



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 08:09 PM BST

PDB ID : 6V4S
Title : A Closed pore conformation of a Pentameric ligand-gated ion channel with additional N-terminal domain
Authors : Delarue, M.; Hu, H.D.
Deposited on : 2019-11-29
Resolution : 3.55 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 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 : 2.13.1
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) : 2.13.1

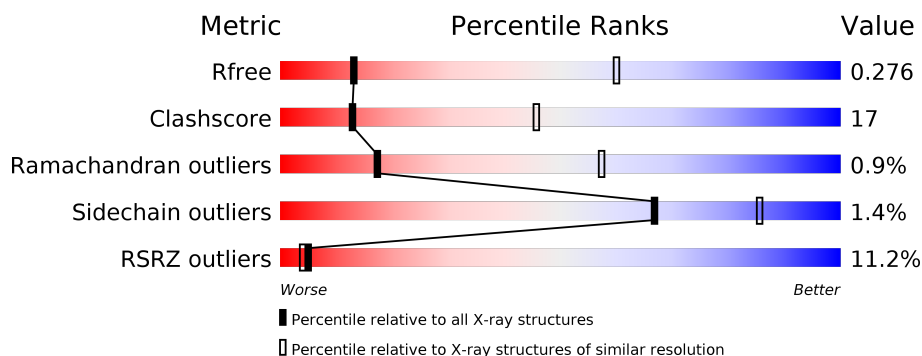
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	642	<div> <div>14%</div> <div> <div>61%</div> <div>27%</div> <div>• 9%</div> </div> </div>
1	B	642	<div> <div>7%</div> <div> <div>63%</div> <div>26%</div> <div>• 9%</div> </div> </div>
1	C	642	<div> <div>9%</div> <div> <div>64%</div> <div>25%</div> <div>• 8%</div> </div> </div>
1	D	642	<div> <div>10%</div> <div> <div>63%</div> <div>27%</div> <div>• 8%</div> </div> </div>
1	E	642	<div> <div>11%</div> <div> <div>63%</div> <div>26%</div> <div>• 8%</div> </div> </div>

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
3	NA	A	704	-	-	-	X
3	NA	B	702	-	-	-	X
4	CL	B	703	-	-	-	X
4	CL	E	702	-	-	-	X
5	LMT	B	706	-	-	-	X
5	LMT	C	706	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 23261 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 Neur_chan_LBD domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4576	2948	752	865	11			
1	E	591	Total	C	N	O	S	0	0	0
			4613	2972	758	872	11			
1	D	591	Total	C	N	O	S	0	0	0
			4613	2972	758	872	11			
1	C	588	Total	C	N	O	S	0	0	0
			4597	2960	756	870	11			
1	B	586	Total	C	N	O	S	0	0	0
			4584	2951	753	869	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	1	0
			1	1		
2	A	2	Total	Ca	2	0
			2	2		
2	C	1	Total	Ca	1	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	3	Total	Na	0	0
			3	3		
3	D	1	Total	Na	0	0
			1	1		

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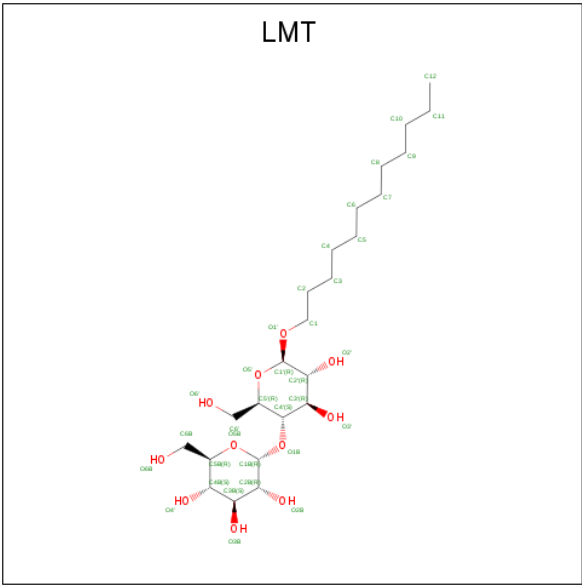
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Na	1	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	14	11		
5	E	1	Total	C	O	0	0
			25	14	11		
5	E	1	Total	C	O	0	0
			25	14	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 25 14 11	0	0
5	D	1	Total C O 26 15 11	0	0
5	C	1	Total C O 25 14 11	0	0
5	C	1	Total C O 27 16 11	0	0
5	B	1	Total C O 25 14 11	0	0
5	B	1	Total C O 26 15 11	0	0
5	B	1	Total C O 27 16 11	0	0

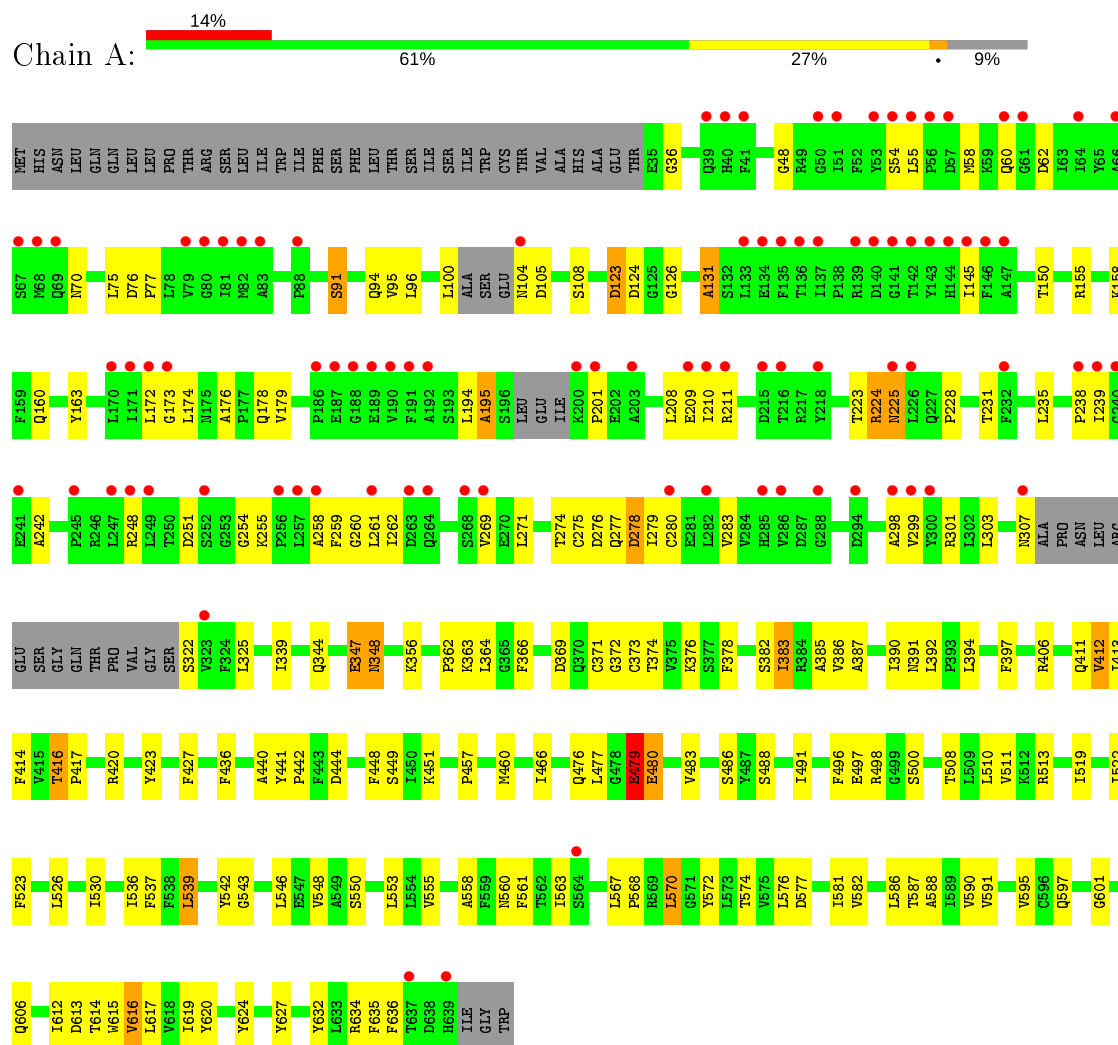
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0
6	E	1	Total O 1 1	0	0
6	D	1	Total O 1 1	0	0
6	C	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0

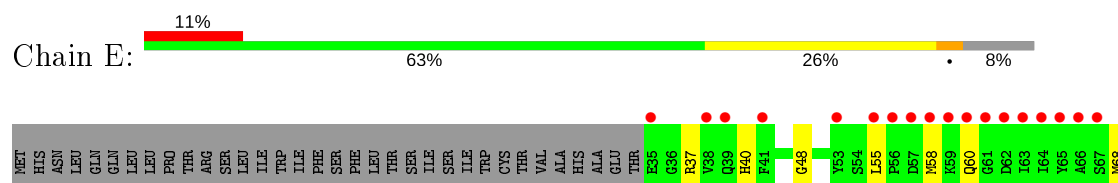
3 Residue-property plots

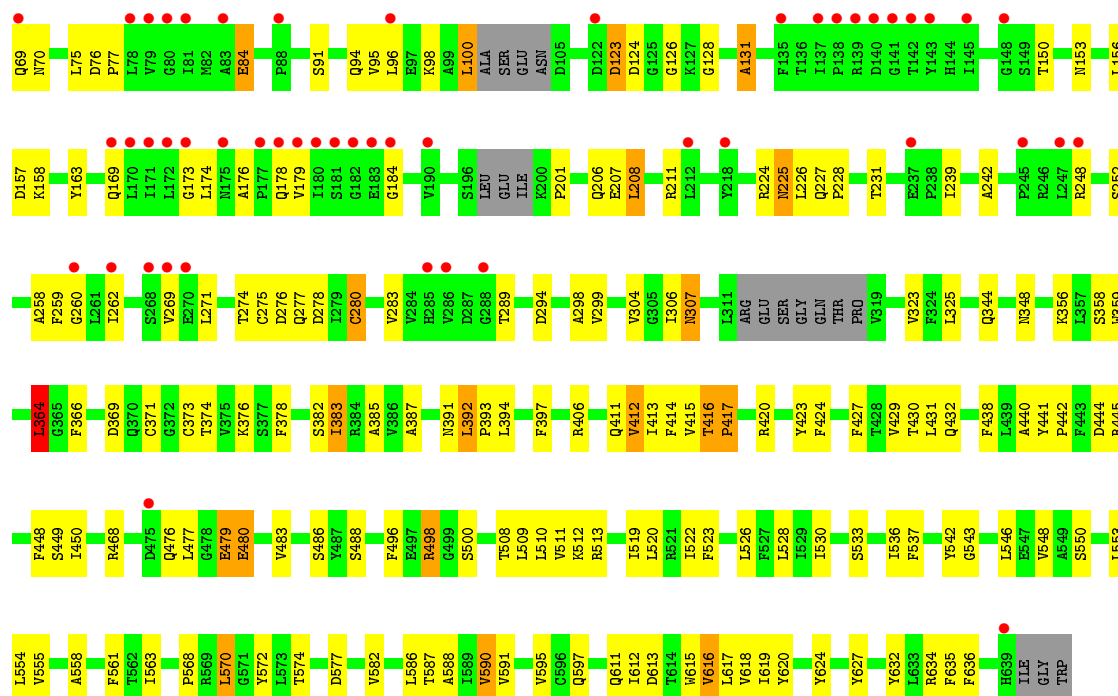
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Neur_chan_LBD domain-containing protein

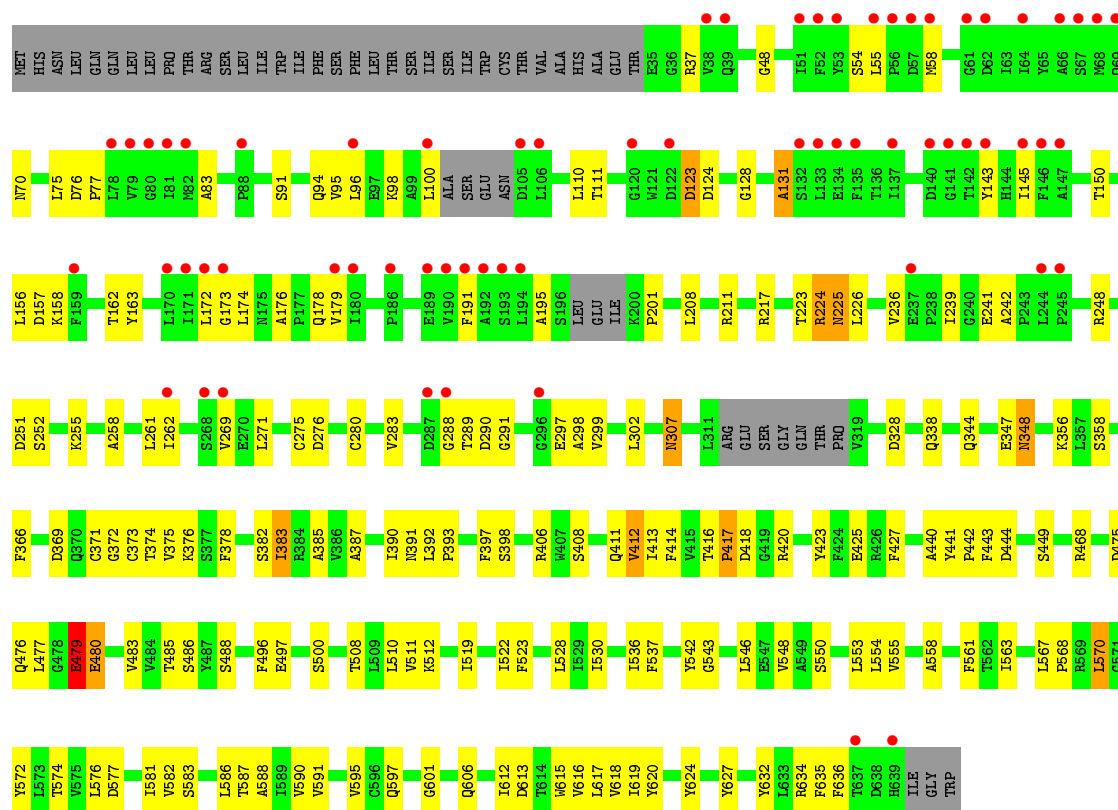


- Molecule 1: Neur_chan_LBD domain-containing protein

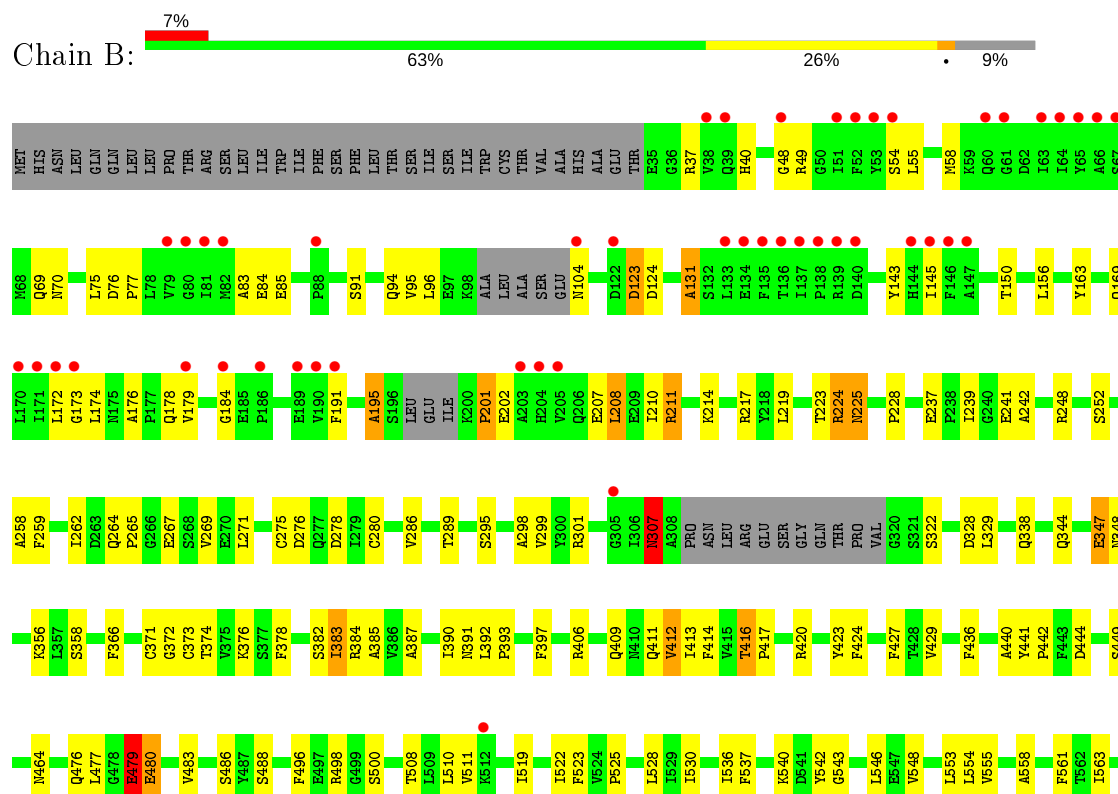




• Molecule 1: Neur_chan_LBD domain-containing protein



• Molecule 1: Neur_chan_LBD domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	159.41Å 337.25Å 111.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 3.55 48.04 – 3.55	Depositor EDS
% Data completeness (in resolution range)	89.0 (48.04-3.55) 89.1 (48.04-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.194 , 0.268 0.206 , 0.276	Depositor DCC
R_{free} test set	3250 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	94.2	Xtriage
Anisotropy	0.916	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23261	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, LMT, CL

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	0.86	4/4678 (0.1%)	1.14	25/6365 (0.4%)
1	B	0.86	3/4687 (0.1%)	1.09	18/6377 (0.3%)
1	C	0.85	2/4700 (0.0%)	1.17	29/6396 (0.5%)
1	D	0.86	4/4716 (0.1%)	1.10	17/6418 (0.3%)
1	E	0.87	1/4716 (0.0%)	1.11	19/6418 (0.3%)
All	All	0.86	14/23497 (0.1%)	1.12	108/31974 (0.3%)

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	5
1	B	0	4
1	C	0	5
1	D	0	4
1	E	0	4
All	All	0	22

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	TYR	CE1-CZ	6.46	1.47	1.38
1	E	620	TYR	CE1-CZ	6.37	1.46	1.38
1	C	620	TYR	CE1-CZ	6.08	1.46	1.38
1	B	620	TYR	CE1-CZ	6.02	1.46	1.38
1	A	457	PRO	N-CD	-5.92	1.39	1.47
1	D	620	TYR	CE1-CZ	5.89	1.46	1.38
1	A	238	PRO	N-CD	5.88	1.56	1.47
1	B	328	ASP	CB-CG	5.79	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	347	GLU	CD-OE1	-5.50	1.19	1.25
1	D	328	ASP	CB-CG	5.19	1.62	1.51
1	D	479	GLU	CG-CD	5.13	1.59	1.51
1	A	36	GLY	N-CA	5.03	1.53	1.46
1	C	328	ASP	CB-CG	5.03	1.62	1.51
1	B	84	GLU	N-CA	5.01	1.56	1.46

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	ARG	NE-CZ-NH2	27.52	134.06	120.30
1	A	513	ARG	NE-CZ-NH2	17.31	128.95	120.30
1	A	513	ARG	NE-CZ-NH1	-14.66	112.97	120.30
1	B	84	GLU	N-CA-C	10.67	139.81	111.00
1	C	513	ARG	NH1-CZ-NH2	-10.03	108.37	119.40
1	C	84	GLU	N-CA-C	9.85	137.60	111.00
1	E	84	GLU	N-CA-C	9.30	136.12	111.00
1	E	392	LEU	CA-CB-CG	8.85	135.66	115.30
1	E	416	THR	C-N-CD	-8.74	101.36	120.60
1	A	195	ALA	N-CA-CB	8.69	122.26	110.10
1	B	416	THR	C-N-CD	-8.47	101.96	120.60
1	C	416	THR	C-N-CD	-8.33	102.27	120.60
1	D	347	GLU	OE1-CD-OE2	-8.31	113.33	123.30
1	A	416	THR	C-N-CD	-7.93	103.16	120.60
1	C	217	ARG	CA-CB-CG	7.55	130.01	113.40
1	D	347	GLU	CG-CD-OE2	7.54	133.39	118.30
1	C	106	LEU	CB-CG-CD2	7.38	123.55	111.00
1	C	498	ARG	N-CA-CB	-7.11	97.81	110.60
1	C	225	ASN	N-CA-C	7.08	130.12	111.00
1	A	225	ASN	N-CA-C	7.00	129.90	111.00
1	E	364	LEU	N-CA-C	-6.98	92.14	111.00
1	E	225	ASN	N-CA-C	6.95	129.75	111.00
1	D	225	ASN	N-CA-C	6.93	129.72	111.00
1	B	225	ASN	N-CA-C	6.92	129.69	111.00
1	C	201	PRO	N-CA-CB	6.89	111.56	103.30
1	B	570	LEU	N-CA-C	-6.70	92.92	111.00
1	C	497	GLU	N-CA-C	6.68	129.05	111.00
1	D	570	LEU	N-CA-C	-6.68	92.97	111.00
1	C	570	LEU	N-CA-C	-6.66	93.01	111.00
1	A	570	LEU	N-CA-C	-6.63	93.09	111.00
1	E	275	CYS	N-CA-C	6.62	128.88	111.00
1	E	420	ARG	NE-CZ-NH1	-6.62	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	ASP	CB-CA-C	-6.59	97.23	110.40
1	A	275	CYS	N-CA-C	6.58	128.75	111.00
1	E	570	LEU	N-CA-C	-6.55	93.33	111.00
1	A	412	VAL	CB-CA-C	-6.46	99.13	111.40
1	B	412	VAL	CB-CA-C	-6.44	99.16	111.40
1	C	480	GLU	N-CA-C	6.37	128.20	111.00
1	D	201	PRO	N-CA-CB	6.36	110.93	103.30
1	D	412	VAL	CB-CA-C	-6.31	99.42	111.40
1	E	412	VAL	CB-CA-C	-6.30	99.42	111.40
1	B	280	CYS	N-CA-C	-6.28	94.05	111.00
1	B	480	GLU	N-CA-C	6.26	127.89	111.00
1	C	412	VAL	CB-CA-C	-6.25	99.53	111.40
1	D	480	GLU	N-CA-C	6.17	127.66	111.00
1	D	226	LEU	CA-CB-CG	6.14	129.44	115.30
1	E	480	GLU	N-CA-C	6.13	127.56	111.00
1	C	490	GLU	N-CA-C	6.11	127.51	111.00
1	A	634	ARG	CG-CD-NE	6.07	124.55	111.80
1	A	480	GLU	N-CA-C	6.07	127.38	111.00
1	B	634	ARG	CG-CD-NE	6.05	124.50	111.80
1	C	280	CYS	N-CA-C	-6.04	94.68	111.00
1	D	280	CYS	N-CA-C	-6.04	94.69	111.00
1	E	280	CYS	N-CA-C	-6.04	94.70	111.00
1	C	634	ARG	CG-CD-NE	5.98	124.36	111.80
1	A	460	MET	CG-SD-CE	5.97	109.75	100.20
1	A	280	CYS	N-CA-CB	5.90	121.22	110.60
1	E	280	CYS	CA-CB-SG	5.89	124.61	114.00
1	C	497	GLU	CA-C-N	5.86	130.09	117.20
1	E	634	ARG	CG-CD-NE	5.83	124.03	111.80
1	D	634	ARG	CG-CD-NE	5.80	123.99	111.80
1	D	290	ASP	CB-CA-C	-5.79	98.82	110.40
1	C	217	ARG	N-CA-C	5.78	126.59	111.00
1	A	479	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	275	CYS	N-CA-C	5.71	126.41	111.00
1	D	275	CYS	N-CA-C	5.70	126.39	111.00
1	C	276	ASP	N-CA-C	5.70	126.38	111.00
1	E	276	ASP	N-CA-C	5.68	126.34	111.00
1	B	211	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	276	ASP	N-CA-C	5.66	126.29	111.00
1	D	276	ASP	N-CA-C	5.65	126.25	111.00
1	C	479	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	A	451	LYS	CD-CE-NZ	5.61	124.60	111.70
1	C	275	CYS	N-CA-C	5.58	126.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	C	123	ASP	N-CA-C	5.53	125.94	111.00
1	A	276	ASP	N-CA-C	5.47	125.76	111.00
1	E	498	ARG	CA-CB-CG	5.46	125.42	113.40
1	A	347	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	C	490	GLU	N-CA-CB	-5.40	100.88	110.60
1	B	85	GLU	N-CA-CB	5.37	120.27	110.60
1	A	280	CYS	N-CA-C	-5.37	96.51	111.00
1	D	123	ASP	N-CA-C	5.37	125.49	111.00
1	E	123	ASP	N-CA-C	5.35	125.45	111.00
1	A	155	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	330	VAL	CA-CB-CG1	5.32	118.89	110.90
1	B	123	ASP	N-CA-C	5.32	125.36	111.00
1	B	347	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	A	261	LEU	CB-CG-CD1	5.27	119.96	111.00
1	C	498	ARG	CB-CA-C	5.27	120.94	110.40
1	C	328	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	211	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	E	208	LEU	N-CA-C	-5.25	96.84	111.00
1	A	123	ASP	N-CA-C	5.22	125.11	111.00
1	B	620	TYR	C-N-CD	5.22	139.36	128.40
1	A	420	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	420	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	D	479	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	364	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	328	ASP	CB-CG-OD1	5.14	122.92	118.30
1	E	513	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	620	TYR	C-N-CD	5.11	139.14	128.40
1	B	328	ASP	CB-CA-C	5.11	120.62	110.40
1	C	535	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	E	616	VAL	N-CA-C	5.08	124.72	111.00
1	B	208	LEU	N-CA-C	-5.06	97.33	111.00
1	B	479	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	A	616	VAL	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASP	Peptide
1	A	224	ARG	Peptide
1	A	278	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	322	SER	Mainchain,Peptide
1	B	104	ASN	Peptide
1	B	123	ASP	Peptide
1	B	195	ALA	Peptide
1	B	224	ARG	Peptide
1	C	123	ASP	Peptide
1	C	217	ARG	Peptide
1	C	224	ARG	Peptide
1	C	321	SER	Peptide
1	C	497	GLU	Peptide
1	D	123	ASP	Peptide
1	D	224	ARG	Peptide
1	D	297	GLU	Peptide
1	D	475	ASP	Peptide
1	E	123	ASP	Peptide
1	E	224	ARG	Peptide
1	E	294	ASP	Peptide
1	E	364	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4576	0	4462	154	0
1	B	4584	0	4469	171	3
1	C	4597	0	4484	171	3
1	D	4613	0	4502	159	3
1	E	4613	0	4502	165	3
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	25	0	23	0	0
5	B	78	0	75	10	0
5	C	52	0	50	0	0
5	D	26	0	25	0	0
5	E	75	0	69	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
All	All	23261	0	22661	759	6

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 17.

All (759) 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:476:GLN:CB	1:C:479:GLU:OE1	1.66	1.42
1:E:207:GLU:O	1:E:208:LEU:CD1	1.77	1.32
1:C:476:GLN:HB2	1:C:479:GLU:OE1	1.21	1.27
1:C:530:ILE:HD13	1:C:624:TYR:CE2	1.70	1.27
1:C:416:THR:OG1	1:C:417:PRO:HD2	1.12	1.23
1:B:530:ILE:HD13	1:B:624:TYR:CE2	1.77	1.19
1:B:416:THR:OG1	1:B:417:PRO:HD2	1.05	1.18
1:B:416:THR:OG1	1:B:417:PRO:CD	1.96	1.14
1:C:476:GLN:HB3	1:C:479:GLU:OE1	1.48	1.13
1:A:416:THR:HB	1:A:417:PRO:HD2	1.11	1.11
1:E:416:THR:CB	1:E:417:PRO:HD2	1.69	1.07
1:C:416:THR:OG1	1:C:417:PRO:CD	2.04	1.06
1:B:416:THR:CB	1:B:417:PRO:HD2	1.75	1.05
1:E:416:THR:HB	1:E:417:PRO:HD2	1.09	1.04
1:E:207:GLU:C	1:E:208:LEU:HD12	1.77	1.03
1:B:344:GLN:HE22	1:B:568:PRO:HG3	1.22	1.01
1:C:344:GLN:HE22	1:C:568:PRO:HG3	1.25	1.01
1:C:416:THR:CB	1:C:417:PRO:HD2	1.80	1.00
1:C:530:ILE:CD1	1:C:624:TYR:HE2	1.74	0.99
1:A:344:GLN:HE22	1:A:568:PRO:HG3	1.21	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:GLU:O	1:E:208:LEU:HD12	0.81	0.98
1:E:289:THR:HG22	1:E:289:THR:O	1.61	0.97
1:D:416:THR:OG1	1:D:417:PRO:HD2	1.63	0.97
1:A:416:THR:CB	1:A:417:PRO:HD2	1.75	0.97
1:E:344:GLN:HE22	1:E:568:PRO:HG3	1.32	0.94
1:B:530:ILE:CD1	1:B:624:TYR:HE2	1.80	0.94
1:D:344:GLN:HE22	1:D:568:PRO:HG3	1.34	0.93
1:C:211:ARG:HG2	1:C:299:VAL:CG2	1.99	0.93
1:E:498:ARG:HE	1:D:414:PHE:HE2	0.97	0.93
1:C:530:ILE:HD13	1:C:624:TYR:HE2	1.12	0.92
1:B:599:ARG:HG2	5:B:706:LMT:O4'	1.70	0.91
1:C:476:GLN:HB3	1:C:479:GLU:CD	1.91	0.91
1:C:476:GLN:CB	1:C:479:GLU:CD	2.38	0.91
1:A:555:VAL:HG11	1:B:553:LEU:HD23	1.54	0.89
1:E:498:ARG:NE	1:D:414:PHE:HE2	1.71	0.89
1:A:194:LEU:O	1:A:194:LEU:HD12	1.72	0.89
1:C:553:LEU:HD23	1:B:555:VAL:HG11	1.53	0.88
1:B:530:ILE:HD13	1:B:624:TYR:HE2	1.20	0.88
1:D:553:LEU:HD23	1:C:555:VAL:HG11	1.54	0.88
1:A:553:LEU:HD23	1:E:555:VAL:HG11	1.56	0.87
1:B:391:ASN:O	1:B:392:LEU:HD12	1.75	0.86
1:A:466:ILE:HG23	1:A:491:ILE:HD11	1.58	0.85
1:E:416:THR:HB	1:E:417:PRO:CD	2.03	0.85
1:C:211:ARG:HG2	1:C:299:VAL:HG23	1.56	0.85
1:E:553:LEU:HD23	1:D:555:VAL:HG11	1.56	0.84
1:A:62:ASP:HB3	1:A:174:LEU:HD11	1.60	0.83
1:E:526:LEU:O	1:E:530:ILE:HD12	1.80	0.82
1:D:289:THR:O	1:D:289:THR:HG22	1.81	0.80
1:A:441:TYR:HB3	1:A:574:THR:OG1	1.81	0.80
1:D:441:TYR:HB3	1:D:574:THR:OG1	1.82	0.80
1:E:441:TYR:HB3	1:E:574:THR:OG1	1.82	0.80
1:A:344:GLN:NE2	1:A:568:PRO:HG3	1.98	0.79
1:E:289:THR:CG2	1:E:289:THR:O	2.29	0.79
1:C:441:TYR:HB3	1:C:574:THR:OG1	1.82	0.79
1:B:599:ARG:CG	5:B:706:LMT:O4'	2.31	0.79
1:A:371:CYS:SG	1:A:373:CYS:N	2.56	0.79
1:E:498:ARG:NE	1:D:414:PHE:CE2	2.46	0.78
1:C:530:ILE:CD1	1:C:624:TYR:CE2	2.54	0.78
1:C:371:CYS:SG	1:C:373:CYS:N	2.57	0.78
1:D:391:ASN:O	1:D:392:LEU:HD12	1.84	0.78
1:E:371:CYS:SG	1:E:373:CYS:N	2.57	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:HE22	1:B:568:PRO:CG	1.97	0.77
1:B:344:GLN:NE2	1:B:568:PRO:HG3	1.98	0.77
1:A:526:LEU:O	1:A:530:ILE:HD12	1.85	0.77
1:B:441:TYR:HB3	1:B:574:THR:OG1	1.83	0.77
1:E:226:LEU:HB2	1:E:280:CYS:SG	2.25	0.77
1:C:289:THR:O	1:C:289:THR:HG22	1.84	0.77
1:B:496:PHE:N	1:B:500:SER:O	2.18	0.76
1:B:441:TYR:HE2	1:B:567:LEU:HD12	1.51	0.76
1:D:371:CYS:SG	1:D:373:CYS:N	2.57	0.76
1:D:441:TYR:HE2	1:D:567:LEU:HD22	1.49	0.76
1:B:371:CYS:SG	1:B:373:CYS:N	2.57	0.76
1:C:496:PHE:N	1:C:500:SER:O	2.18	0.76
1:A:441:TYR:HE2	1:A:567:LEU:HD12	1.52	0.75
1:C:344:GLN:NE2	1:C:568:PRO:HG3	2.01	0.75
1:E:364:LEU:HD22	1:E:415:VAL:HG11	1.68	0.75
1:E:304:VAL:HG13	1:E:323:VAL:HG11	1.68	0.74
1:A:496:PHE:N	1:A:500:SER:O	2.19	0.74
1:B:416:THR:HG1	1:B:417:PRO:HD2	1.48	0.74
1:C:416:THR:HG1	1:C:417:PRO:HD2	1.51	0.74
1:D:496:PHE:N	1:D:500:SER:O	2.19	0.74
1:B:211:ARG:HG2	1:B:299:VAL:HG23	1.70	0.74
1:A:614:THR:HG21	5:B:706:LMT:H32	1.68	0.74
1:C:476:GLN:O	1:C:479:GLU:HG2	1.87	0.74
1:A:416:THR:HB	1:A:417:PRO:CD	2.06	0.73
1:A:344:GLN:HE22	1:A:568:PRO:CG	2.01	0.73
1:E:496:PHE:N	1:E:500:SER:O	2.19	0.73
1:C:227:GLN:HB3	1:C:228:PRO:HD2	1.70	0.73
1:B:211:ARG:HG2	1:B:299:VAL:CG2	2.20	0.72
1:C:211:ARG:HG2	1:C:299:VAL:HG21	1.71	0.72
1:C:258:ALA:CB	1:C:271:LEU:HD11	2.20	0.71
1:D:530:ILE:HD11	1:D:583:SER:OG	1.89	0.71
1:A:283:VAL:HG11	1:E:156:LEU:HD22	1.71	0.71
1:B:289:THR:O	1:B:289:THR:HG22	1.90	0.71
1:B:546:LEU:HD11	1:B:595:VAL:CG2	2.20	0.71
1:E:546:LEU:HD11	1:E:595:VAL:CG2	2.20	0.70
1:E:206:GLN:HG2	1:E:208:LEU:HD11	1.73	0.70
1:D:110:LEU:HD12	1:D:111:THR:N	2.05	0.70
1:B:382:SER:O	1:B:383:ILE:C	2.28	0.70
1:C:289:THR:O	1:C:289:THR:CG2	2.39	0.70
1:C:391:ASN:O	1:C:392:LEU:HD12	1.92	0.69
1:A:546:LEU:HD11	1:A:595:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:GLN:HB2	1:C:479:GLU:CD	2.08	0.69
1:B:599:ARG:NE	5:B:706:LMT:O4'	2.24	0.69
1:D:546:LEU:HD21	1:C:548:VAL:HG21	1.74	0.69
1:B:530:ILE:CD1	1:B:624:TYR:CE2	2.59	0.69
1:E:211:ARG:HG3	1:E:299:VAL:HG12	1.74	0.69
1:C:546:LEU:HD11	1:C:595:VAL:CG2	2.22	0.69
1:C:429:VAL:HG22	1:C:431:LEU:CD1	2.23	0.69
1:E:206:GLN:HB2	1:E:323:VAL:HG12	1.73	0.68
1:D:289:THR:O	1:D:289:THR:CG2	2.40	0.68
1:C:476:GLN:O	1:C:479:GLU:CG	2.40	0.68
1:C:211:ARG:CG	1:C:299:VAL:HG23	2.24	0.68
1:C:249:LEU:HB2	1:C:271:LEU:HD21	1.76	0.68
1:D:344:GLN:HE22	1:D:568:PRO:CG	2.06	0.68
1:A:239:ILE:HD11	1:A:301:ARG:HG3	1.76	0.67
1:D:77:PRO:O	1:D:124:ASP:N	2.27	0.67
1:A:548:VAL:HG21	1:B:546:LEU:HD21	1.75	0.67
1:A:391:ASN:O	1:A:392:LEU:HD12	1.94	0.67
1:A:77:PRO:O	1:A:124:ASP:N	2.28	0.67
1:C:382:SER:O	1:C:383:ILE:C	2.33	0.67
1:C:429:VAL:HG22	1:C:431:LEU:HD12	1.76	0.67
1:B:406:ARG:HD3	1:B:429:VAL:CG1	2.25	0.67
1:C:60:GLN:HB3	1:C:139:ARG:HA	1.76	0.67
1:E:77:PRO:O	1:E:124:ASP:N	2.28	0.66
1:D:546:LEU:HD11	1:D:595:VAL:CG2	2.25	0.66
1:A:382:SER:O	1:A:383:ILE:C	2.33	0.66
1:C:77:PRO:O	1:C:124:ASP:N	2.28	0.66
1:B:77:PRO:O	1:B:124:ASP:N	2.27	0.66
1:C:597:GLN:NE2	1:C:612:ILE:HG22	2.11	0.66
1:D:597:GLN:NE2	1:D:612:ILE:HG22	2.11	0.66
1:E:597:GLN:NE2	1:E:612:ILE:HG22	2.11	0.66
1:D:344:GLN:NE2	1:D:568:PRO:HG3	2.08	0.66
1:B:416:THR:HG21	1:B:420:ARG:HE	1.61	0.66
1:A:224:ARG:HB2	1:A:325:LEU:HB2	1.78	0.65
1:A:382:SER:O	1:A:385:ALA:N	2.29	0.65
1:A:390:ILE:HG22	1:A:392:LEU:HD13	1.77	0.65
1:A:548:VAL:CG2	1:B:546:LEU:HD21	2.26	0.65
1:A:597:GLN:NE2	1:A:612:ILE:HG22	2.11	0.65
1:B:597:GLN:NE2	1:B:612:ILE:HG22	2.10	0.65
1:D:546:LEU:HD21	1:C:548:VAL:CG2	2.25	0.65
1:A:77:PRO:N	1:A:124:ASP:CB	2.58	0.65
1:D:77:PRO:N	1:D:124:ASP:CB	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:PRO:N	1:C:124:ASP:CB	2.60	0.65
1:E:77:PRO:N	1:E:124:ASP:CB	2.59	0.65
1:B:77:PRO:N	1:B:124:ASP:CB	2.59	0.65
1:E:382:SER:O	1:E:383:ILE:C	2.34	0.65
1:C:382:SER:O	1:C:385:ALA:N	2.29	0.65
1:D:382:SER:O	1:D:385:ALA:N	2.30	0.65
1:C:258:ALA:HB3	1:C:271:LEU:HD11	1.79	0.64
1:B:382:SER:O	1:B:385:ALA:N	2.30	0.64
1:E:522:ILE:HG12	1:E:563:ILE:HD11	1.79	0.64
1:B:406:ARG:CD	1:B:429:VAL:CG1	2.75	0.64
1:D:595:VAL:HG11	1:C:535:VAL:HG12	1.78	0.64
1:D:416:THR:HG21	1:D:420:ARG:HE	1.62	0.64
1:A:522:ILE:HG12	1:A:563:ILE:HD11	1.80	0.64
1:B:344:GLN:NE2	1:B:568:PRO:CG	2.60	0.64
1:D:522:ILE:HG12	1:D:563:ILE:HD11	1.80	0.64
1:C:344:GLN:HE22	1:C:568:PRO:CG	2.04	0.64
1:E:382:SER:O	1:E:385:ALA:N	2.30	0.64
1:B:522:ILE:HG12	1:B:563:ILE:HD11	1.80	0.63
1:A:546:LEU:HD21	1:E:548:VAL:CG2	2.29	0.63
1:C:522:ILE:HG12	1:C:563:ILE:HD11	1.79	0.63
1:D:546:LEU:HD11	1:D:595:VAL:HG22	1.80	0.63
1:E:546:LEU:HD21	1:D:548:VAL:CG2	2.28	0.63
1:C:416:THR:HG21	1:C:420:ARG:HE	1.62	0.63
1:A:208:LEU:HD23	1:A:209:GLU:C	2.19	0.63
1:A:586:LEU:HD12	1:A:624:TYR:CE1	2.33	0.62
1:D:382:SER:O	1:D:383:ILE:C	2.36	0.62
1:C:546:LEU:HD21	1:B:548:VAL:CG2	2.29	0.62
1:B:329:LEU:HB2	1:B:464:ASN:HB2	1.81	0.62
1:B:546:LEU:HD11	1:B:595:VAL:HG22	1.82	0.62
1:E:211:ARG:HG3	1:E:299:VAL:CG1	2.30	0.62
1:A:546:LEU:HD21	1:E:548:VAL:HG21	1.82	0.62
1:E:429:VAL:HG22	1:E:431:LEU:HD12	1.82	0.61
1:C:546:LEU:HD21	1:B:548:VAL:HG21	1.80	0.61
1:D:248:ARG:HA	1:D:271:LEU:CD1	2.30	0.61
1:A:248:ARG:HA	1:A:271:LEU:CD1	2.30	0.61
1:B:248:ARG:HA	1:B:271:LEU:CD1	2.31	0.61
1:C:546:LEU:HD11	1:C:595:VAL:HG22	1.82	0.61
1:D:242:ALA:HB1	1:D:298:ALA:HB1	1.83	0.61
1:E:416:THR:CB	1:E:417:PRO:CD	2.61	0.61
1:C:283:VAL:HG11	1:B:156:LEU:HD22	1.81	0.61
1:B:289:THR:O	1:B:289:THR:CG2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:GLN:HG2	1:E:208:LEU:CD1	2.30	0.61
1:E:586:LEU:HD12	1:E:624:TYR:CE1	2.36	0.61
1:A:158:LYS:HE3	1:A:160:GLN:HG3	1.83	0.61
1:A:344:GLN:NE2	1:A:568:PRO:CG	2.63	0.61
1:E:248:ARG:HA	1:E:271:LEU:CD1	2.31	0.61
1:E:546:LEU:HD11	1:E:595:VAL:HG23	1.82	0.61
1:D:374:THR:O	1:D:417:PRO:HD3	2.01	0.61
1:A:546:LEU:HD11	1:A:595:VAL:HG22	1.83	0.60
1:E:283:VAL:HG11	1:D:156:LEU:HD22	1.83	0.60
1:E:546:LEU:HD21	1:D:548:VAL:HG21	1.81	0.60
1:A:242:ALA:HB1	1:A:298:ALA:HB1	1.83	0.60
1:D:601:GLY:HA2	1:D:606:GLN:HG2	1.84	0.59
1:C:173:GLY:HA3	1:C:179:VAL:HG21	1.84	0.59
1:E:366:PHE:CZ	1:E:376:LYS:HD2	2.36	0.59
1:C:553:LEU:CD2	1:B:555:VAL:HG11	2.28	0.59
1:A:208:LEU:HD22	1:A:210:ILE:HG22	1.84	0.59
1:D:418:ASP:OD1	1:D:418:ASP:O	2.21	0.59
1:E:429:VAL:HG22	1:E:431:LEU:CD1	2.33	0.59
1:C:574:THR:HG22	1:C:577:ASP:CG	2.23	0.59
1:B:242:ALA:HB1	1:B:298:ALA:HB1	1.85	0.59
1:B:258:ALA:HB3	1:B:271:LEU:HD21	1.85	0.58
1:C:418:ASP:O	1:C:418:ASP:OD1	2.20	0.58
1:E:258:ALA:HB3	1:E:271:LEU:HD21	1.85	0.58
1:E:344:GLN:NE2	1:E:568:PRO:HG3	2.11	0.58
1:B:391:ASN:C	1:B:392:LEU:HD12	2.24	0.58
1:C:390:ILE:HG23	1:C:392:LEU:HD13	1.85	0.58
1:A:553:LEU:CD2	1:E:555:VAL:HG11	2.31	0.58
1:E:588:ALA:HB3	1:D:528:LEU:HD23	1.85	0.58
1:C:444:ASP:OD1	1:C:513:ARG:NH1	2.36	0.58
1:E:476:GLN:HB3	1:E:479:GLU:OE1	2.03	0.58
1:A:476:GLN:HB3	1:A:479:GLU:OE1	2.04	0.58
1:D:173:GLY:HA3	1:D:179:VAL:HG21	1.85	0.58
1:B:366:PHE:CZ	1:B:376:LYS:HD2	2.39	0.58
1:E:546:LEU:HD11	1:E:595:VAL:HG22	1.86	0.58
1:B:522:ILE:CG1	1:B:563:ILE:HD11	2.34	0.58
1:A:173:GLY:HA3	1:A:179:VAL:HG21	1.85	0.57
1:A:522:ILE:CG1	1:A:563:ILE:HD11	2.34	0.57
1:B:173:GLY:HA3	1:B:179:VAL:HG21	1.85	0.57
1:D:236:VAL:CG1	1:D:302:LEU:HD13	2.34	0.57
1:D:485:THR:OG1	1:D:510:LEU:HB2	2.04	0.57
1:A:386:VAL:HG23	1:A:394:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:HD12	1:C:174:LEU:O	2.04	0.57
1:C:476:GLN:HB3	1:C:479:GLU:OE2	2.05	0.57
1:C:258:ALA:HB1	1:C:271:LEU:HD11	1.87	0.57
1:C:344:GLN:NE2	1:C:568:PRO:CG	2.67	0.57
1:C:366:PHE:CZ	1:C:376:LYS:HD2	2.39	0.57
1:E:344:GLN:HE22	1:E:568:PRO:CG	2.13	0.57
1:D:522:ILE:CG1	1:D:563:ILE:HD11	2.35	0.57
1:E:522:ILE:CG1	1:E:563:ILE:HD11	2.34	0.57
1:B:416:THR:HG21	1:B:420:ARG:NE	2.19	0.57
1:A:519:ILE:HA	1:A:523:PHE:HB2	1.87	0.57
1:C:522:ILE:CG1	1:C:563:ILE:HD11	2.35	0.57
1:E:483:VAL:O	1:E:511:VAL:HA	2.05	0.56
1:E:546:LEU:HD12	1:E:595:VAL:N	2.20	0.56
1:A:258:ALA:HB3	1:A:271:LEU:HD21	1.86	0.56
1:A:555:VAL:HG11	1:B:553:LEU:CD2	2.31	0.56
1:A:612:ILE:HA	1:A:615:TRP:HB3	1.88	0.56
1:B:546:LEU:HD11	1:B:595:VAL:HG23	1.87	0.56
1:D:519:ILE:HA	1:D:523:PHE:HB2	1.86	0.56
1:C:416:THR:HG21	1:C:420:ARG:NE	2.20	0.56
1:C:485:THR:OG1	1:C:510:LEU:HB2	2.05	0.56
1:C:519:ILE:HA	1:C:523:PHE:HB2	1.87	0.56
1:D:416:THR:HG21	1:D:420:ARG:NE	2.20	0.56
1:E:206:GLN:CB	1:E:323:VAL:HG12	2.36	0.56
1:D:476:GLN:HB3	1:D:479:GLU:CG	2.36	0.55
1:A:211:ARG:HA	1:A:299:VAL:HG23	1.88	0.55
1:D:476:GLN:CB	1:D:479:GLU:HG2	2.36	0.55
1:A:466:ILE:HG23	1:A:491:ILE:CD1	2.34	0.55
1:C:91:SER:O	1:C:95:VAL:HG23	2.07	0.55
1:B:519:ILE:HA	1:B:523:PHE:HB2	1.87	0.55
1:D:283:VAL:HG11	1:C:156:LEU:HD22	1.89	0.55
1:A:588:ALA:HB3	1:E:528:LEU:HD23	1.88	0.55
1:B:201:PRO:HG2	1:B:307:ASN:HD22	1.71	0.55
1:D:546:LEU:CD1	1:D:595:VAL:HA	2.36	0.55
1:E:519:ILE:HA	1:E:523:PHE:HB2	1.87	0.55
1:D:91:SER:O	1:D:95:VAL:HG23	2.06	0.55
1:A:546:LEU:HD12	1:A:595:VAL:N	2.22	0.55
1:B:476:GLN:HB3	1:B:479:GLU:OE1	2.07	0.55
1:B:488:SER:O	1:B:508:THR:HG22	2.06	0.55
1:E:91:SER:O	1:E:95:VAL:HG23	2.07	0.55
1:D:366:PHE:CZ	1:D:376:LYS:HD2	2.41	0.54
1:E:553:LEU:CD2	1:D:555:VAL:HG11	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:CD1	1:A:595:VAL:HA	2.38	0.54
1:C:217:ARG:NH1	1:C:289:THR:HA	2.22	0.54
1:E:445:ARG:HH12	1:E:512:LYS:HD3	1.72	0.54
1:B:91:SER:O	1:B:95:VAL:HG23	2.06	0.54
1:A:91:SER:O	1:A:95:VAL:HG23	2.07	0.54
1:D:553:LEU:CD2	1:C:555:VAL:HG11	2.32	0.54
1:C:546:LEU:HD11	1:C:595:VAL:HG23	1.89	0.54
1:E:612:ILE:HA	1:E:615:TRP:HB3	1.88	0.54
1:B:582:VAL:HG21	1:B:627:TYR:CZ	2.42	0.54
1:A:372:GLY:O	1:B:252:SER:HB3	2.08	0.54
1:C:546:LEU:HD12	1:C:595:VAL:N	2.23	0.54
1:C:587:THR:O	1:C:590:VAL:HG22	2.08	0.54
1:C:582:VAL:HG21	1:C:627:TYR:CZ	2.43	0.54
1:A:546:LEU:HD11	1:A:595:VAL:HG23	1.90	0.54
1:D:587:THR:O	1:D:590:VAL:HG22	2.08	0.54
1:E:582:VAL:HG21	1:E:627:TYR:CZ	2.42	0.54
1:A:104:ASN:O	1:A:108:SER:HB2	2.08	0.54
1:A:574:THR:HG22	1:A:577:ASP:CG	2.28	0.54
1:A:587:THR:O	1:A:590:VAL:HG22	2.08	0.54
1:A:366:PHE:CZ	1:A:376:LYS:HD2	2.42	0.53
1:D:476:GLN:HB3	1:D:479:GLU:HG2	1.90	0.53
1:D:582:VAL:HG21	1:D:627:TYR:CZ	2.43	0.53
1:B:546:LEU:HD12	1:B:595:VAL:N	2.23	0.53
1:C:430:THR:C	1:C:431:LEU:HD12	2.29	0.53
1:D:236:VAL:HG12	1:D:302:LEU:HD13	1.89	0.53
1:E:173:GLY:HA3	1:E:179:VAL:HG21	1.90	0.53
1:A:60:GLN:O	1:A:60:GLN:HG2	2.08	0.53
1:C:290:ASP:C	1:C:290:ASP:OD1	2.44	0.53
1:C:546:LEU:CD1	1:C:595:VAL:HA	2.38	0.53
1:D:537:PHE:O	1:D:613:ASP:OD2	2.26	0.53
1:E:498:ARG:CZ	1:D:375:VAL:HG11	2.38	0.53
1:E:537:PHE:O	1:E:613:ASP:OD2	2.26	0.53
1:A:582:VAL:HG21	1:A:627:TYR:CZ	2.43	0.53
1:B:587:THR:O	1:B:590:VAL:HG22	2.07	0.53
1:D:574:THR:HG22	1:D:577:ASP:CG	2.29	0.53
1:E:430:THR:C	1:E:431:LEU:HD12	2.29	0.53
1:A:537:PHE:O	1:A:613:ASP:OD2	2.27	0.53
1:B:537:PHE:O	1:B:613:ASP:OD2	2.27	0.53
1:C:391:ASN:C	1:C:392:LEU:HD12	2.28	0.53
1:E:252:SER:HB3	1:D:372:GLY:O	2.09	0.53
1:D:488:SER:O	1:D:508:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:GLN:O	1:E:60:GLN:HG2	2.09	0.53
1:D:391:ASN:C	1:D:392:LEU:HD12	2.29	0.53
1:B:479:GLU:N	1:B:479:GLU:OE2	2.42	0.52
1:C:497:GLU:HG2	1:B:424:PHE:CE2	2.44	0.52
1:C:488:SER:O	1:C:508:THR:HG22	2.09	0.52
1:B:406:ARG:HD3	1:B:429:VAL:HG12	1.90	0.52
5:B:706:LMT:O3'	5:B:706:LMT:H1B	2.08	0.52
1:E:574:THR:HG22	1:E:577:ASP:CG	2.29	0.52
1:B:522:ILE:HG23	1:B:563:ILE:CD1	2.40	0.52
1:D:344:GLN:NE2	1:D:568:PRO:CG	2.69	0.52
1:E:431:LEU:HD21	1:E:450:ILE:HG23	1.92	0.52
1:E:488:SER:O	1:E:508:THR:HG22	2.10	0.52
1:E:55:LEU:HD23	1:E:58:MET:SD	2.50	0.52
1:A:239:ILE:CD1	1:A:301:ARG:HG3	2.38	0.52
1:C:104:ASN:O	1:C:108:SER:HB2	2.09	0.52
1:C:553:LEU:HD12	1:C:587:THR:HG22	1.92	0.52
1:E:37:ARG:CZ	1:E:174:LEU:HD13	2.39	0.52
1:A:391:ASN:C	1:A:392:LEU:HD12	2.30	0.52
1:B:546:LEU:CD1	1:B:595:VAL:HA	2.39	0.52
1:B:174:LEU:HD12	1:B:174:LEU:O	2.10	0.52
1:C:537:PHE:O	1:C:613:ASP:OD2	2.27	0.52
1:D:55:LEU:HD23	1:D:58:MET:SD	2.50	0.52
1:A:248:ARG:HA	1:A:271:LEU:HD11	1.92	0.52
1:C:242:ALA:HB1	1:C:298:ALA:HB1	1.91	0.52
1:D:553:LEU:HD12	1:D:587:THR:HG22	1.92	0.52
1:B:211:ARG:HA	1:B:299:VAL:HG23	1.92	0.51
1:C:211:ARG:HA	1:C:299:VAL:HG23	1.92	0.51
1:C:55:LEU:HD23	1:C:58:MET:SD	2.50	0.51
1:D:217:ARG:NE	1:D:288:GLY:O	2.35	0.51
1:A:55:LEU:HD23	1:A:58:MET:SD	2.50	0.51
1:E:242:ALA:HB1	1:E:298:ALA:HB1	1.90	0.51
1:B:374:THR:O	1:B:417:PRO:HD3	2.11	0.51
1:B:601:GLY:HA2	1:B:606:GLN:HG2	1.92	0.51
1:C:290:ASP:OD1	1:C:291:GLY:N	2.44	0.51
1:C:522:ILE:HG23	1:C:563:ILE:CD1	2.41	0.51
1:D:476:GLN:HB3	1:D:479:GLU:OE1	2.09	0.51
1:E:277:GLN:NE2	1:D:128:GLY:O	2.44	0.51
1:E:304:VAL:HG13	1:E:323:VAL:CG1	2.38	0.51
1:A:374:THR:O	1:A:417:PRO:HD3	2.11	0.51
1:D:522:ILE:HG23	1:D:563:ILE:CD1	2.40	0.51
1:A:486:SER:OG	1:A:510:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:PHE:CD2	1:B:616:VAL:HG11	2.46	0.51
1:B:55:LEU:HD23	1:B:58:MET:SD	2.50	0.51
1:E:537:PHE:CD2	1:E:616:VAL:HG11	2.46	0.51
1:C:258:ALA:HB1	1:C:271:LEU:CD1	2.39	0.51
1:E:126:GLY:HA3	1:E:369:ASP:OD2	2.10	0.51
1:A:208:LEU:HD22	1:A:210:ILE:CG2	2.40	0.50
1:B:392:LEU:HB3	1:B:393:PRO:HD2	1.92	0.50
1:B:412:VAL:HG11	1:B:414:PHE:HE1	1.76	0.50
1:C:486:SER:OG	1:C:510:LEU:HD12	2.11	0.50
1:D:542:TYR:O	1:D:543:GLY:C	2.49	0.50
1:B:553:LEU:HD12	1:B:587:THR:HG22	1.94	0.50
1:C:537:PHE:CD2	1:C:616:VAL:HG11	2.47	0.50
1:A:488:SER:O	1:A:508:THR:HG22	2.11	0.50
1:A:537:PHE:CD2	1:A:616:VAL:HG11	2.47	0.50
1:E:522:ILE:HG23	1:E:563:ILE:CD1	2.41	0.50
1:A:479:GLU:OE2	1:A:479:GLU:N	2.45	0.50
1:A:601:GLY:HA2	1:A:606:GLN:HG2	1.94	0.50
1:A:522:ILE:HG23	1:A:563:ILE:CD1	2.40	0.50
1:B:542:TYR:O	1:B:543:GLY:C	2.49	0.50
1:D:110:LEU:C	1:D:110:LEU:HD12	2.31	0.50
1:A:62:ASP:HB3	1:A:174:LEU:CD1	2.38	0.50
1:E:248:ARG:HA	1:E:271:LEU:HD11	1.93	0.50
1:B:207:GLU:OE1	1:B:301:ARG:HD2	2.12	0.50
1:D:546:LEU:HD12	1:D:595:VAL:N	2.27	0.50
1:E:479:GLU:N	1:E:479:GLU:OE2	2.44	0.50
1:D:479:GLU:N	1:D:479:GLU:OE2	2.45	0.50
1:E:546:LEU:CD1	1:E:595:VAL:HA	2.42	0.50
1:A:277:GLN:HB3	1:A:279:ILE:O	2.12	0.50
1:A:542:TYR:O	1:A:543:GLY:C	2.49	0.50
1:C:542:TYR:O	1:C:543:GLY:C	2.49	0.50
1:D:486:SER:OG	1:D:510:LEU:HD12	2.12	0.50
1:B:174:LEU:HD23	1:B:191:PHE:CD1	2.46	0.49
1:B:211:ARG:CG	1:B:299:VAL:HG23	2.41	0.49
1:B:612:ILE:HA	1:B:615:TRP:HB3	1.94	0.49
1:C:374:THR:O	1:C:417:PRO:HD3	2.12	0.49
1:D:398:SER:HB2	1:C:409:GLN:HE21	1.77	0.49
1:B:210:ILE:CD1	1:B:219:LEU:HD22	2.43	0.49
1:C:252:SER:HB3	1:B:372:GLY:O	2.12	0.49
1:C:106:LEU:O	1:C:106:LEU:HD23	2.11	0.49
1:C:574:THR:HG23	1:C:577:ASP:H	1.77	0.49
1:E:616:VAL:HA	1:E:619:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:OE1	1:B:241:GLU:HA	2.12	0.49
1:D:174:LEU:O	1:D:174:LEU:HD12	2.12	0.49
1:E:374:THR:O	1:E:417:PRO:HD3	2.12	0.49
1:A:553:LEU:HD12	1:A:587:THR:HG22	1.93	0.49
1:B:248:ARG:HA	1:B:271:LEU:HD11	1.95	0.49
1:D:248:ARG:HA	1:D:271:LEU:HD11	1.94	0.49
1:D:217:ARG:NH1	1:D:291:GLY:O	2.46	0.49
1:E:48:GLY:HA3	1:E:163:TYR:HB3	1.95	0.49
1:A:616:VAL:HA	1:A:619:ILE:HG12	1.95	0.49
1:B:37:ARG:NH2	1:B:174:LEU:HD21	2.27	0.49
1:D:537:PHE:CD2	1:D:616:VAL:HG11	2.46	0.49
1:E:344:GLN:HG2	1:E:438:PHE:CZ	2.47	0.49
1:A:208:LEU:HD23	1:A:209:GLU:O	2.12	0.49
1:C:239:ILE:HB	1:C:299:VAL:HG13	1.95	0.49
1:D:616:VAL:HA	1:D:619:ILE:HG12	1.95	0.49
1:C:535:VAL:O	1:C:535:VAL:HG12	2.12	0.49
1:E:542:TYR:O	1:E:543:GLY:C	2.49	0.49
1:B:616:VAL:HA	1:B:619:ILE:HG12	1.94	0.48
1:E:348:ASN:C	1:E:348:ASN:OD1	2.52	0.48
1:E:412:VAL:HG11	1:E:414:PHE:HE1	1.77	0.48
1:A:348:ASN:OD1	1:A:348:ASN:C	2.52	0.48
1:A:126:GLY:HA3	1:A:369:ASP:OD2	2.13	0.48
1:A:412:VAL:HG11	1:A:414:PHE:HE1	1.78	0.48
1:B:441:TYR:HD2	1:B:574:THR:HG21	1.78	0.48
1:D:412:VAL:HG11	1:D:414:PHE:HE1	1.79	0.48
1:A:497:GLU:HG2	1:E:424:PHE:CE2	2.48	0.48
1:E:476:GLN:CB	1:E:479:GLU:HG2	2.44	0.48
5:B:706:LMT:O4'	5:B:706:LMT:O2B	2.24	0.48
1:C:390:ILE:HG22	1:C:392:LEU:HB2	1.96	0.48
1:C:616:VAL:HA	1:C:619:ILE:HG12	1.96	0.48
1:D:258:ALA:HB3	1:D:271:LEU:HD21	1.96	0.48
1:B:406:ARG:CD	1:B:429:VAL:HG12	2.43	0.48
1:C:412:VAL:HG11	1:C:414:PHE:HE1	1.79	0.48
1:E:553:LEU:HD12	1:E:587:THR:HG22	1.94	0.48
1:D:595:VAL:CG1	1:C:535:VAL:HG12	2.41	0.48
1:B:574:THR:HG22	1:B:577:ASP:CG	2.35	0.47
1:D:174:LEU:HD23	1:D:191:PHE:CD1	2.49	0.47
1:D:37:ARG:NH2	1:D:174:LEU:HD21	2.29	0.47
1:B:210:ILE:HD11	1:B:219:LEU:HD22	1.96	0.47
1:B:486:SER:OG	1:B:510:LEU:HD12	2.14	0.47
1:C:348:ASN:C	1:C:348:ASN:OD1	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:611:GLN:O	1:E:615:TRP:N	2.47	0.47
1:B:387:ALA:O	1:B:391:ASN:N	2.48	0.47
1:C:387:ALA:O	1:C:391:ASN:N	2.47	0.47
1:D:48:GLY:HA3	1:D:163:TYR:HB3	1.95	0.47
1:B:348:ASN:C	1:B:348:ASN:OD1	2.52	0.47
1:B:406:ARG:HD3	1:B:429:VAL:HG11	1.97	0.47
1:C:48:GLY:HA3	1:C:163:TYR:HB3	1.96	0.47
1:A:277:GLN:OE1	1:E:128:GLY:O	2.32	0.47
1:B:382:SER:O	1:B:384:ARG:N	2.48	0.47
1:C:174:LEU:HD23	1:C:191:PHE:CD1	2.49	0.47
1:D:558:ALA:HA	1:D:561:PHE:CE2	2.50	0.47
1:A:560:ASN:ND2	4:A:706:CL:CL	2.84	0.47
1:E:486:SER:OG	1:E:510:LEU:HD12	2.14	0.47
1:A:228:PRO:HD3	1:A:278:ASP:HA	1.97	0.47
1:A:378:PHE:HB2	1:A:413:ILE:HG23	1.97	0.47
1:A:449:SER:HA	1:A:508:THR:HA	1.96	0.47
1:A:558:ALA:HA	1:A:561:PHE:CE2	2.50	0.47
1:B:586:LEU:HD23	1:B:624:TYR:CE1	2.50	0.47
1:D:441:TYR:CD1	1:D:442:PRO:HA	2.50	0.47
1:E:554:LEU:CD1	1:D:555:VAL:HG22	2.45	0.47
1:B:392:LEU:HB3	1:B:393:PRO:CD	2.45	0.46
1:B:537:PHE:CE2	1:B:616:VAL:HG11	2.51	0.46
1:C:366:PHE:H	1:C:417:PRO:HA	1.80	0.46
1:D:497:GLU:HG2	1:C:424:PHE:CE2	2.50	0.46
1:D:408:SER:OG	1:D:425:GLU:OE1	2.30	0.46
1:B:239:ILE:HB	1:B:299:VAL:HG13	1.97	0.46
1:B:616:VAL:O	1:B:617:LEU:C	2.54	0.46
1:D:348:ASN:C	1:D:348:ASN:OD1	2.52	0.46
1:E:558:ALA:HA	1:E:561:PHE:CE2	2.51	0.46
1:D:252:SER:HB3	1:C:372:GLY:O	2.15	0.46
1:C:601:GLY:HA2	1:C:606:GLN:HG2	1.96	0.46
1:A:235:LEU:HG	1:A:303:LEU:HB3	1.97	0.46
1:C:530:ILE:HD11	1:C:624:TYR:HE2	1.73	0.46
1:E:441:TYR:CD1	1:E:442:PRO:HA	2.51	0.46
1:B:378:PHE:HB2	1:B:413:ILE:HG23	1.98	0.46
1:C:378:PHE:HB2	1:C:413:ILE:HG23	1.98	0.46
1:E:537:PHE:CE2	1:E:616:VAL:HG11	2.51	0.46
1:A:387:ALA:O	1:A:391:ASN:N	2.49	0.46
1:A:616:VAL:O	1:A:617:LEU:C	2.54	0.46
1:C:537:PHE:CE2	1:C:616:VAL:HG11	2.51	0.46
1:A:441:TYR:CD1	1:A:442:PRO:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PHE:CE2	1:A:616:VAL:HG11	2.51	0.46
1:B:211:ARG:HG2	1:B:299:VAL:HG21	1.96	0.46
1:B:558:ALA:HA	1:B:561:PHE:CE2	2.50	0.46
1:D:387:ALA:O	1:D:391:ASN:N	2.49	0.46
1:B:449:SER:HA	1:B:508:THR:HA	1.98	0.46
1:B:635:PHE:C	1:B:636:PHE:HD1	2.19	0.46
1:E:533:SER:HB3	1:E:590:VAL:HG21	1.98	0.46
1:D:483:VAL:O	1:D:511:VAL:HA	2.15	0.46
1:D:567:LEU:HD23	1:D:576:LEU:HD23	1.98	0.46
1:A:48:GLY:HA3	1:A:163:TYR:HB3	1.97	0.45
1:C:441:TYR:CD1	1:C:442:PRO:HA	2.51	0.45
1:C:558:ALA:HA	1:C:561:PHE:CE2	2.51	0.45
1:A:476:GLN:CB	1:A:479:GLU:HG2	2.46	0.45
1:C:477:LEU:O	1:C:480:GLU:HG3	2.16	0.45
1:E:387:ALA:O	1:E:391:ASN:N	2.49	0.45
1:E:570:LEU:HB3	1:E:572:TYR:CE1	2.51	0.45
1:D:546:LEU:HD11	1:D:595:VAL:HG23	1.99	0.45
1:E:258:ALA:CB	1:E:271:LEU:HD21	2.46	0.45
1:E:306:ILE:HG12	1:E:323:VAL:HG23	1.98	0.45
1:A:231:THR:HA	1:A:274:THR:HA	1.97	0.45
1:B:48:GLY:HA3	1:B:163:TYR:HB3	1.98	0.45
1:B:262:ILE:HG13	1:B:269:VAL:HG22	1.99	0.45
1:D:241:GLU:OE1	1:D:241:GLU:HA	2.16	0.45
1:D:76:ASP:O	1:D:150:THR:HG22	2.17	0.45
1:E:356:LYS:HA	1:E:423:TYR:O	2.16	0.45
1:A:279:ILE:HG13	1:A:279:ILE:O	2.17	0.45
1:A:363:LYS:HA	1:A:363:LYS:HE2	1.99	0.45
1:C:498:ARG:HB2	1:B:414:PHE:CE2	2.51	0.45
1:B:477:LEU:O	1:B:480:GLU:HG3	2.17	0.45
1:B:69:GLN:HG2	1:B:169:GLN:HB3	1.98	0.45
1:C:76:ASP:O	1:C:150:THR:HG22	2.17	0.45
1:D:537:PHE:CE2	1:D:616:VAL:HG11	2.52	0.45
1:A:477:LEU:O	1:A:480:GLU:HG3	2.17	0.45
1:C:369:ASP:OD1	1:C:369:ASP:N	2.50	0.45
1:D:369:ASP:N	1:D:369:ASP:OD1	2.50	0.45
1:D:449:SER:HA	1:D:508:THR:HA	1.98	0.45
1:E:378:PHE:HB2	1:E:413:ILE:HG23	1.99	0.45
1:B:237:GLU:OE1	1:B:301:ARG:NH2	2.50	0.45
1:E:449:SER:HA	1:E:508:THR:HA	1.98	0.45
1:A:406:ARG:HD2	1:A:427:PHE:HB2	1.99	0.45
1:B:397:PHE:CD1	1:B:397:PHE:C	2.91	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:ILE:HG22	1:D:392:LEU:HD13	1.98	0.45
1:E:344:GLN:NE2	1:E:568:PRO:CG	2.77	0.45
1:E:77:PRO:CD	1:E:124:ASP:CB	2.95	0.45
1:A:498:ARG:NH1	1:E:157:ASP:OD2	2.50	0.45
1:A:635:PHE:C	1:A:636:PHE:HD1	2.20	0.45
1:B:70:ASN:HD22	1:B:75:LEU:HB3	1.82	0.45
1:C:262:ILE:HG13	1:C:269:VAL:HG22	1.99	0.45
1:C:429:VAL:CG2	1:C:431:LEU:HD11	2.47	0.45
1:D:262:ILE:HG13	1:D:269:VAL:HG22	1.99	0.45
1:A:574:THR:HG23	1:A:577:ASP:H	1.82	0.44
1:C:406:ARG:HD2	1:C:427:PHE:HB2	2.00	0.44
1:C:635:PHE:C	1:C:636:PHE:HD1	2.20	0.44
1:D:98:LYS:HD3	1:D:100:LEU:HD11	1.99	0.44
1:A:262:ILE:HG13	1:A:269:VAL:HG22	1.99	0.44
1:A:77:PRO:CD	1:A:124:ASP:CB	2.95	0.44
1:D:477:LEU:O	1:D:480:GLU:HG3	2.17	0.44
1:E:397:PHE:C	1:E:397:PHE:CD1	2.91	0.44
1:E:635:PHE:C	1:E:636:PHE:HD1	2.20	0.44
1:A:258:ALA:CB	1:A:271:LEU:HD21	2.47	0.44
1:A:581:ILE:HD13	1:E:520:LEU:HB3	1.99	0.44
1:B:258:ALA:CB	1:B:271:LEU:HD21	2.46	0.44
1:D:398:SER:HB2	1:C:409:GLN:NE2	2.31	0.44
1:D:406:ARG:HD2	1:D:427:PHE:HB2	1.99	0.44
1:D:70:ASN:HD22	1:D:75:LEU:HB3	1.82	0.44
1:A:356:LYS:HA	1:A:423:TYR:O	2.17	0.44
1:B:347:GLU:OE2	1:B:436:PHE:O	2.35	0.44
1:C:616:VAL:O	1:C:617:LEU:C	2.54	0.44
1:D:378:PHE:HB2	1:D:413:ILE:HG23	1.98	0.44
1:D:635:PHE:C	1:D:636:PHE:HD1	2.20	0.44
1:E:477:LEU:O	1:E:480:GLU:HG3	2.17	0.44
1:E:483:VAL:HG23	1:E:512:LYS:HG2	1.99	0.44
1:B:441:TYR:CD1	1:B:442:PRO:HA	2.51	0.44
1:D:586:LEU:HD23	1:D:624:TYR:CE1	2.52	0.44
1:E:76:ASP:O	1:E:150:THR:HG22	2.17	0.44
1:A:124:ASP:HA	1:A:131:ALA:HB2	2.00	0.44
1:A:239:ILE:HB	1:A:299:VAL:HG13	1.99	0.44
1:A:411:GLN:O	1:A:412:VAL:HG22	2.18	0.44
1:B:76:ASP:O	1:B:150:THR:HG22	2.16	0.44
1:B:616:VAL:HG12	1:B:617:LEU:N	2.33	0.44
1:C:37:ARG:NH2	1:C:174:LEU:HD21	2.33	0.44
1:E:498:ARG:NE	1:D:375:VAL:HG11	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:THR:HG23	1:E:577:ASP:H	1.82	0.44
1:A:397:PHE:CD1	1:A:397:PHE:C	2.91	0.44
1:C:411:GLN:O	1:C:412:VAL:HG22	2.18	0.44
1:C:347:GLU:OE2	1:C:436:PHE:O	2.36	0.44
1:C:449:SER:HA	1:C:508:THR:HA	1.98	0.44
1:C:70:ASN:HD22	1:C:75:LEU:HB3	1.82	0.44
1:A:536:ILE:HG21	1:A:548:VAL:HG11	2.00	0.44
1:A:616:VAL:HG12	1:A:617:LEU:N	2.33	0.44
1:B:77:PRO:CD	1:B:124:ASP:CB	2.96	0.44
1:D:124:ASP:HA	1:D:131:ALA:HB2	1.99	0.44
1:D:356:LYS:HA	1:D:423:TYR:O	2.17	0.44
1:D:597:GLN:NE2	1:D:612:ILE:CG2	2.81	0.44
1:E:231:THR:HA	1:E:274:THR:HA	2.00	0.44
1:E:406:ARG:HD2	1:E:427:PHE:HB2	1.99	0.44
1:A:347:GLU:OE2	1:A:436:PHE:O	2.36	0.44
1:A:539:LEU:CD1	1:B:595:VAL:HG13	2.48	0.44
1:B:49:ARG:NH2	1:B:202:GLU:OE1	2.51	0.44
1:B:536:ILE:HG21	1:B:548:VAL:HG11	2.00	0.44
1:D:397:PHE:C	1:D:397:PHE:CD1	2.91	0.44
1:A:76:ASP:O	1:A:150:THR:HG22	2.17	0.43
1:B:124:ASP:HA	1:B:131:ALA:HB2	1.99	0.43
1:B:210:ILE:HD11	1:B:219:LEU:CD2	2.48	0.43
1:B:329:LEU:O	1:B:329:LEU:HD12	2.18	0.43
1:B:522:ILE:HG23	1:B:563:ILE:HD11	2.00	0.43
1:C:356:LYS:HA	1:C:423:TYR:O	2.18	0.43
1:D:124:ASP:HA	1:D:131:ALA:CB	2.48	0.43
1:D:239:ILE:HB	1:D:299:VAL:HG13	2.00	0.43
1:D:411:GLN:O	1:D:412:VAL:HG22	2.18	0.43
1:E:429:VAL:HG13	1:E:431:LEU:CD1	2.48	0.43
1:E:536:ILE:HG21	1:E:548:VAL:HG11	2.00	0.43
1:E:616:VAL:O	1:E:617:LEU:C	2.53	0.43
1:E:616:VAL:HG12	1:E:617:LEU:N	2.33	0.43
1:A:277:GLN:CD	1:E:128:GLY:HA2	2.38	0.43
1:A:522:ILE:HG23	1:A:563:ILE:HD11	2.00	0.43
1:B:145:ILE:HD13	1:B:172:LEU:HD21	2.01	0.43
1:C:211:ARG:CG	1:C:299:VAL:CG2	2.83	0.43
1:C:611:GLN:O	1:C:615:TRP:N	2.48	0.43
1:D:616:VAL:O	1:D:617:LEU:C	2.54	0.43
1:D:77:PRO:CD	1:D:124:ASP:CB	2.96	0.43
1:B:356:LYS:HA	1:B:423:TYR:O	2.18	0.43
1:E:259:PHE:C	1:E:271:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:GLN:O	1:E:412:VAL:HG22	2.18	0.43
1:E:441:TYR:HD2	1:E:574:THR:HG21	1.83	0.43
1:E:91:SER:HA	1:E:94:GLN:HB2	2.01	0.43
1:A:339:ILE:HG21	1:A:448:PHE:CE2	2.54	0.43
1:A:570:LEU:HB3	1:A:572:TYR:CE1	2.53	0.43
1:B:264:GLN:HB3	1:B:265:PRO:CD	2.48	0.43
1:B:406:ARG:HB2	1:B:429:VAL:HG12	2.00	0.43
1:B:411:GLN:O	1:B:412:VAL:HG22	2.18	0.43
1:C:397:PHE:CD1	1:C:397:PHE:C	2.91	0.43
1:C:616:VAL:HG12	1:C:617:LEU:N	2.33	0.43
1:D:145:ILE:HD13	1:D:172:LEU:HD21	1.99	0.43
1:D:536:ILE:HG21	1:D:548:VAL:HG11	2.00	0.43
1:D:574:THR:HG23	1:D:577:ASP:H	1.83	0.43
1:A:254:GLY:O	1:E:153:ASN:HB3	2.18	0.43
1:C:124:ASP:HA	1:C:131:ALA:CB	2.49	0.43
1:E:359:TRP:HH2	1:E:394:LEU:HD22	1.84	0.43
1:A:260:GLY:N	1:A:271:LEU:HD12	2.33	0.43
1:C:124:ASP:HA	1:C:131:ALA:HB2	2.00	0.43
1:E:570:LEU:HD23	1:E:572:TYR:CE1	2.53	0.43
1:B:530:ILE:HD13	1:B:624:TYR:CD2	2.44	0.43
1:C:570:LEU:HB3	1:C:572:TYR:CE1	2.53	0.43
1:B:264:GLN:HB3	1:B:265:PRO:HD3	2.00	0.43
1:B:210:ILE:HD13	1:B:286:VAL:HG11	2.01	0.43
1:B:382:SER:C	1:B:384:ARG:N	2.70	0.43
1:B:570:LEU:HD23	1:B:572:TYR:CE1	2.54	0.43
1:C:429:VAL:HG22	1:C:431:LEU:HD11	2.00	0.43
1:C:612:ILE:HA	1:C:615:TRP:HB3	2.01	0.43
1:E:69:GLN:HB2	1:E:169:GLN:HB3	2.00	0.43
1:A:91:SER:HA	1:A:94:GLN:HB2	2.01	0.43
1:B:611:GLN:O	1:B:615:TRP:N	2.50	0.43
1:B:259:PHE:C	1:B:271:LEU:HD12	2.39	0.43
1:C:214:LYS:HD2	1:C:217:ARG:HD2	2.01	0.43
1:D:392:LEU:HB3	1:D:393:PRO:HD2	2.01	0.43
1:D:483:VAL:HG23	1:D:512:LYS:HG2	1.99	0.43
1:E:84:GLU:N	1:E:84:GLU:OE1	2.51	0.43
1:B:597:GLN:NE2	1:B:612:ILE:CG2	2.81	0.42
1:C:145:ILE:HD13	1:C:172:LEU:HD21	2.00	0.42
1:E:432:GLN:HB3	1:D:338:GLN:HE22	1.84	0.42
1:E:70:ASN:HD22	1:E:75:LEU:HB3	1.83	0.42
1:A:124:ASP:HA	1:A:131:ALA:CB	2.49	0.42
1:A:362:PRO:HG2	1:A:363:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PHE:HD2	1:B:498:ARG:HE	1.67	0.42
1:A:70:ASN:HD22	1:A:75:LEU:HB3	1.82	0.42
1:B:267:GLU:O	1:B:267:GLU:HG3	2.18	0.42
1:B:406:ARG:HD2	1:B:427:PHE:HB2	2.00	0.42
1:A:145:ILE:HD13	1:A:172:LEU:HD21	2.01	0.42
1:B:228:PRO:HD3	1:B:278:ASP:HA	2.01	0.42
1:C:223:THR:HG23	1:C:282:LEU:O	2.19	0.42
1:C:483:VAL:HG23	1:C:512:LYS:HG2	2.00	0.42
1:D:581:ILE:HD13	1:C:520:LEU:HB3	2.01	0.42
1:C:616:VAL:C	1:C:618:VAL:N	2.72	0.42
1:D:476:GLN:CB	1:D:479:GLU:CG	2.96	0.42
1:E:228:PRO:HD3	1:E:278:ASP:HA	2.01	0.42
1:E:554:LEU:HD12	1:D:555:VAL:HG22	2.00	0.42
1:B:599:ARG:CD	5:B:706:LMT:O4'	2.67	0.42
1:C:536:ILE:HG21	1:C:548:VAL:HG11	2.00	0.42
1:D:261:LEU:HD11	1:C:104:ASN:ND2	2.35	0.42
1:D:441:TYR:HE2	1:D:567:LEU:CD2	2.26	0.42
1:D:554:LEU:CD1	1:C:555:VAL:HG22	2.50	0.42
1:E:124:ASP:HA	1:E:131:ALA:HB2	2.00	0.42
1:A:54:SER:CB	1:A:195:ALA:HB2	2.50	0.42
1:C:77:PRO:CD	1:C:124:ASP:CB	2.97	0.42
1:D:223:THR:HG22	1:D:224:ARG:N	2.35	0.42
1:E:262:ILE:HG13	1:E:269:VAL:HG22	2.00	0.42
1:A:597:GLN:NE2	1:A:612:ILE:CG2	2.81	0.42
1:E:124:ASP:HA	1:E:131:ALA:CB	2.49	0.42
1:A:176:ALA:HB1	1:A:178:GLN:NE2	2.34	0.42
1:A:259:PHE:C	1:A:271:LEU:HD12	2.40	0.42
1:B:124:ASP:HA	1:B:131:ALA:CB	2.48	0.42
1:C:390:ILE:CG2	1:C:392:LEU:HB2	2.48	0.42
1:D:522:ILE:HG23	1:D:563:ILE:HD11	2.01	0.42
1:E:260:GLY:N	1:E:271:LEU:HD12	2.35	0.42
1:E:530:ILE:HG12	1:E:624:TYR:CE2	2.54	0.42
1:C:632:TYR:CD1	1:C:632:TYR:C	2.93	0.42
1:D:570:LEU:HB3	1:D:572:TYR:CE1	2.54	0.42
1:D:546:LEU:HD12	1:D:595:VAL:HA	2.02	0.42
1:D:616:VAL:HG12	1:D:617:LEU:N	2.33	0.42
1:E:445:ARG:NH1	1:E:512:LYS:HD3	2.34	0.42
1:B:91:SER:HA	1:B:94:GLN:HB2	2.01	0.42
1:D:588:ALA:HB3	1:C:528:LEU:HD23	2.02	0.42
1:E:632:TYR:CD1	1:E:632:TYR:C	2.93	0.42
1:B:176:ALA:HB1	1:B:178:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ALA:O	1:B:444:ASP:N	2.53	0.42
1:A:614:THR:HB	5:B:706:LMT:O6'	2.19	0.42
1:C:251:ASP:OD1	1:C:255:LYS:N	2.53	0.42
1:C:416:THR:CG2	1:C:420:ARG:HB2	2.50	0.42
1:C:483:VAL:O	1:C:511:VAL:HA	2.20	0.42
1:C:91:SER:HA	1:C:94:GLN:HB2	2.01	0.42
1:A:441:TYR:HD2	1:A:574:THR:HG21	1.84	0.41
1:A:555:VAL:HG22	1:B:554:LEU:CD1	2.50	0.41
1:C:584:PHE:CE2	1:B:525:PRO:HB3	2.55	0.41
1:D:176:ALA:HB1	1:D:178:GLN:NE2	2.35	0.41
1:D:612:ILE:HA	1:D:615:TRP:HB3	2.01	0.41
1:B:599:ARG:HG2	5:B:706:LMT:C4B	2.47	0.41
1:E:40:HIS:NE2	1:E:184:GLY:O	2.47	0.41
1:A:483:VAL:O	1:A:511:VAL:HA	2.20	0.41
1:A:632:TYR:CD1	1:A:632:TYR:C	2.93	0.41
1:C:588:ALA:HB3	1:B:528:LEU:HD23	2.01	0.41
1:B:616:VAL:C	1:B:618:VAL:N	2.72	0.41
1:D:440:ALA:O	1:D:444:ASP:N	2.53	0.41
1:D:91:SER:HA	1:D:94:GLN:HB2	2.01	0.41
1:E:157:ASP:O	1:E:158:LYS:HG3	2.21	0.41
1:E:176:ALA:HB1	1:E:178:GLN:NE2	2.36	0.41
1:A:70:ASN:ND2	1:A:75:LEU:HB3	2.35	0.41
1:B:214:LYS:HA	1:B:217:ARG:HE	1.85	0.41
1:B:416:THR:OG1	1:B:417:PRO:CG	2.65	0.41
1:B:483:VAL:O	1:B:511:VAL:HA	2.21	0.41
1:B:540:LYS:NZ	5:B:705:LMT:O6'	2.54	0.41
1:C:522:ILE:HG23	1:C:563:ILE:HD11	2.02	0.41
1:D:616:VAL:C	1:D:618:VAL:N	2.72	0.41
1:E:369:ASP:OD1	1:E:369:ASP:N	2.51	0.41
1:E:392:LEU:CD1	1:E:393:PRO:HD2	2.50	0.41
1:C:440:ALA:O	1:C:444:ASP:N	2.53	0.41
1:D:416:THR:HG1	1:D:417:PRO:HD2	1.75	0.41
1:D:570:LEU:HD23	1:D:572:TYR:CE1	2.55	0.41
1:D:70:ASN:ND2	1:D:75:LEU:HB3	2.36	0.41
1:E:440:ALA:O	1:E:444:ASP:N	2.53	0.41
1:A:550:SER:HA	1:A:591:VAL:HG21	2.02	0.41
1:E:448:PHE:O	1:E:509:LEU:N	2.50	0.41
1:E:616:VAL:C	1:E:618:VAL:N	2.72	0.41
1:A:440:ALA:O	1:A:444:ASP:N	2.53	0.41
1:B:344:GLN:NE2	1:B:568:PRO:CB	2.84	0.41
1:B:70:ASN:ND2	1:B:75:LEU:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:NH2	1:E:174:LEU:HD13	2.36	0.41
1:A:223:THR:HG22	1:A:224:ARG:N	2.36	0.41
1:B:570:LEU:HB3	1:B:572:TYR:CE1	2.55	0.41
1:C:530:ILE:HD13	1:C:624:TYR:CD2	2.42	0.41
1:E:392:LEU:HD13	1:E:393:PRO:HD2	2.01	0.41
1:E:522:ILE:HG23	1:E:563:ILE:HD11	2.01	0.41
1:E:550:SER:HA	1:E:591:VAL:HG21	2.03	0.41
1:E:68:MET:HA	1:E:169:GLN:O	2.20	0.41
1:E:70:ASN:ND2	1:E:75:LEU:HB3	2.36	0.41
1:A:251:ASP:OD1	1:A:255:LYS:N	2.53	0.41
1:A:555:VAL:HG22	1:B:554:LEU:HD12	2.02	0.41
1:B:632:TYR:C	1:B:632:TYR:CD1	2.93	0.41
1:D:441:TYR:HD2	1:D:574:THR:HG21	1.84	0.41
1:D:632:TYR:CD1	1:D:632:TYR:C	2.93	0.41
1:E:239:ILE:HB	1:E:299:VAL:HG23	2.02	0.41
1:B:54:SER:CB	1:B:195:ALA:HB2	2.51	0.41
1:C:570:LEU:HD23	1:C:572:TYR:CE1	2.55	0.41
1:C:550:SER:HA	1:C:591:VAL:HG21	2.03	0.41
1:C:70:ASN:ND2	1:C:75:LEU:HB3	2.36	0.41
1:E:98:LYS:HD3	1:E:100:LEU:HD11	2.03	0.41
1:A:104:ASN:O	1:A:108:SER:CB	2.69	0.40
1:B:223:THR:HG22	1:B:224:ARG:N	2.36	0.40
1:D:251:ASP:OD1	1:D:255:LYS:N	2.53	0.40
1:D:54:SER:CB	1:D:195:ALA:HB2	2.51	0.40
1:D:550:SER:HA	1:D:591:VAL:HG21	2.03	0.40
1:E:476:GLN:HB3	1:E:479:GLU:CG	2.51	0.40
1:A:211:ARG:CA	1:A:299:VAL:HG23	2.50	0.40
1:A:570:LEU:HD23	1:A:572:TYR:CE1	2.56	0.40
1:B:441:TYR:CE2	1:B:567:LEU:HD12	2.42	0.40
1:C:431:LEU:HD21	1:C:450:ILE:HG23	2.04	0.40
1:D:162:THR:HG22	1:D:163:TYR:N	2.36	0.40
1:D:83:ALA:HB2	1:D:143:TYR:CE2	2.56	0.40
1:B:40:HIS:NE2	1:B:184:GLY:O	2.47	0.40
1:C:54:SER:CB	1:C:195:ALA:HB2	2.51	0.40
1:C:432:GLN:HB3	1:B:338:GLN:HE22	1.87	0.40
1:D:440:ALA:O	1:D:443:PHE:N	2.55	0.40
1:A:54:SER:OG	1:A:195:ALA:HB2	2.22	0.40
1:D:157:ASP:O	1:D:158:LYS:HG3	2.21	0.40
1:E:597:GLN:NE2	1:E:612:ILE:CG2	2.81	0.40
1:A:567:LEU:HD13	1:A:576:LEU:HD23	2.04	0.40
1:B:83:ALA:HB2	1:B:143:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:THR:HA	1:D:417:PRO:HD3	1.91	0.40

All (6) 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:E:468:ARG:NH2	1:B:262:ILE:CG2[4_479]	1.05	1.15
1:D:468:ARG:NH2	1:C:262:ILE:CG2[4_4710]	1.27	0.93
1:D:468:ARG:NH2	1:C:262:ILE:CB[4_4710]	1.40	0.80
1:D:468:ARG:NH2	1:C:262:ILE:CG1[4_4710]	1.88	0.32
1:E:468:ARG:CZ	1:B:262:ILE:CG2[4_479]	2.00	0.20
1:E:468:ARG:NH2	1:B:262:ILE:CB[4_479]	2.12	0.08

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	577/642 (90%)	544 (94%)	28 (5%)	5 (1%)	17	57
1	B	578/642 (90%)	545 (94%)	27 (5%)	6 (1%)	15	55
1	C	580/642 (90%)	548 (94%)	28 (5%)	4 (1%)	22	62
1	D	583/642 (91%)	551 (94%)	27 (5%)	5 (1%)	17	57
1	E	583/642 (91%)	554 (95%)	23 (4%)	6 (1%)	15	55
All	All	2901/3210 (90%)	2742 (94%)	133 (5%)	26 (1%)	17	57

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ALA
1	A	383	ILE
1	E	131	ALA

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Mol	Chain	Res	Type
1	E	307	ASN
1	E	383	ILE
1	D	131	ALA
1	D	307	ASN
1	D	383	ILE
1	C	131	ALA
1	C	307	ASN
1	B	131	ALA
1	B	307	ASN
1	A	225	ASN
1	E	225	ASN
1	D	225	ASN
1	C	225	ASN
1	C	383	ILE
1	B	225	ASN
1	A	201	PRO
1	B	322	SER
1	B	383	ILE
1	A	105	ASP
1	E	201	PRO
1	B	201	PRO
1	D	417	PRO
1	E	417	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/557 (89%)	489 (99%)	7 (1%)	67	85
1	B	498/557 (89%)	490 (98%)	8 (2%)	62	83
1	C	499/557 (90%)	493 (99%)	6 (1%)	71	87
1	D	500/557 (90%)	494 (99%)	6 (1%)	71	87
1	E	500/557 (90%)	492 (98%)	8 (2%)	62	83
All	All	2493/2785 (90%)	2458 (99%)	35 (1%)	67	85

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	SER
1	A	96	LEU
1	A	100	LEU
1	A	307	ASN
1	A	348	ASN
1	A	479	GLU
1	A	539	LEU
1	E	96	LEU
1	E	100	LEU
1	E	227	GLN
1	E	307	ASN
1	E	325	LEU
1	E	358	SER
1	E	479	GLU
1	E	590	VAL
1	D	96	LEU
1	D	208	LEU
1	D	307	ASN
1	D	348	ASN
1	D	358	SER
1	D	479	GLU
1	C	96	LEU
1	C	208	LEU
1	C	218	TYR
1	C	307	ASN
1	C	358	SER
1	C	479	GLU
1	B	96	LEU
1	B	208	LEU
1	B	295	SER
1	B	307	ASN
1	B	358	SER
1	B	390	ILE
1	B	409	GLN
1	B	479	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	154	GLN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	175	ASN
1	A	178	GLN
1	A	338	GLN
1	A	344	GLN
1	A	403	GLN
1	A	432	GLN
1	A	489	GLN
1	A	545	GLN
1	A	597	GLN
1	E	70	ASN
1	E	154	GLN
1	E	175	ASN
1	E	178	GLN
1	E	277	GLN
1	E	338	GLN
1	E	403	GLN
1	E	432	GLN
1	E	489	GLN
1	E	545	GLN
1	E	597	GLN
1	D	70	ASN
1	D	154	GLN
1	D	175	ASN
1	D	178	GLN
1	D	338	GLN
1	D	344	GLN
1	D	403	GLN
1	D	432	GLN
1	D	489	GLN
1	D	545	GLN
1	D	597	GLN
1	C	70	ASN
1	C	104	ASN
1	C	154	GLN
1	C	175	ASN
1	C	338	GLN
1	C	344	GLN
1	C	403	GLN
1	C	432	GLN
1	C	489	GLN
1	C	545	GLN

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Mol	Chain	Res	Type
1	C	597	GLN
1	B	70	ASN
1	B	175	ASN
1	B	338	GLN
1	B	344	GLN
1	B	403	GLN
1	B	432	GLN
1	B	489	GLN
1	B	545	GLN
1	B	597	GLN

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 ⓘ

Of 27 ligands modelled in this entry, 17 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
5	LMT	E	705	-	26,26,36	1.40	3 (11%)	37,37,47	2.28	10 (27%)
5	LMT	B	704	-	26,26,36	1.10	1 (3%)	37,37,47	1.60	7 (18%)
5	LMT	C	706	-	28,28,36	1.25	1 (3%)	39,39,47	2.14	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LMT	E	703	-	26,26,36	1.05	1 (3%)	37,37,47	1.60	5 (13%)
5	LMT	B	705	-	27,27,36	1.22	1 (3%)	37,38,47	1.82	10 (27%)
5	LMT	C	705	-	26,26,36	1.14	1 (3%)	37,37,47	1.77	9 (24%)
5	LMT	B	706	-	28,28,36	0.50	0	39,39,47	1.24	6 (15%)
5	LMT	E	704	-	26,26,36	0.98	1 (3%)	37,37,47	2.02	13 (35%)
5	LMT	D	703	-	27,27,36	1.28	1 (3%)	37,38,47	2.41	9 (24%)
5	LMT	A	707	-	26,26,36	1.24	2 (7%)	37,37,47	1.97	8 (21%)

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
5	LMT	E	705	-	-	5/11/51/61	0/2/2/2
5	LMT	B	704	-	-	5/11/51/61	0/2/2/2
5	LMT	C	706	-	-	3/13/53/61	0/2/2/2
5	LMT	E	703	-	-	5/11/51/61	0/2/2/2
5	LMT	B	705	-	-	6/12/52/61	0/2/2/2
5	LMT	C	705	-	-	6/11/51/61	0/2/2/2
5	LMT	B	706	-	-	5/13/53/61	0/2/2/2
5	LMT	E	704	-	-	8/11/51/61	0/2/2/2
5	LMT	D	703	-	-	5/12/52/61	0/2/2/2
5	LMT	A	707	-	-	5/11/51/61	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	705	LMT	O1'-C1'	4.59	1.48	1.40
5	D	703	LMT	O1'-C1'	4.47	1.47	1.40
5	A	707	LMT	O1'-C1'	4.12	1.47	1.40
5	B	705	LMT	O1'-C1'	4.07	1.47	1.40
5	C	705	LMT	O1'-C1'	3.99	1.47	1.40
5	C	706	LMT	O1'-C1'	3.80	1.46	1.40
5	B	704	LMT	O1'-C1'	3.61	1.46	1.40
5	E	703	LMT	O1'-C1'	2.92	1.45	1.40
5	E	704	LMT	O1'-C1'	2.85	1.45	1.40
5	E	705	LMT	O1B-C1B	2.41	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	707	LMT	O1B-C1B	2.10	1.47	1.41
5	E	705	LMT	O5B-C1B	2.09	1.47	1.41

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	703	LMT	C1B-O5B-C5B	7.63	128.66	113.69
5	D	703	LMT	C1-O1'-C1'	7.17	125.73	113.84
5	E	705	LMT	C1B-O5B-C5B	6.72	126.89	113.69
5	C	706	LMT	C1B-O5B-C5B	5.85	125.17	113.69
5	E	705	LMT	C1'-O5'-C5'	5.52	124.52	113.69
5	A	707	LMT	O1B-C1B-C2B	5.49	122.32	108.10
5	A	707	LMT	C1B-O1B-C4'	5.03	130.41	117.96
5	E	705	LMT	O5'-C5'-C4'	4.88	120.05	109.75
5	E	703	LMT	O1B-C1B-C2B	4.79	120.51	108.10
5	A	707	LMT	C1'-O5'-C5'	4.67	122.85	113.69
5	D	703	LMT	C1'-O5'-C5'	4.42	122.37	113.69
5	E	703	LMT	C1'-O5'-C5'	4.35	122.23	113.69
5	B	705	LMT	C1B-O5B-C5B	4.29	122.11	113.69
5	E	703	LMT	C1B-O1B-C4'	4.27	128.53	117.96
5	B	704	LMT	C1'-O5'-C5'	4.25	122.03	113.69
5	B	705	LMT	C1-O1'-C1'	4.24	120.87	113.84
5	C	705	LMT	O1B-C1B-C2B	4.16	118.89	108.10
5	C	706	LMT	C1-O1'-C1'	4.05	120.56	113.84
5	C	706	LMT	C3B-C4B-C5B	3.94	117.26	110.24
5	A	707	LMT	C1B-O5B-C5B	3.92	121.38	113.69
5	C	706	LMT	O1'-C1'-C2'	3.87	114.35	108.30
5	E	704	LMT	C4B-C3B-C2B	3.80	117.46	110.82
5	C	705	LMT	O2B-C2B-C1B	3.73	119.12	110.05
5	C	706	LMT	O1B-C4'-C3'	3.70	117.12	107.28
5	B	704	LMT	O5'-C5'-C4'	3.68	117.52	109.75
5	E	704	LMT	C3B-C4B-C5B	3.65	116.75	110.24
5	E	704	LMT	C1B-O1B-C4'	3.63	126.96	117.96
5	B	705	LMT	C3B-C4B-C5B	3.61	116.68	110.24
5	B	704	LMT	C1B-O1B-C4'	3.61	126.89	117.96
5	C	706	LMT	O5'-C1'-C2'	-3.52	102.89	110.35
5	E	705	LMT	O5B-C5B-C4B	3.52	116.08	109.69
5	C	706	LMT	O5B-C5B-C6B	3.51	115.16	106.44
5	C	705	LMT	O1'-C1'-C2'	3.45	113.69	108.30
5	E	704	LMT	C1B-O5B-C5B	3.43	120.42	113.69
5	E	705	LMT	C2'-C3'-C4'	3.42	117.48	109.68
5	E	704	LMT	O5B-C5B-C6B	3.35	114.77	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	704	LMT	O1B-C1B-C2B	-3.30	99.55	108.10
5	B	706	LMT	O1B-C4'-C3'	3.30	116.06	107.28
5	D	703	LMT	O5'-C1'-C2'	-3.30	103.37	110.35
5	D	703	LMT	O5'-C5'-C4'	3.22	116.53	109.75
5	B	706	LMT	C1B-O5B-C5B	3.18	119.92	113.69
5	B	706	LMT	C4B-C3B-C2B	-3.17	105.29	110.82
5	B	704	LMT	O1B-C1B-C2B	3.16	116.29	108.10
5	C	705	LMT	C1B-O1B-C4'	3.12	125.69	117.96
5	D	703	LMT	C3B-C4B-C5B	3.12	115.80	110.24
5	D	703	LMT	C2'-C3'-C4'	3.10	116.77	109.68
5	C	706	LMT	C2'-C3'-C4'	3.09	116.74	109.68
5	E	704	LMT	O1'-C1'-C2'	3.08	113.11	108.30
5	B	705	LMT	O1'-C1'-C2'	3.03	113.03	108.30
5	B	705	LMT	O5'-C1'-C2'	-2.99	104.02	110.35
5	E	704	LMT	O5'-C1'-C2'	-2.94	104.12	110.35
5	B	706	LMT	O5B-C5B-C4B	2.91	114.97	109.69
5	C	706	LMT	O5'-C5'-C4'	2.86	115.79	109.75
5	E	703	LMT	O2B-C2B-C1B	2.85	116.97	110.05
5	E	705	LMT	C1B-O1B-C4'	2.77	124.82	117.96
5	C	705	LMT	O5'-C5'-C4'	2.77	115.58	109.75
5	E	704	LMT	C1'-O5'-C5'	2.73	119.04	113.69
5	B	705	LMT	C2'-C3'-C4'	2.72	115.89	109.68
5	C	705	LMT	C1'-O5'-C5'	2.70	118.99	113.69
5	E	705	LMT	C1'-C2'-C3'	2.67	115.56	110.00
5	C	706	LMT	C1B-O1B-C4'	2.67	124.56	117.96
5	E	705	LMT	O1'-C1'-C2'	2.59	112.35	108.30
5	E	704	LMT	C1B-C2B-C3B	2.57	115.34	110.00
5	D	703	LMT	O1B-C1B-C2B	2.56	114.74	108.10
5	B	705	LMT	C1B-O1B-C4'	2.49	124.14	117.96
5	B	704	LMT	O2B-C2B-C1B	2.47	116.06	110.05
5	A	707	LMT	O2B-C2B-C1B	2.44	115.97	110.05
5	B	704	LMT	O1'-C1'-C2'	2.42	112.08	108.30
5	B	705	LMT	O1B-C4'-C3'	2.41	113.70	107.28
5	B	704	LMT	O5B-C5B-C6B	2.41	112.42	106.44
5	C	705	LMT	O5'-C1'-C2'	-2.39	105.28	110.35
5	C	706	LMT	O5B-C5B-C4B	2.39	114.03	109.69
5	E	704	LMT	O5'-C5'-C6'	2.37	112.33	106.44
5	B	705	LMT	O5'-C5'-C4'	2.36	114.73	109.75
5	A	707	LMT	O5'-C5'-C4'	2.33	114.66	109.75
5	E	703	LMT	O5'-C5'-C4'	2.32	114.65	109.75
5	E	705	LMT	C1-O1'-C1'	2.26	119.03	113.92
5	A	707	LMT	O1'-C1'-C2'	2.25	111.82	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	706	LMT	C6B-C5B-C4B	-2.19	107.88	113.00
5	C	705	LMT	O5B-C5B-C6B	2.13	111.72	106.44
5	B	706	LMT	O5B-C1B-C2B	2.10	114.79	110.35
5	C	705	LMT	C1-O1'-C1'	2.10	118.66	113.92
5	E	705	LMT	O1B-C4'-C3'	2.10	112.86	107.28
5	C	706	LMT	C1'-C2'-C3'	2.08	114.34	110.00
5	E	704	LMT	O1B-C4'-C3'	2.07	112.79	107.28
5	E	704	LMT	C1-O1'-C1'	2.03	118.50	113.92
5	D	703	LMT	O5B-C5B-C4B	2.01	113.35	109.69
5	A	707	LMT	O5B-C5B-C4B	2.01	113.34	109.69
5	B	705	LMT	O5B-C5B-C4B	2.00	113.33	109.69

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	705	LMT	C2B-C1B-O1B-C4'
5	E	703	LMT	C2B-C1B-O1B-C4'
5	D	703	LMT	C2'-C1'-O1'-C1
5	D	703	LMT	O5'-C1'-O1'-C1
5	A	707	LMT	C2B-C1B-O1B-C4'
5	B	704	LMT	C2'-C1'-O1'-C1
5	B	704	LMT	O5'-C1'-O1'-C1
5	E	704	LMT	C2'-C1'-O1'-C1
5	E	704	LMT	O5'-C1'-O1'-C1
5	B	706	LMT	C3'-C4'-O1B-C1B
5	B	704	LMT	C2B-C1B-O1B-C4'
5	B	706	LMT	O5'-C5'-C6'-O6'
5	B	705	LMT	O5B-C5B-C6B-O6B
5	B	706	LMT	C4B-C5B-C6B-O6B
5	C	706	LMT	O5B-C5B-C6B-O6B
5	B	706	LMT	O5B-C5B-C6B-O6B
5	E	703	LMT	O5B-C5B-C6B-O6B
5	B	706	LMT	C4'-C5'-C6'-O6'
5	D	703	LMT	C4B-C5B-C6B-O6B
5	C	706	LMT	O5'-C1'-O1'-C1
5	E	703	LMT	C4'-C5'-C6'-O6'
5	B	705	LMT	C4B-C5B-C6B-O6B
5	E	704	LMT	O5'-C5'-C6'-O6'
5	E	703	LMT	C4B-C5B-C6B-O6B
5	C	705	LMT	O5B-C5B-C6B-O6B
5	D	703	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	E	705	LMT	C4'-C5'-C6'-O6'
5	E	704	LMT	O5B-C1B-O1B-C4'
5	C	706	LMT	C2'-C1'-O1'-C1
5	E	704	LMT	O5B-C5B-C6B-O6B
5	E	705	LMT	O5'-C5'-C6'-O6'
5	E	703	LMT	O5'-C5'-C6'-O6'
5	D	703	LMT	O1'-C1-C2-C3
5	B	704	LMT	O5'-C5'-C6'-O6'
5	E	704	LMT	C5'-C4'-O1B-C1B
5	E	704	LMT	C3'-C4'-O1B-C1B
5	A	707	LMT	O5B-C5B-C6B-O6B
5	E	705	LMT	O5B-C5B-C6B-O6B
5	B	704	LMT	O5B-C5B-C6B-O6B
5	B	705	LMT	C3'-C4'-O1B-C1B
5	C	705	LMT	O5'-C5'-C6'-O6'
5	A	707	LMT	O5'-C5'-C6'-O6'
5	B	705	LMT	C5'-C4'-O1B-C1B
5	E	704	LMT	C2-C1-O1'-C1'
5	B	705	LMT	C4'-C5'-C6'-O6'
5	C	705	LMT	C4B-C5B-C6B-O6B
5	B	705	LMT	O1'-C1-C2-C3
5	A	707	LMT	O5B-C1B-O1B-C4'
5	E	705	LMT	O5'-C1'-O1'-C1
5	E	705	LMT	C2'-C1'-O1'-C1
5	C	705	LMT	O5'-C1'-O1'-C1
5	A	707	LMT	C5'-C4'-O1B-C1B
5	C	705	LMT	C2'-C1'-O1'-C1

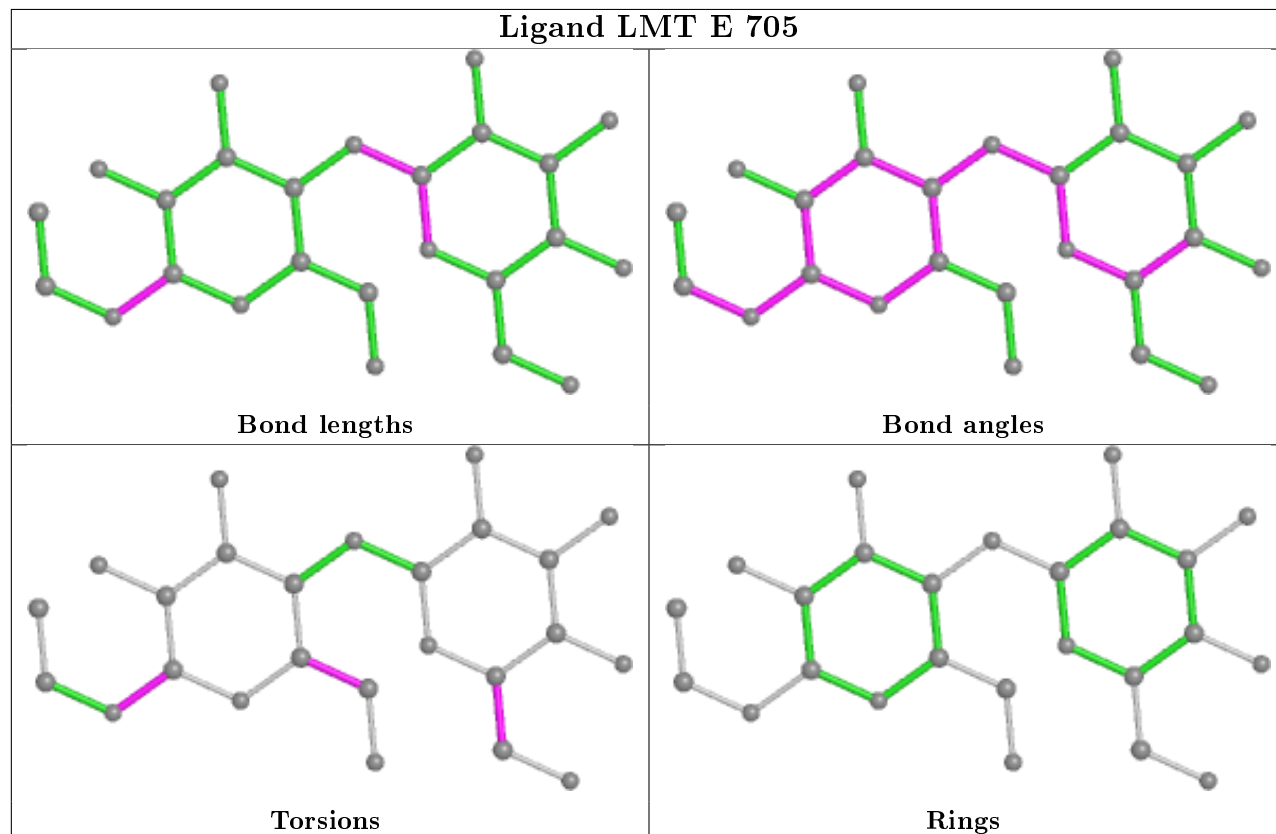
There are no ring outliers.

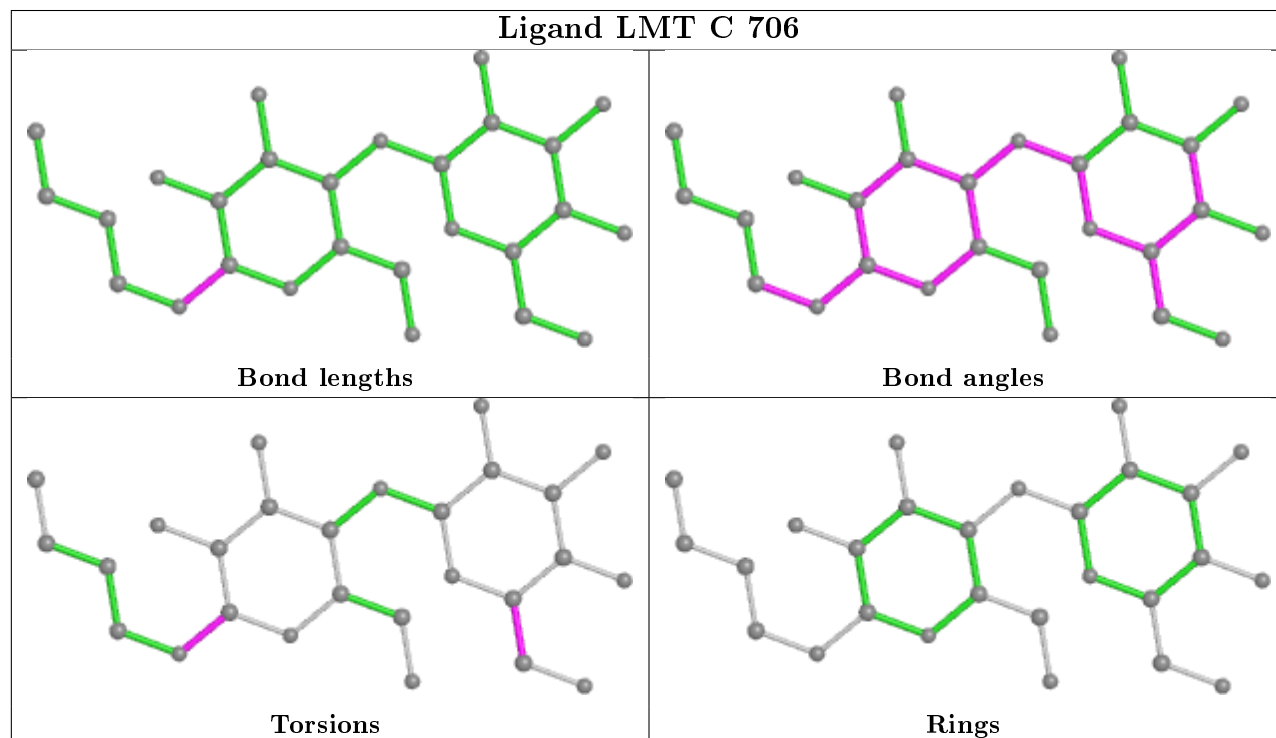
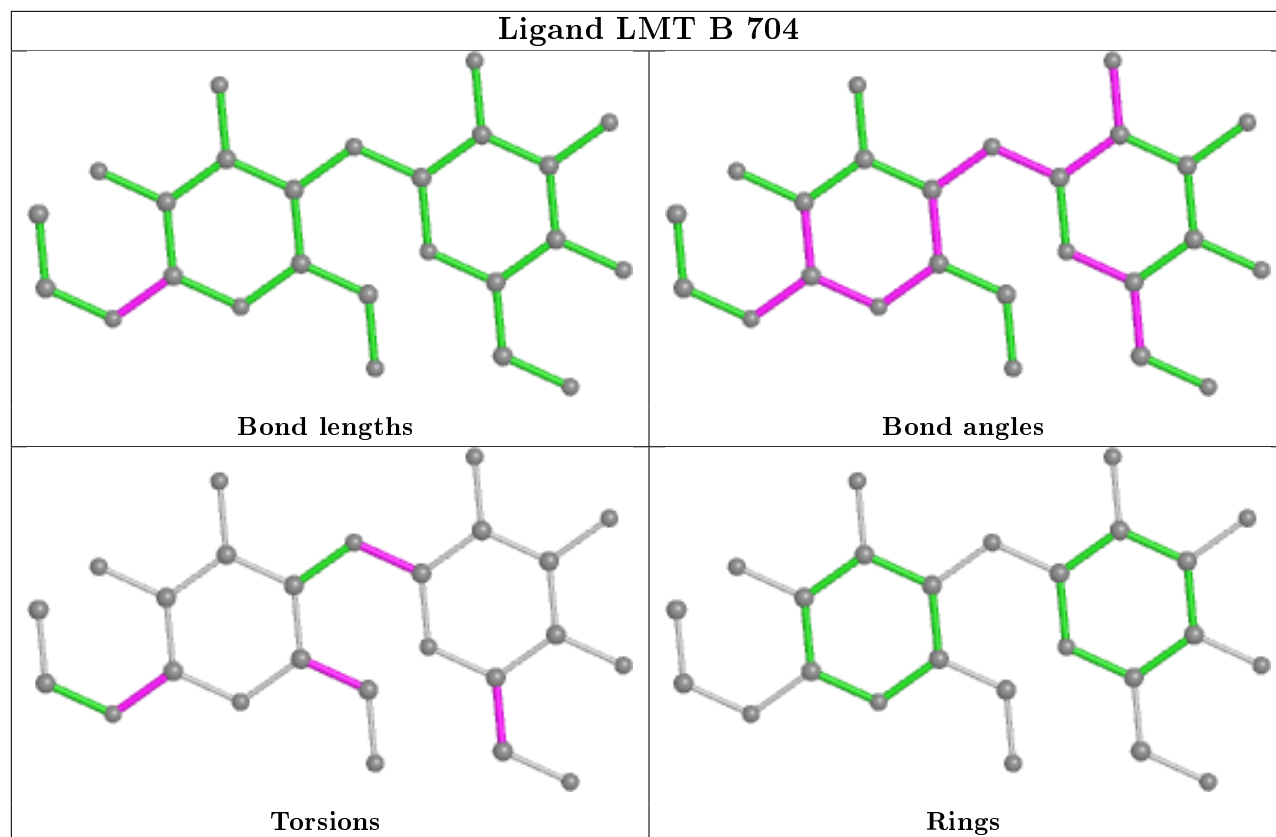
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	705	LMT	1	0
5	B	706	LMT	9	0

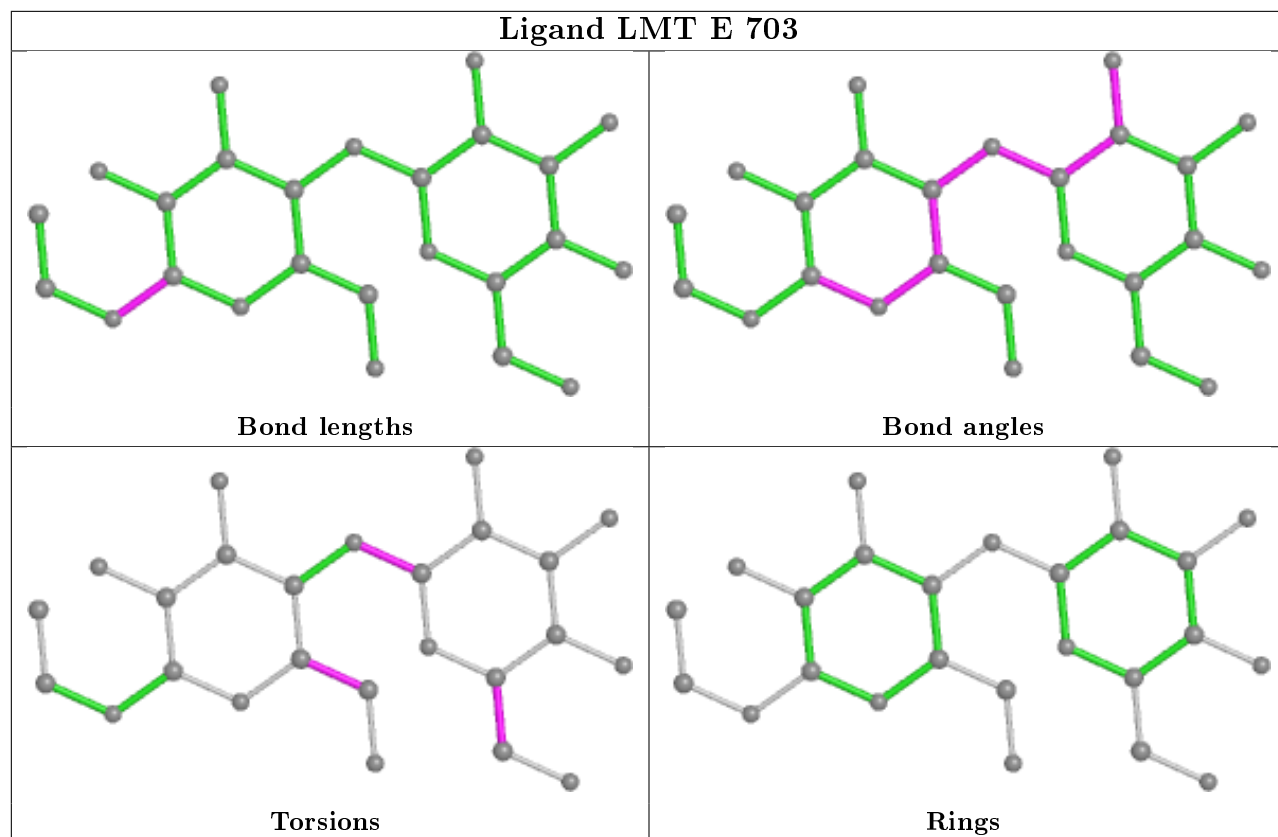
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

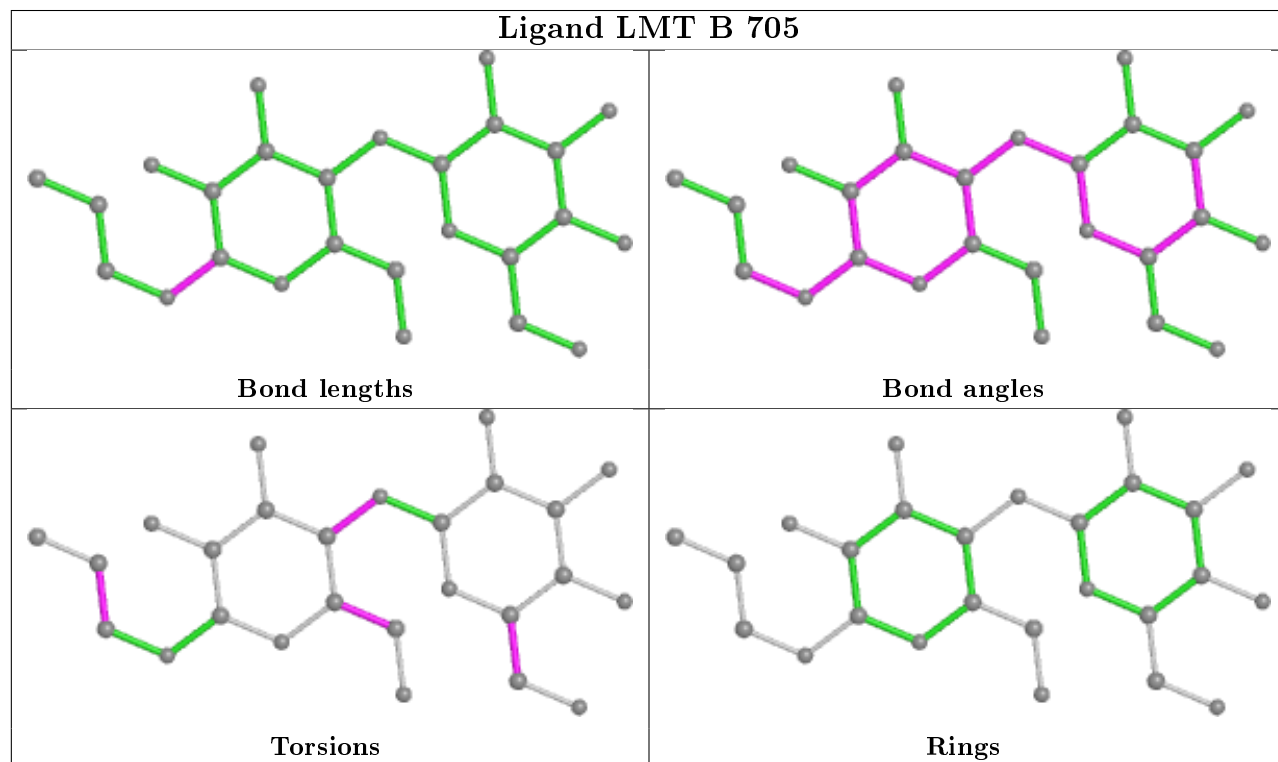


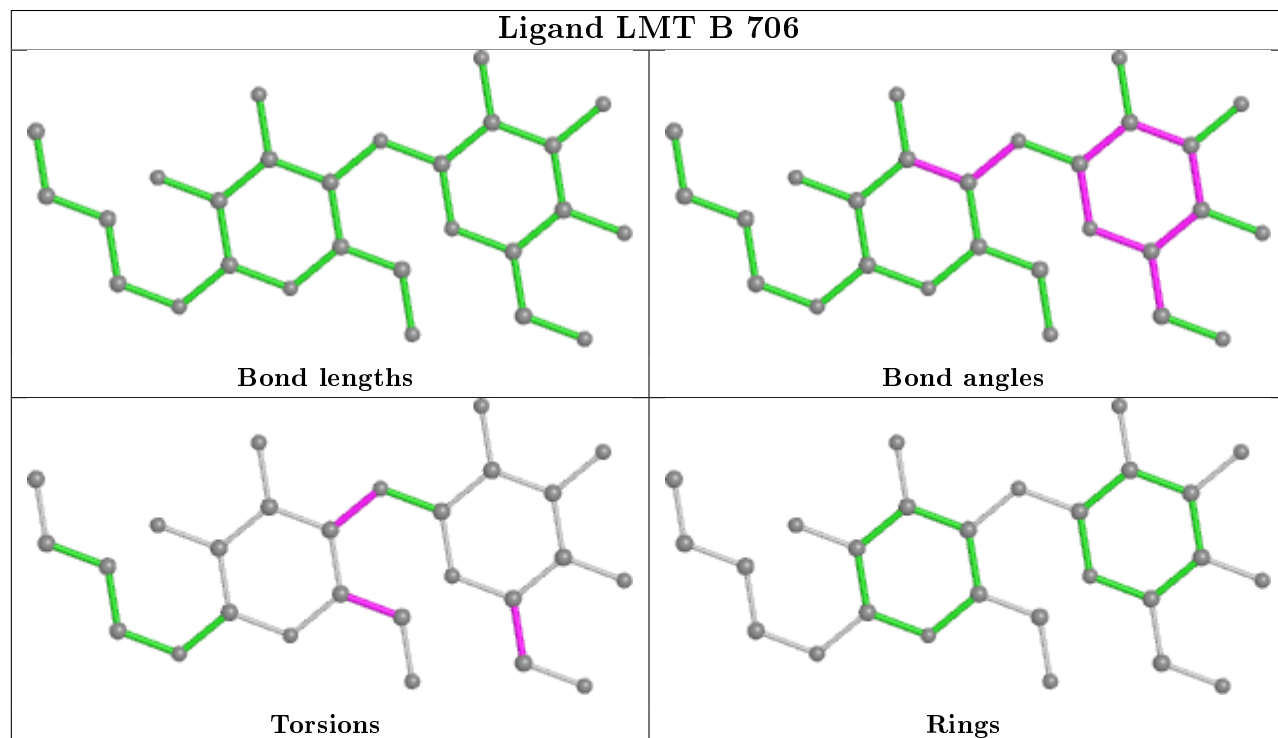
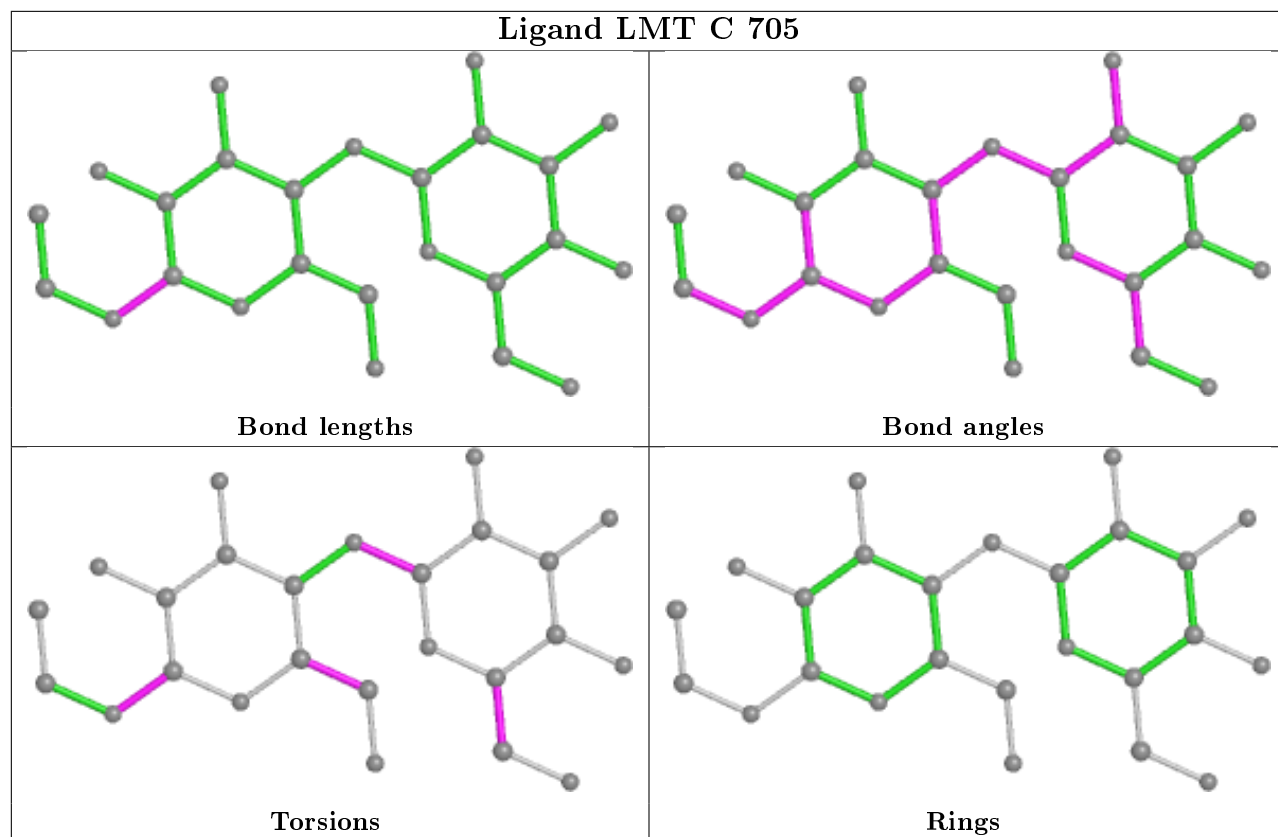


Ligand LMT E 703

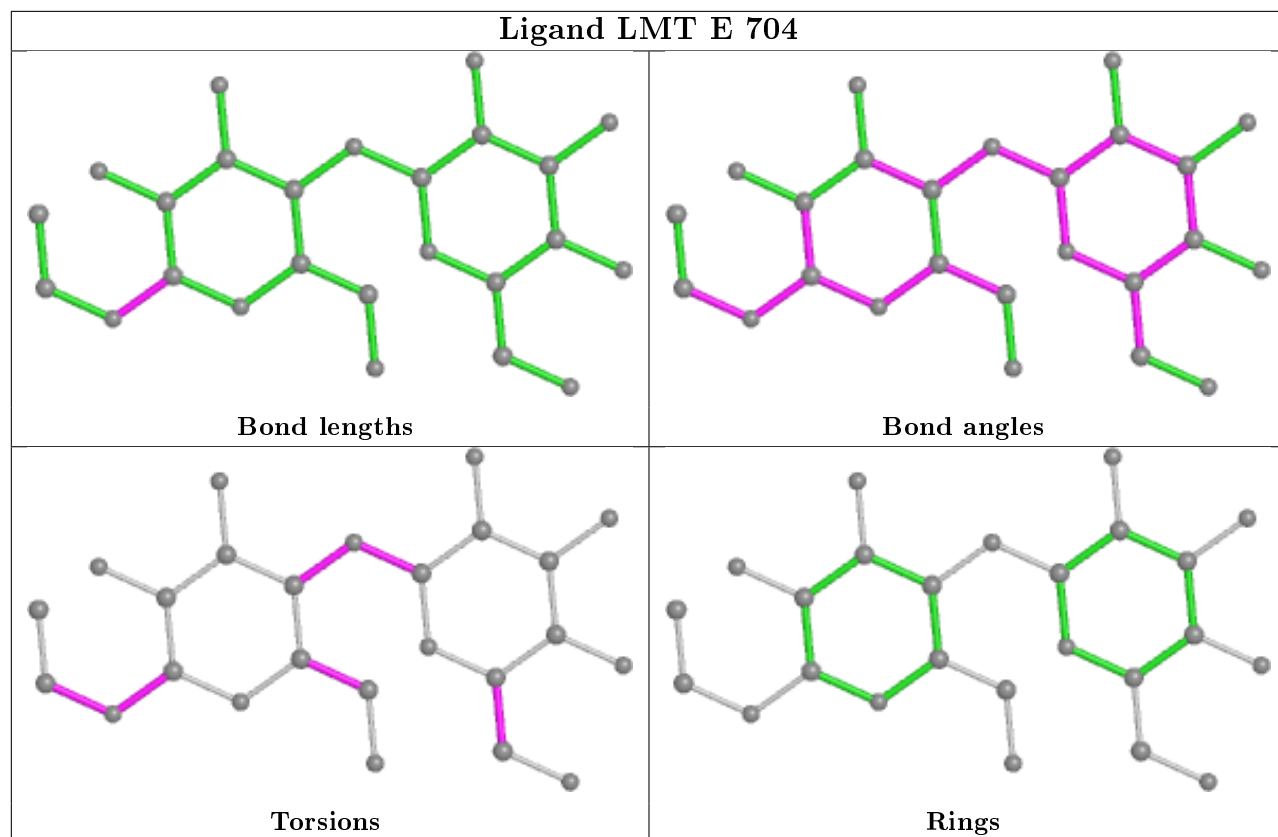


Ligand LMT B 705

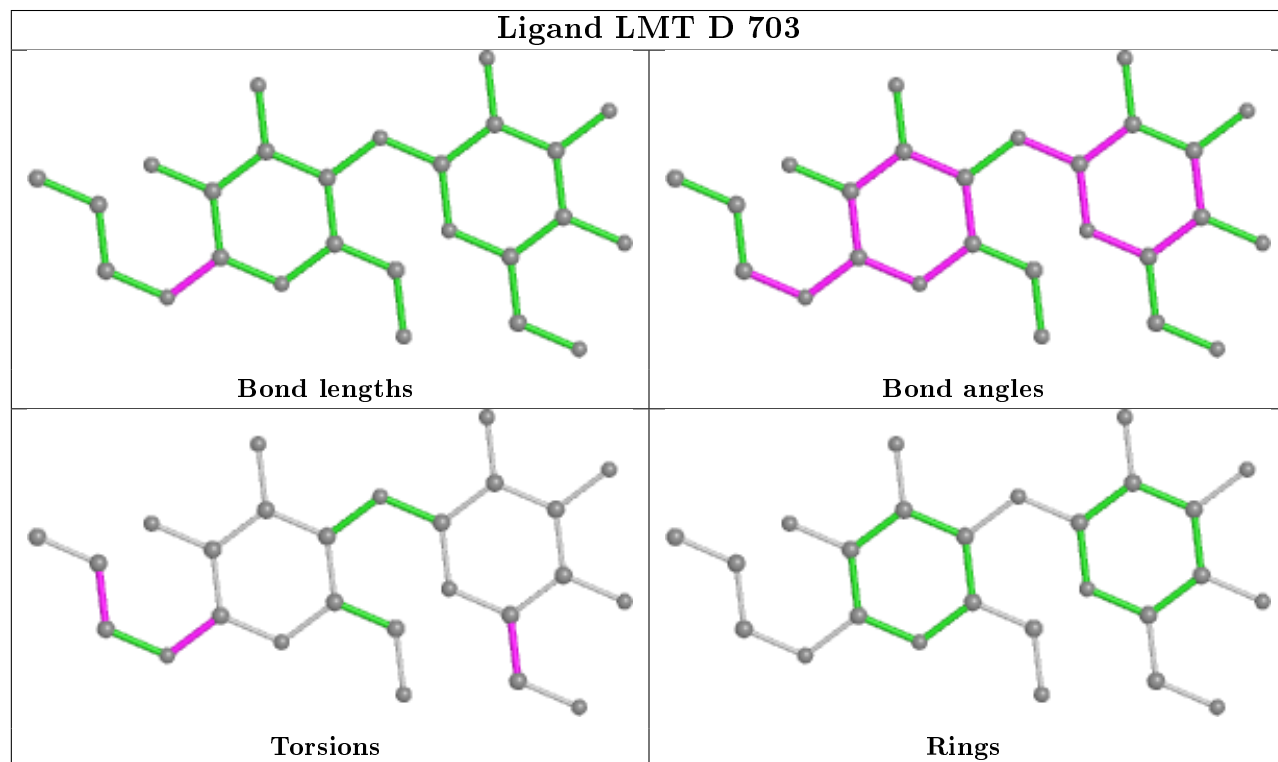


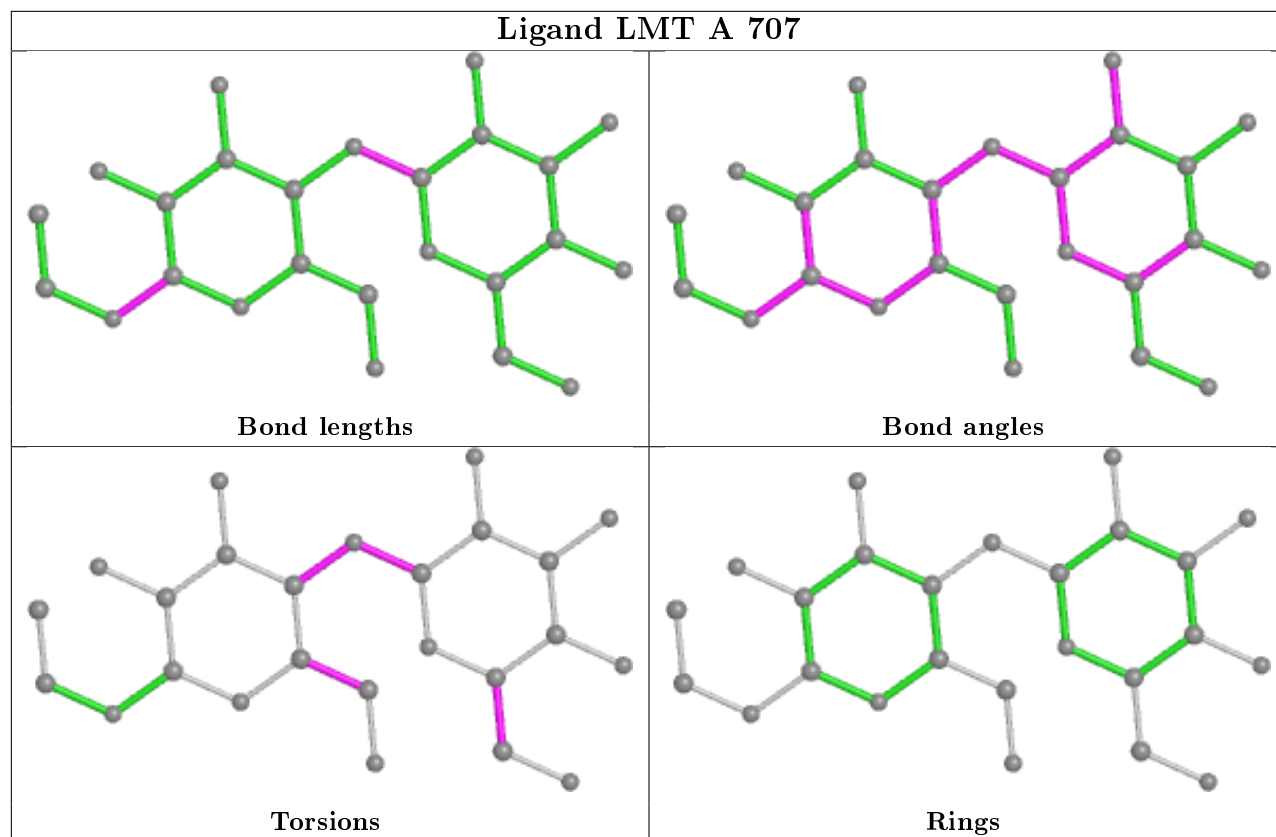


Ligand LMT E 704



Ligand LMT D 703





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	585/642 (91%)	0.58	92 (15%) 2 1	58, 149, 242, 288	0
1	B	586/642 (91%)	0.26	48 (8%) 11 8	55, 137, 203, 228	0
1	C	588/642 (91%)	0.27	55 (9%) 8 5	57, 133, 208, 238	0
1	D	591/642 (92%)	0.38	65 (10%) 5 4	53, 136, 216, 239	0
1	E	591/642 (92%)	0.40	68 (11%) 4 4	52, 146, 238, 265	0
All	All	2941/3210 (91%)	0.38	328 (11%) 5 4	52, 139, 226, 288	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ALA	9.7
1	C	171	ILE	9.5
1	D	80	GLY	9.5
1	A	173	GLY	9.0
1	A	226	LEU	8.7
1	D	172	LEU	8.2
1	C	172	LEU	8.1
1	E	79	VAL	7.7
1	E	182	GLY	7.7
1	B	80	GLY	7.7
1	E	64	ILE	7.4
1	A	66	ALA	7.3
1	C	66	ALA	7.3
1	A	53	TYR	7.2
1	D	79	VAL	7.0
1	A	144	HIS	7.0
1	A	248	ARG	6.9
1	D	88	PRO	6.9
1	A	172	LEU	6.8
1	A	143	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	58	MET	6.4
1	C	173	GLY	6.3
1	B	88	PRO	6.3
1	C	39	GLN	6.2
1	B	173	GLY	6.2
1	C	191	PHE	6.2
1	A	145	ILE	6.2
1	C	182	GLY	6.0
1	D	53	TYR	6.0
1	D	145	ILE	5.9
1	E	57	ASP	5.9
1	A	189	GLU	5.9
1	D	39	GLN	5.8
1	B	79	VAL	5.8
1	C	639	HIS	5.8
1	A	56	PRO	5.8
1	C	67	SER	5.7
1	B	53	TYR	5.7
1	A	80	GLY	5.7
1	A	247	LEU	5.6
1	E	80	GLY	5.6
1	D	146	PHE	5.5
1	B	172	LEU	5.5
1	A	55	LEU	5.5
1	E	137	ILE	5.4
1	C	189	GLU	5.4
1	E	62	ASP	5.4
1	D	66	ALA	5.3
1	C	79	VAL	5.3
1	C	53	TYR	5.2
1	A	258	ALA	5.1
1	C	88	PRO	5.1
1	D	140	ASP	5.0
1	D	141	GLY	5.0
1	B	133	LEU	4.9
1	C	41	PHE	4.9
1	B	171	ILE	4.8
1	A	285	HIS	4.8
1	A	67	SER	4.8
1	C	64	ILE	4.8
1	D	57	ASP	4.8
1	B	52	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	143	TYR	4.6
1	E	269	VAL	4.6
1	D	81	ILE	4.6
1	C	38	VAL	4.6
1	A	81	ILE	4.5
1	B	145	ILE	4.5
1	A	249	LEU	4.5
1	B	184	GLY	4.5
1	E	66	ALA	4.5
1	C	170	LEU	4.5
1	E	268	SER	4.5
1	A	88	PRO	4.5
1	E	171	ILE	4.5
1	B	146	PHE	4.5
1	A	280	CYS	4.4
1	E	39	GLN	4.4
1	A	200	LYS	4.4
1	D	51	ILE	4.4
1	E	56	PRO	4.3
1	D	190	VAL	4.3
1	C	80	GLY	4.3
1	D	64	ILE	4.3
1	D	133	LEU	4.2
1	D	52	PHE	4.2
1	A	39	GLN	4.2
1	A	54	SER	4.2
1	C	179	VAL	4.2
1	A	57	ASP	4.1
1	E	88	PRO	4.1
1	E	237	GLU	4.1
1	E	170	LEU	4.0
1	C	133	LEU	4.0
1	A	256	PRO	4.0
1	A	218	TYR	4.0
1	E	60	GLN	4.0
1	B	147	ALA	4.0
1	A	245	PRO	4.0
1	E	145	ILE	4.0
1	A	239	ILE	3.9
1	D	173	GLY	3.9
1	C	132	SER	3.9
1	A	64	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	639	HIS	3.9
1	E	141	GLY	3.9
1	E	59	LYS	3.9
1	C	187	GLU	3.9
1	C	190	VAL	3.8
1	B	134	GLU	3.8
1	B	64	ILE	3.8
1	A	188	GLY	3.8
1	E	67	SER	3.8
1	B	138	PRO	3.8
1	D	189	GLU	3.8
1	E	175	ASN	3.7
1	D	191	PHE	3.7
1	B	140	ASP	3.7
1	A	134	GLU	3.7
1	A	232	PHE	3.6
1	E	173	GLY	3.6
1	C	58	MET	3.6
1	E	148	GLY	3.6
1	E	140	ASP	3.6
1	C	135	PHE	3.6
1	A	299	VAL	3.5
1	B	67	SER	3.5
1	E	172	LEU	3.5
1	E	218	TYR	3.5
1	C	37	ARG	3.5
1	D	56	PRO	3.5
1	C	142	THR	3.5
1	A	264	GLN	3.4
1	B	39	GLN	3.4
1	A	190	VAL	3.4
1	D	192	ALA	3.4
1	D	143	TYR	3.4
1	D	639	HIS	3.4
1	D	58	MET	3.4
1	D	120	GLY	3.4
1	A	142	THR	3.4
1	E	55	LEU	3.4
1	A	192	ALA	3.4
1	D	171	ILE	3.3
1	E	184	GLY	3.3
1	C	188	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	169	GLN	3.3
1	A	191	PHE	3.3
1	D	193	SER	3.3
1	C	136	THR	3.3
1	D	147	ALA	3.3
1	D	142	THR	3.3
1	C	56	PRO	3.3
1	C	174	LEU	3.3
1	C	140	ASP	3.2
1	E	262	ILE	3.2
1	E	41	PHE	3.2
1	B	136	THR	3.2
1	E	78	LEU	3.2
1	E	288	GLY	3.2
1	A	261	LEU	3.2
1	A	60	GLN	3.2
1	A	140	ASP	3.2
1	C	186	PRO	3.1
1	A	286	VAL	3.1
1	E	135	PHE	3.1
1	D	186	PRO	3.1
1	D	62	ASP	3.1
1	C	145	ILE	3.1
1	B	137	ILE	3.1
1	D	100	LEU	3.1
1	A	146	PHE	3.1
1	A	136	THR	3.1
1	A	240	GLY	3.1
1	D	135	PHE	3.1
1	C	141	GLY	3.0
1	C	62	ASP	3.0
1	A	104	ASN	3.0
1	B	191	PHE	3.0
1	D	268	SER	3.0
1	A	82	MET	3.0
1	A	215	ASP	3.0
1	C	184	GLY	3.0
1	D	179	VAL	3.0
1	C	57	ASP	3.0
1	A	79	VAL	3.0
1	A	147	ALA	2.9
1	E	69	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	211	ARG	2.9
1	D	96	LEU	2.9
1	B	190	VAL	2.9
1	C	40	HIS	2.9
1	D	134	GLU	2.9
1	D	69	GLN	2.9
1	A	288	GLY	2.9
1	E	61	GLY	2.9
1	B	203	ALA	2.9
1	E	38	VAL	2.9
1	D	67	SER	2.9
1	A	225	ASN	2.9
1	E	139	ARG	2.9
1	E	260	GLY	2.8
1	C	48	GLY	2.8
1	D	137	ILE	2.8
1	B	189	GLU	2.8
1	C	194	LEU	2.8
1	B	205	VAL	2.8
1	E	35	GLU	2.8
1	E	142	THR	2.8
1	A	171	ILE	2.8
1	C	55	LEU	2.8
1	A	83	ALA	2.8
1	E	178	GLN	2.7
1	D	82	MET	2.7
1	B	82	MET	2.7
1	A	201	PRO	2.7
1	A	135	PHE	2.7
1	E	65	TYR	2.7
1	D	269	VAL	2.7
1	E	122	ASP	2.7
1	A	216	THR	2.7
1	B	139	ARG	2.7
1	A	133	LEU	2.7
1	A	639	HIS	2.7
1	E	183	GLU	2.7
1	E	247	LEU	2.7
1	A	141	GLY	2.7
1	E	180	ILE	2.7
1	D	244	LEU	2.7
1	C	137	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLN	2.6
1	E	190	VAL	2.6
1	D	637	THR	2.6
1	B	135	PHE	2.6
1	E	286	VAL	2.6
1	A	263	ASP	2.6
1	E	212	LEU	2.6
1	A	203	ALA	2.6
1	B	305	GLY	2.6
1	A	298	ALA	2.6
1	D	237	GLU	2.6
1	C	81	ILE	2.6
1	A	257	LEU	2.5
1	B	179	VAL	2.5
1	E	63	ILE	2.5
1	A	252	SER	2.5
1	C	193	SER	2.5
1	A	241	GLU	2.5
1	C	143	TYR	2.5
1	D	132	SER	2.5
1	A	268	SER	2.5
1	D	38	VAL	2.5
1	A	307	ASN	2.5
1	E	245	PRO	2.4
1	E	96	LEU	2.4
1	E	177	PRO	2.4
1	D	288	GLY	2.4
1	A	637	THR	2.4
1	A	61	GLY	2.4
1	C	82	MET	2.4
1	B	63	ILE	2.4
1	A	187	GLU	2.4
1	B	122	ASP	2.4
1	D	122	ASP	2.4
1	A	139	ARG	2.4
1	D	194	LEU	2.4
1	D	106	LEU	2.3
1	B	204	HIS	2.3
1	A	282	LEU	2.3
1	C	175	ASN	2.3
1	B	104	ASN	2.3
1	D	78	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	65	TYR	2.3
1	B	65	TYR	2.3
1	B	144	HIS	2.3
1	A	41	PHE	2.3
1	C	146	PHE	2.3
1	A	269	VAL	2.3
1	E	475	ASP	2.3
1	D	61	GLY	2.3
1	C	60	GLN	2.3
1	A	68	MET	2.3
1	A	50	GLY	2.3
1	E	179	VAL	2.3
1	B	48	GLY	2.2
1	B	81	ILE	2.2
1	A	69	GLN	2.2
1	B	38	VAL	2.2
1	B	170	LEU	2.2
1	A	186	PRO	2.2
1	A	238	PRO	2.2
1	D	296	GLY	2.2
1	A	40	HIS	2.2
1	A	51	ILE	2.2
1	D	170	LEU	2.2
1	D	245	PRO	2.2
1	C	637	THR	2.2
1	C	180	ILE	2.2
1	D	159	PHE	2.2
1	B	51	ILE	2.2
1	A	170	LEU	2.1
1	E	248	ARG	2.1
1	D	68	MET	2.1
1	E	53	TYR	2.1
1	A	294	ASP	2.1
1	D	287	ASP	2.1
1	E	81	ILE	2.1
1	C	176	ALA	2.1
1	A	137	ILE	2.1
1	B	186	PRO	2.1
1	D	55	LEU	2.1
1	A	300	TYR	2.1
1	D	180	ILE	2.1
1	A	323	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	181	SER	2.1
1	D	105	ASP	2.1
1	A	564	SER	2.1
1	B	54	SER	2.1
1	A	209	GLU	2.1
1	E	270	GLU	2.1
1	B	61	GLY	2.1
1	B	512	LYS	2.1
1	A	210	ILE	2.1
1	C	226	LEU	2.1
1	E	83	ALA	2.0
1	E	285	HIS	2.0
1	D	262	ILE	2.0
1	E	138	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	B	701	1/1	-	-	170,170,170,170	1
5	LMT	E	704	25/35	0.62	0.29	94,203,246,254	0
4	CL	D	702	1/1	0.84	0.42	110,110,110,110	0
2	CA	E	701	1/1	0.98	0.11	140,140,140,140	0
2	CA	A	701	1/1	-	-	170,170,170,170	1
4	CL	E	702	1/1	0.72	0.67	121,121,121,121	0
3	NA	A	703	1/1	0.92	0.67	66,66,66,66	0
3	NA	C	702	1/1	-	-	170,170,170,170	1
5	LMT	B	704	25/35	0.64	0.24	129,211,244,265	0

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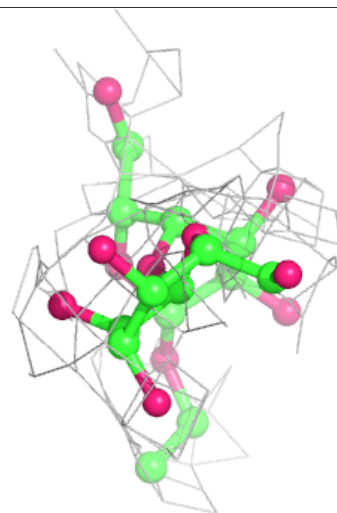
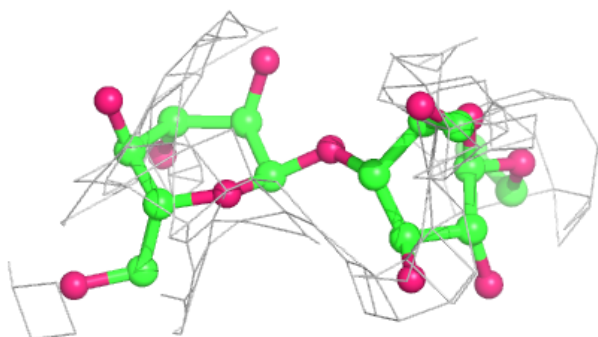
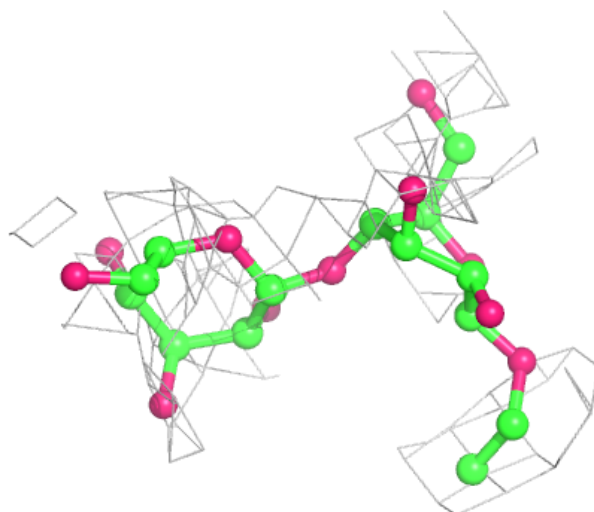
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	A	702	1/1	-	-	170,170,170,170	1
5	LMT	E	705	25/35	0.61	0.25	108,205,239,256	0
5	LMT	D	703	26/35	0.64	0.26	120,205,232,245	0
5	LMT	B	705	26/35	0.64	0.28	100,211,240,272	0
4	CL	B	703	1/1	0.68	0.62	104,104,104,104	0
5	LMT	A	707	25/35	0.70	0.27	105,209,252,279	0
5	LMT	E	703	25/35	0.76	0.20	111,219,250,271	0
3	NA	A	705	1/1	0.90	0.58	71,71,71,71	0
4	CL	A	706	1/1	0.95	0.35	119,119,119,119	0
3	NA	C	703	1/1	0.95	0.51	79,79,79,79	0
2	CA	C	701	1/1	-	-	170,170,170,170	1
5	LMT	C	706	27/35	0.66	0.46	113,203,240,250	0
5	LMT	B	706	27/35	0.69	0.41	93,198,233,234	0
5	LMT	C	705	25/35	0.71	0.23	100,190,244,259	0
3	NA	A	704	1/1	0.73	0.80	107,107,107,107	0
3	NA	B	702	1/1	0.77	0.57	88,88,88,88	0
4	CL	C	704	1/1	0.87	0.39	105,105,105,105	0
3	NA	D	701	1/1	0.95	0.32	63,63,63,63	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.

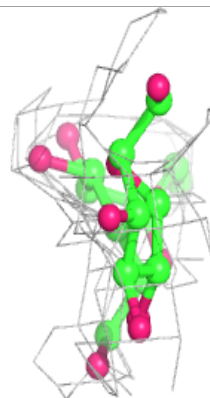
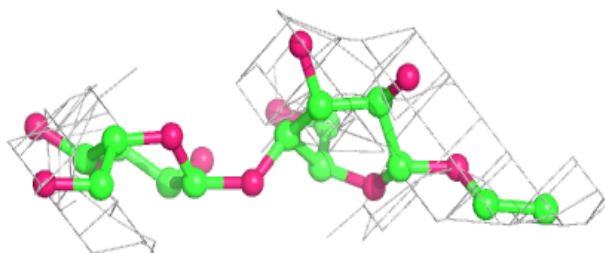
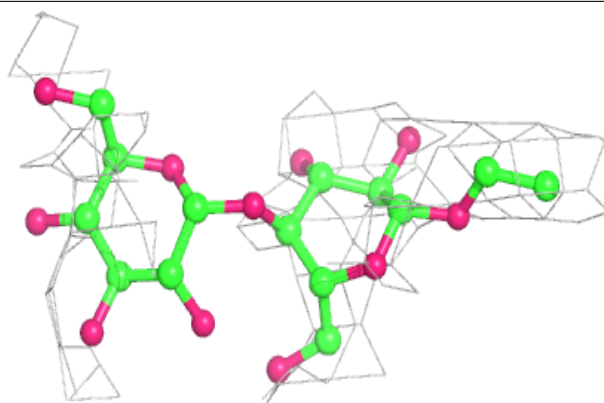
Electron density around LMT E 704:

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

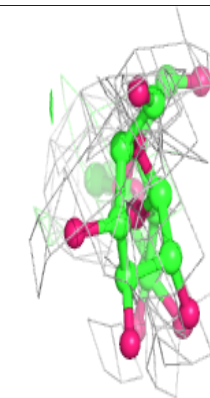
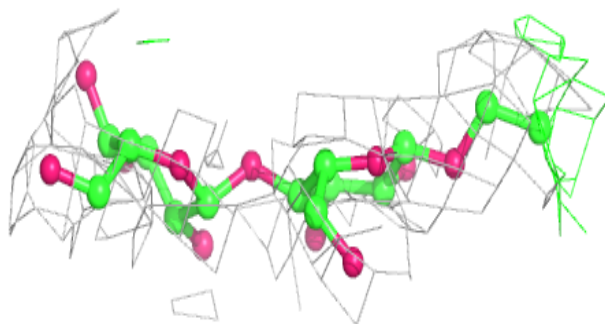
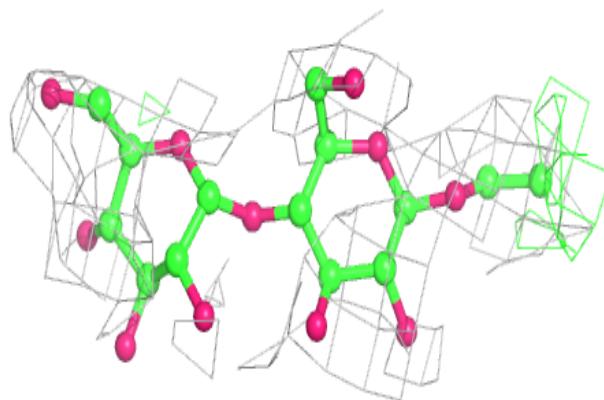


Electron density around LMT B 704:

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

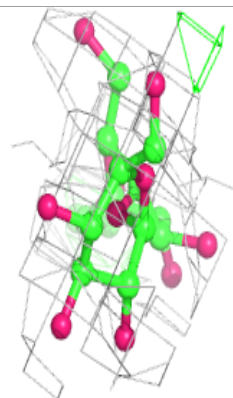
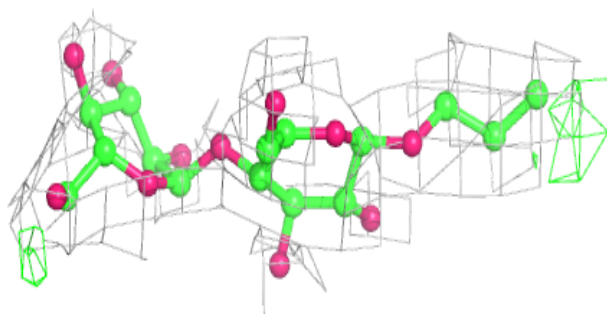
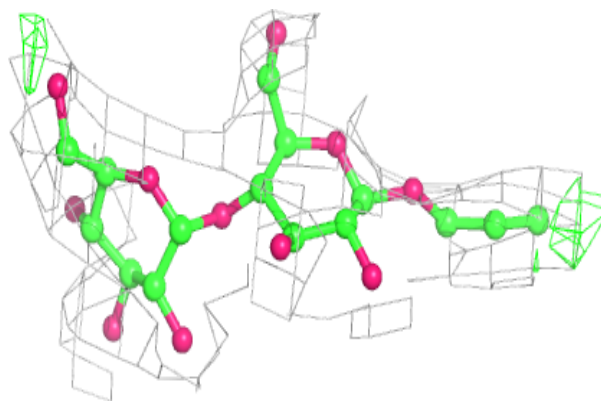
**Electron density around LMT E 705:**

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

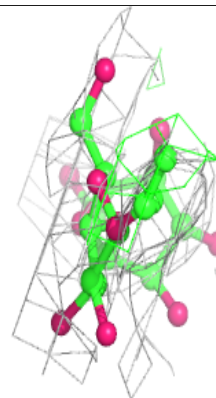
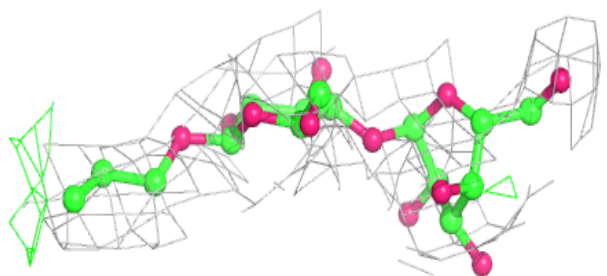
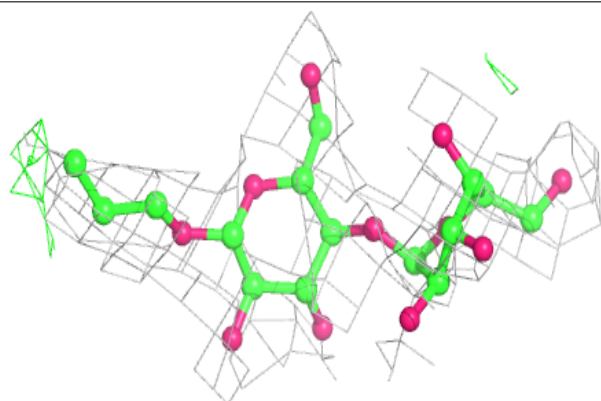


Electron density around LMT D 703:

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

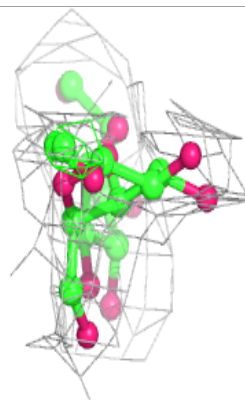
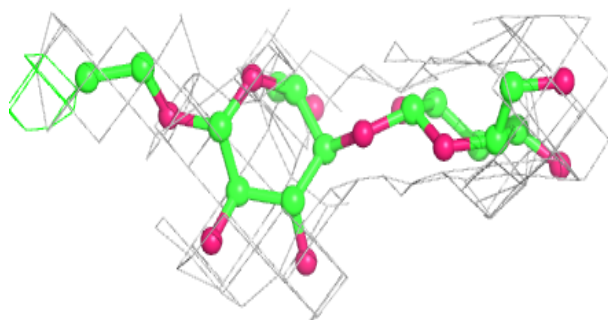
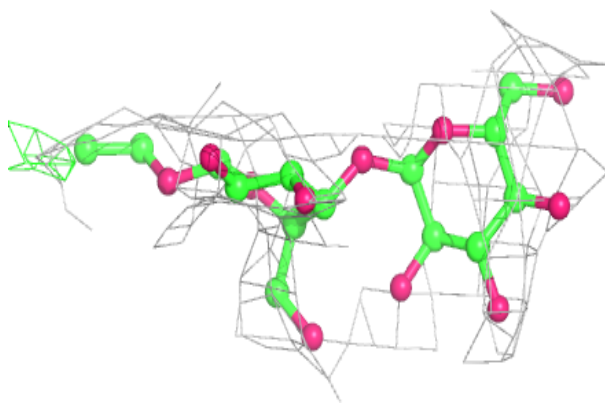
**Electron density around LMT B 705:**

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

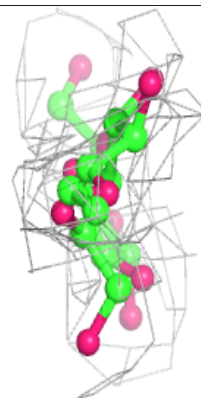
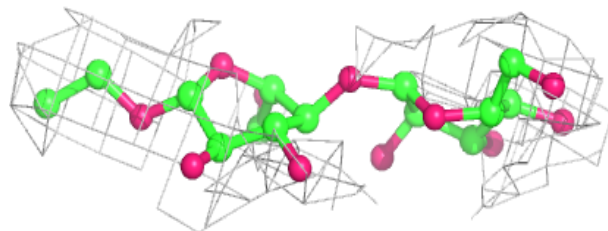
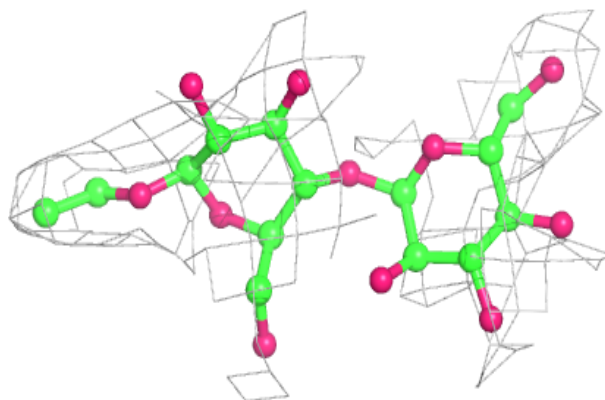


Electron density around LMT A 707:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

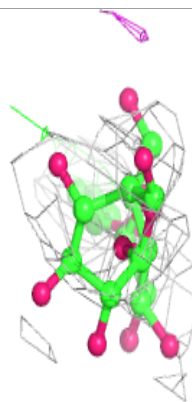
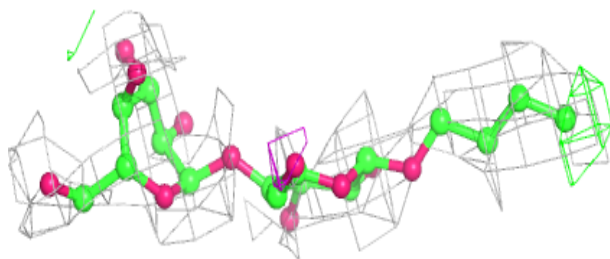
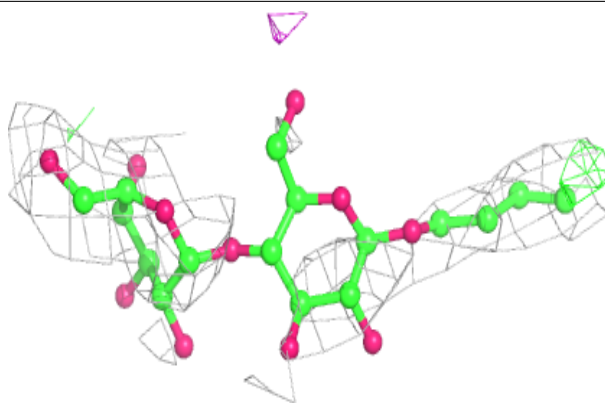
**Electron density around LMT E 703:**

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

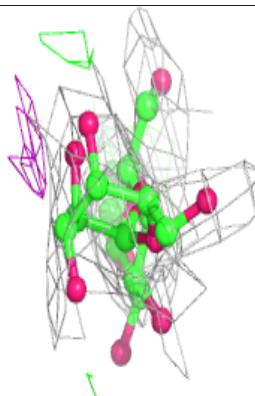
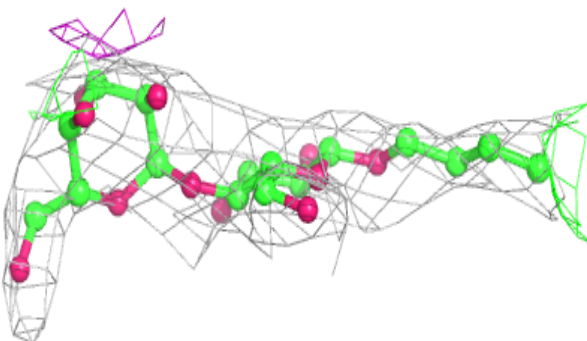
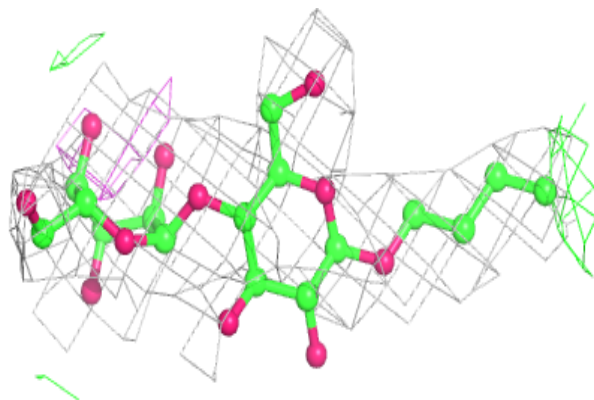


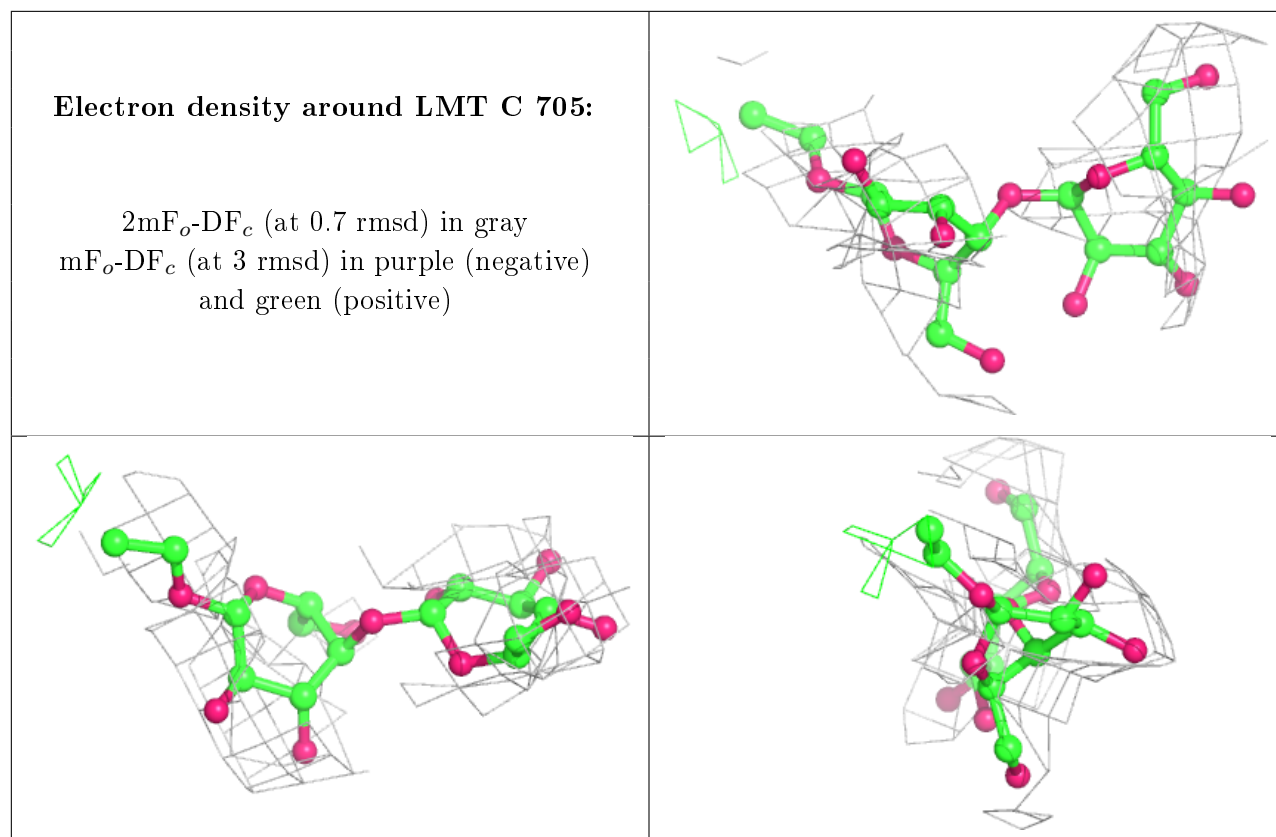
Electron density around LMT C 706:

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

**Electron density around LMT B 706:**

$2mF_o-DF_c$ (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.