	45	28, 56, 102, 130	0
1	C	264/343 (76%)	-0.67	3 (1%)	80	60	31, 47, 83, 127	0
1	D	332/343 (96%)	-0.50	7 (2%)	63	39	31, 57, 105, 134	0
1	E	270/343 (78%)	-0.71	2 (0%)	87	72	29, 52, 81, 109	0
1	F	332/343 (96%)	-0.53	10 (3%)	50	25	28, 50, 128, 148	0
1	G	267/343 (77%)	-0.69	2 (0%)	87	72	28, 50, 72, 118	0
1	H	333/343 (97%)	-0.44	16 (4%)	30	13	29, 49, 134, 151	0
All	All	2396/2744 (87%)	-0.58	49 (2%)	65	41	28, 51, 111, 151	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ASN	7.5
1	D	193	ASN	7.0
1	H	264	GLY	6.2
1	C	193	ASN	5.7
1	F	263	ALA	5.3
1	H	265	ALA	5.1
1	B	194	GLY	5.1
1	A	193	ASN	4.8
1	H	261	ALA	4.6
1	F	266	MET	4.6
1	H	275	GLY	4.5
1	F	267	ALA	4.3
1	H	263	ALA	4.3
1	H	266	MET	4.1
1	D	194	GLY	4.0
1	C	194	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	3.5
1	H	326	LYS	3.4
1	B	-5	VAL	3.3
1	H	304	GLY	3.0
1	D	192	ARG	3.0
1	G	-3	ASP	2.9
1	H	262	GLY	2.9
1	B	192	ARG	2.8
1	F	275	GLY	2.7
1	D	326	LYS	2.7
1	H	274	LYS	2.6
1	H	267	ALA	2.5
1	F	264	GLY	2.5
1	H	268	THR	2.5
1	H	276	GLU	2.5
1	B	196	ARG	2.4
1	F	304	GLY	2.4
1	H	303	GLY	2.4
1	G	-2	ASP	2.4
1	B	197	ASP	2.4
1	F	276	GLU	2.3
1	H	277	GLU	2.3
1	E	-4	ASP	2.3
1	E	-9	HIS	2.3
1	F	303	GLY	2.2
1	F	265	ALA	2.2
1	D	197	ASP	2.1
1	H	305	LYS	2.1
1	D	191	ASP	2.0
1	C	191	ASP	2.0
1	F	274	LYS	2.0
1	D	196	ARG	2.0
1	A	190	TYR	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

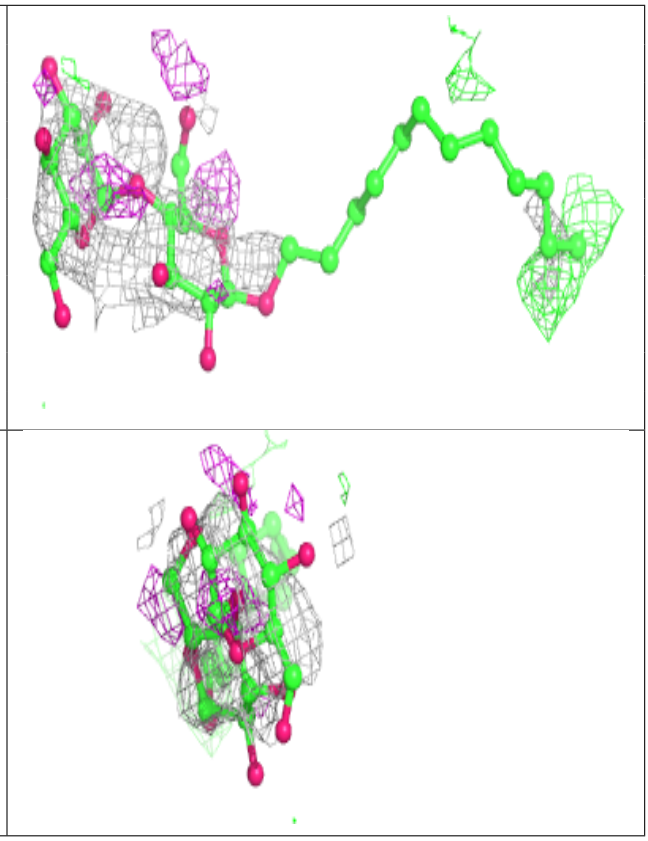
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	G	902	35/35	0.59	0.67	98,146,157,159	0
2	LMT	H	903	35/35	0.68	0.43	98,125,148,148	0
2	LMT	H	902	35/35	0.75	0.37	91,144,159,159	0
2	LMT	F	902	35/35	0.79	0.32	71,121,126,126	0
2	LMT	F	901	35/35	0.89	0.24	77,111,113,114	0
2	LMT	E	901	35/35	0.90	0.22	72,97,100,102	0
2	LMT	G	901	35/35	0.91	0.21	65,88,94,95	0
2	LMT	H	901	35/35	0.91	0.23	94,108,113,114	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.

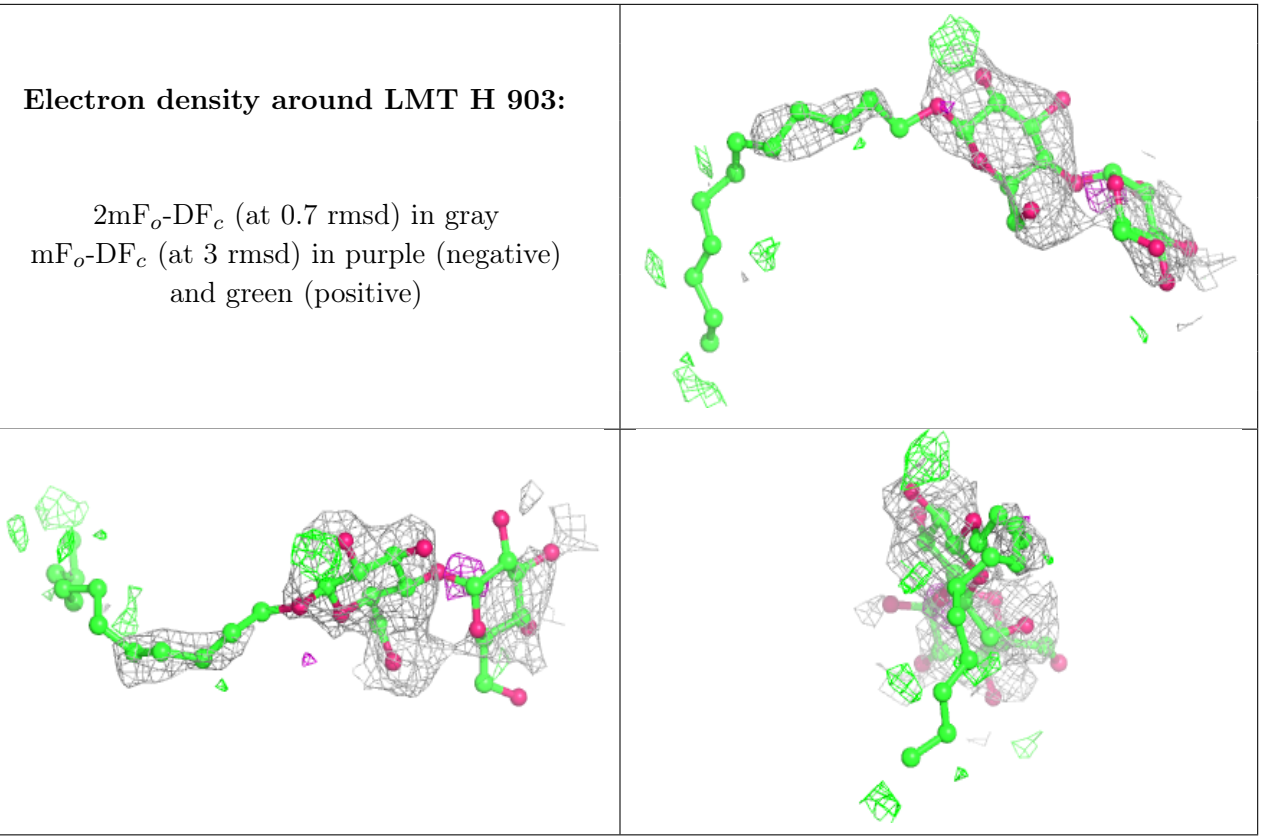
Electron density around LMT G 902:

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



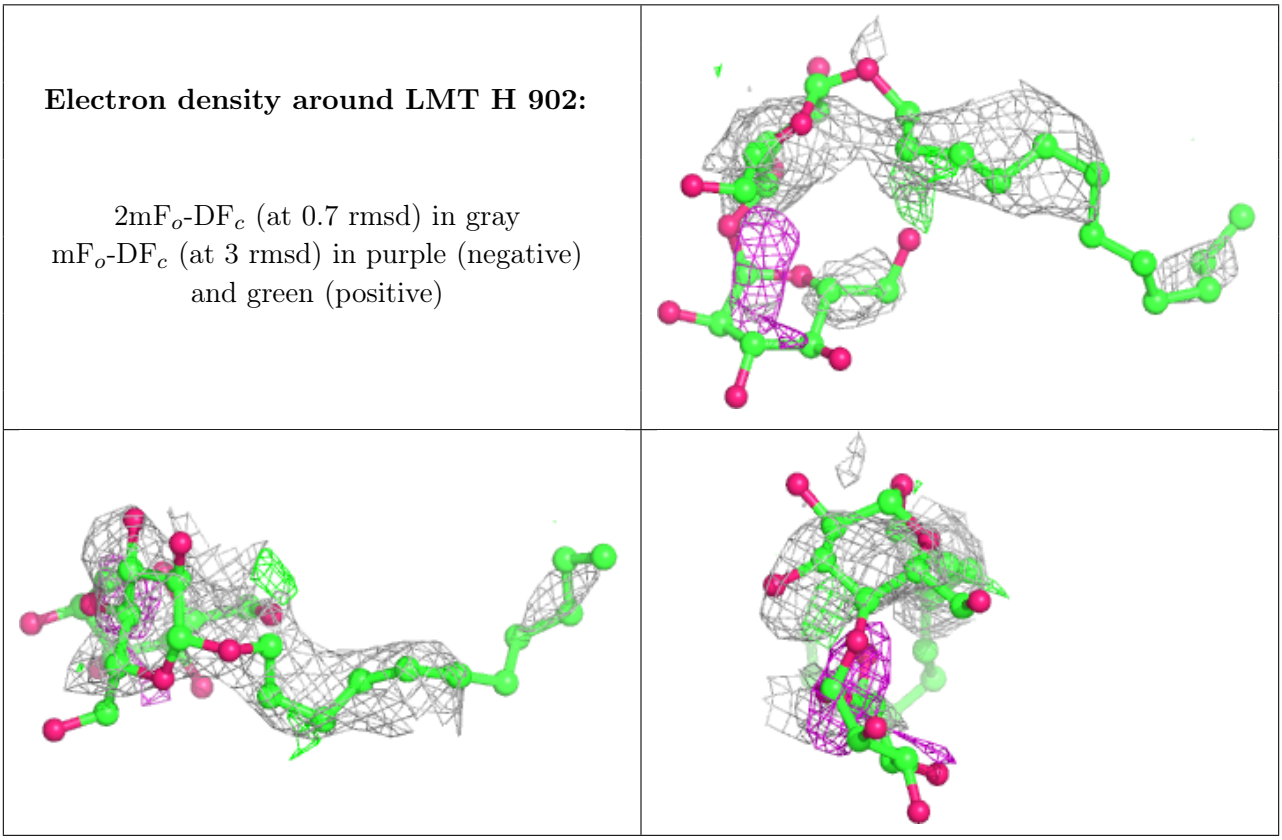
Electron density around LMT H 903:

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



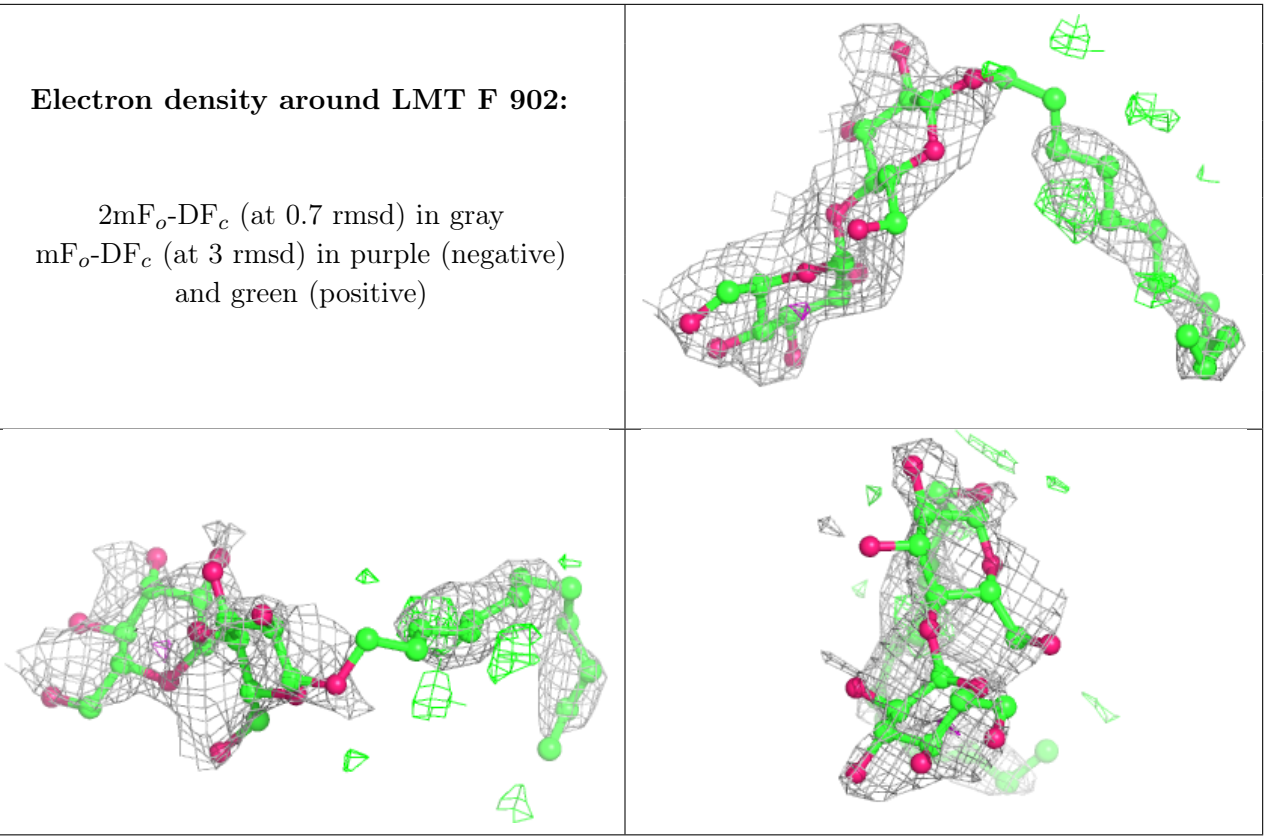
Electron density around LMT H 902:

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



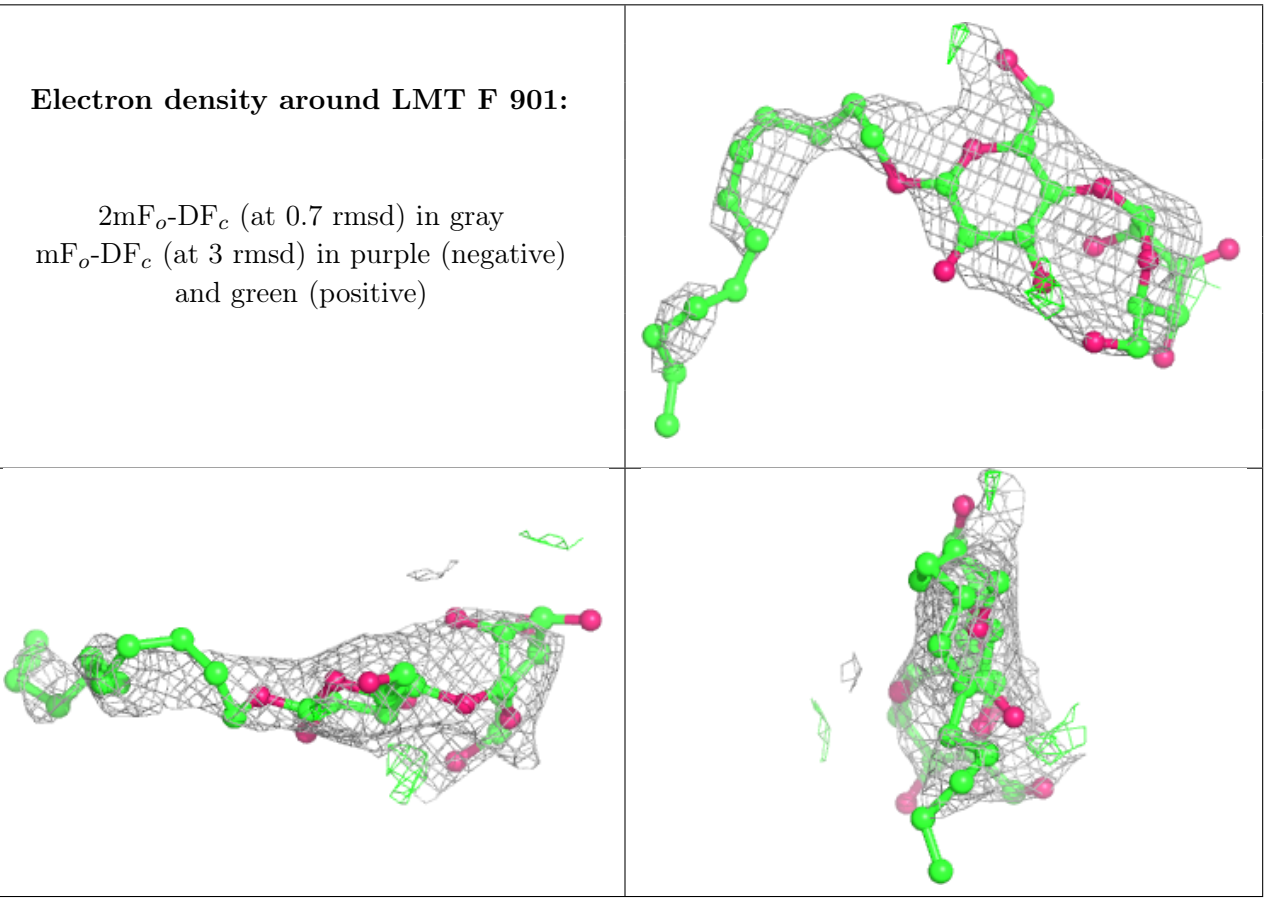
Electron density around LMT F 902:

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



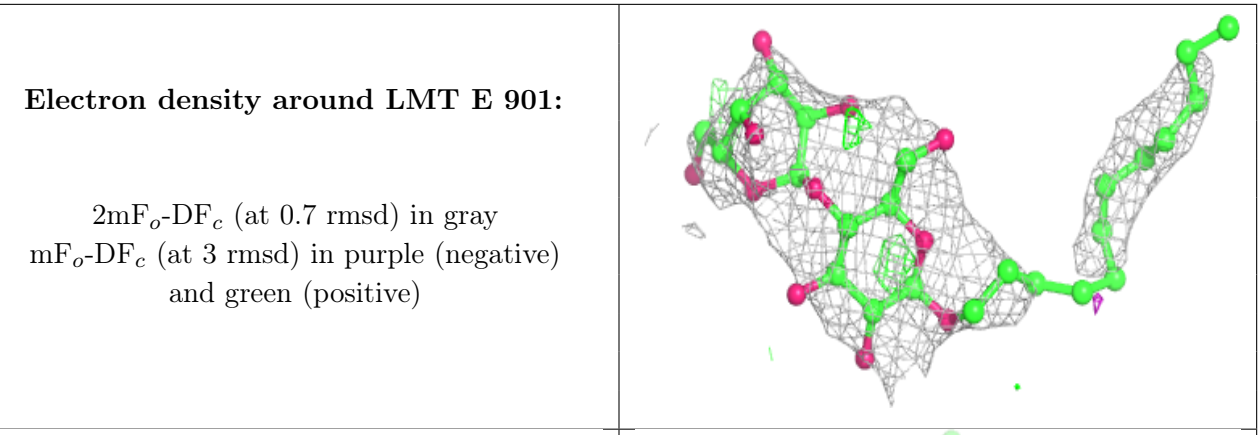
Electron density around LMT F 901:

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



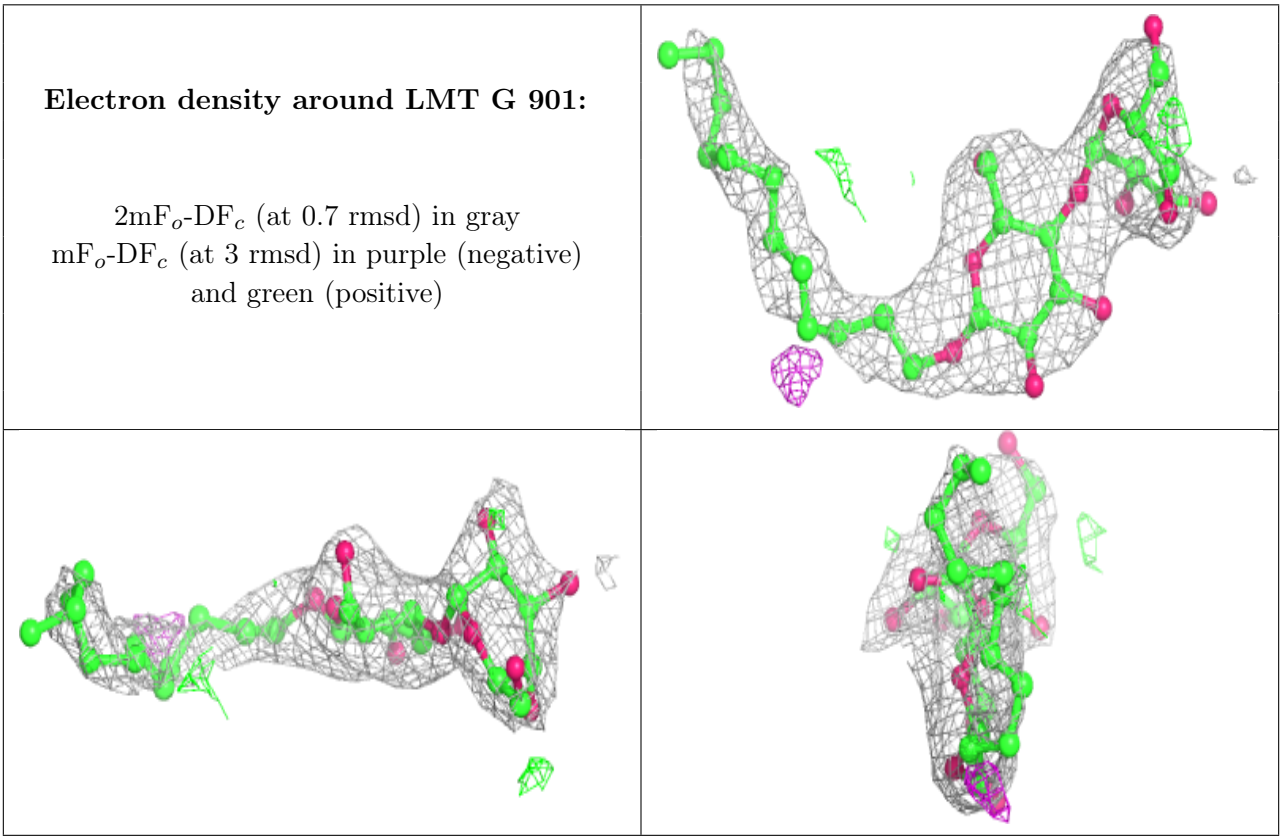
Electron density around LMT E 901:

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



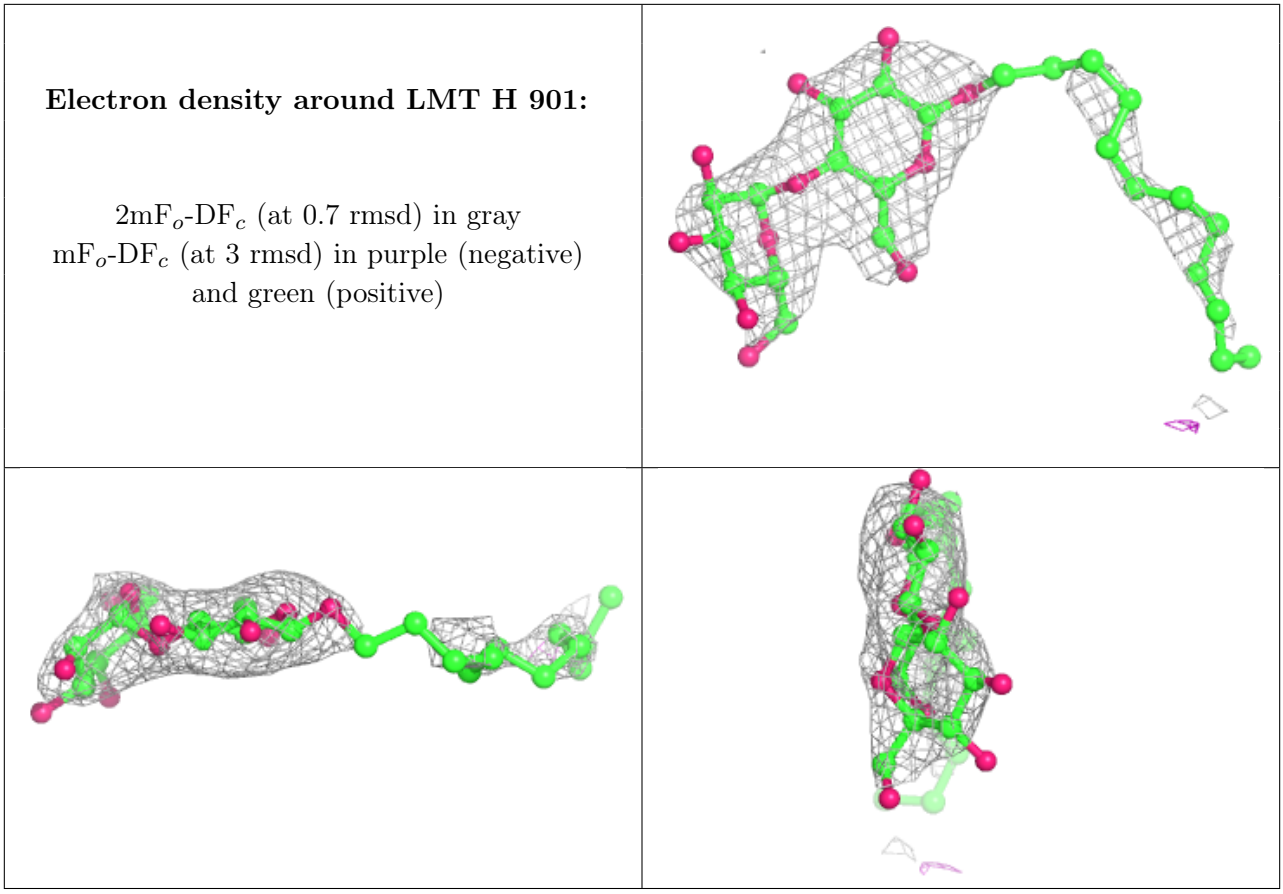
Electron density around LMT G 901:

$2mF_o$-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 H 901:

$2mF_o$-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

There are no such residues in this entry.