



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:50 PM UTC

PDB ID : 8ITT / pdb_00008itt
Title : Crystal structure of lysophosphatidylcholine in complex with human serum albumin and myristate
Authors : Wang, Y.; Jiang, L.G.; Huang, M.D.
Deposited on : 2023-03-22
Resolution : 3.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

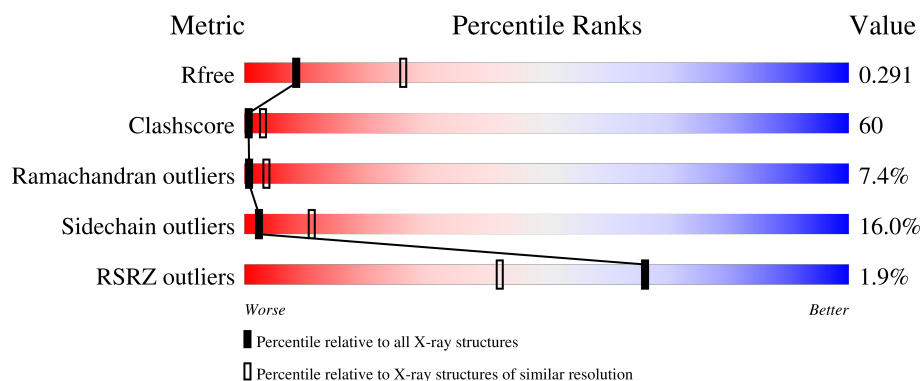
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	580	2% 33% 43% 20% .
1	B	580	2% 36% 45% 15% .

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	MYR	B	601	-	-	X	-
2	MYR	B	602	-	-	X	-
3	LPC	A	604	-	-	X	-
3	LPC	A	605	-	-	X	-
3	LPC	A	606	-	-	X	-
3	LPC	B	603	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9167 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.

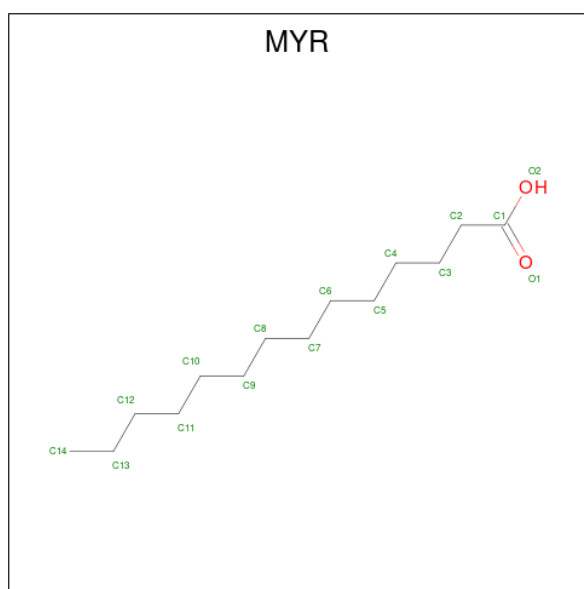
- Molecule 1 is a protein called Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4443	2808	750	844	41			
1	B	579	Total	C	N	O	S	0	0	0
			4442	2807	752	842	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	580	GLU	GLN	conflict	UNP P02768
B	580	GLU	GLN	conflict	UNP P02768

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$) (labeled as "Ligand of Interest" by depositor).



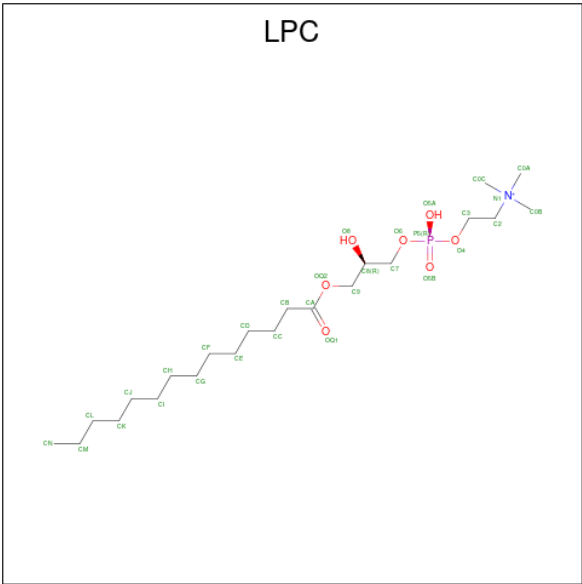
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 3 is [1-MYRISTOYL-GLYCEROL-3-YL]PHOSPHONYLCHOLINE (CCD ID: LPC) (formula: C₂₂H₄₇NO₇P) (labeled as "Ligand of Interest" by depositor).

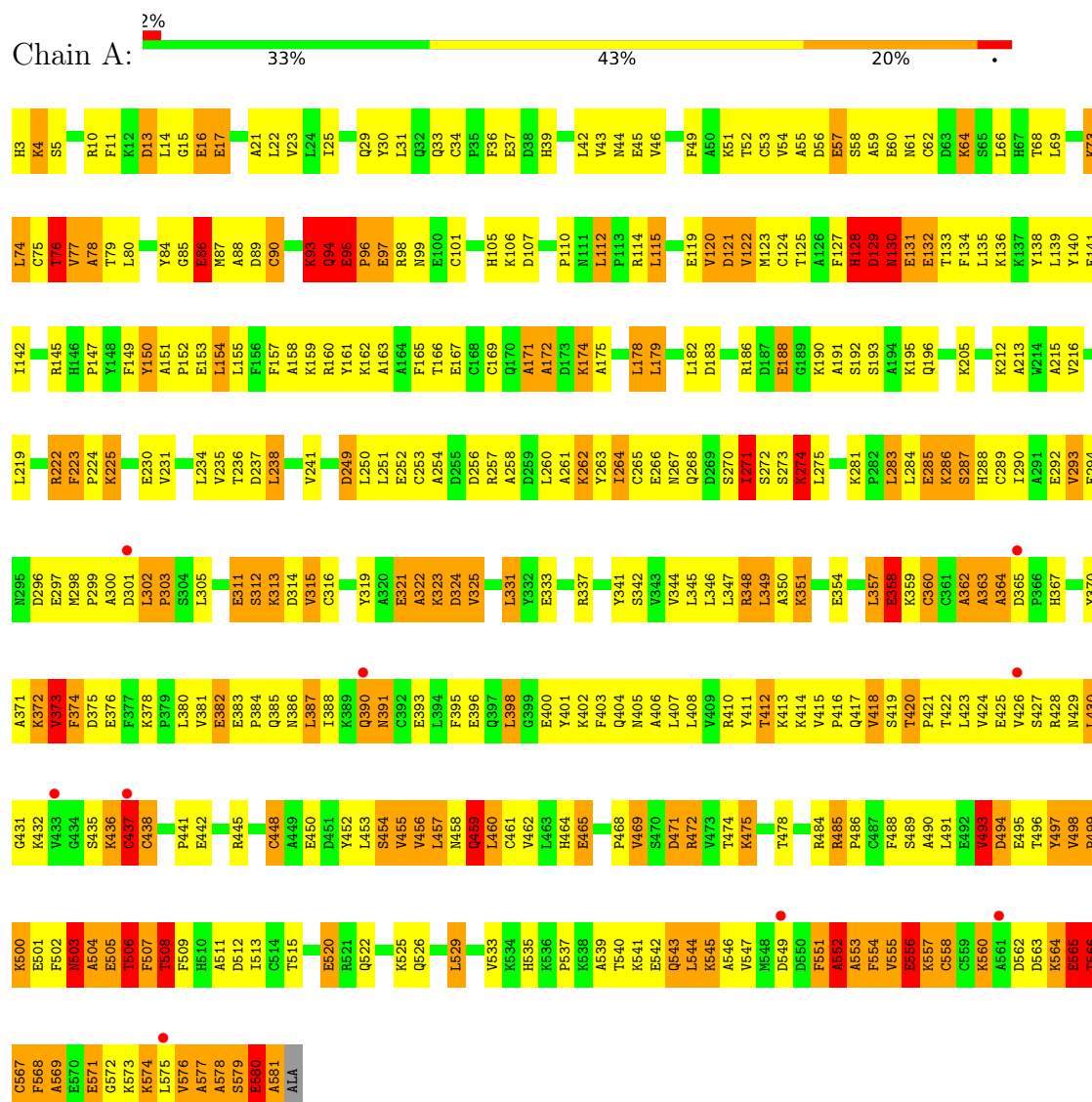


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	22	1	7	1		
3	A	1	Total	C	N	O	P	0	0
			31	22	1	7	1		
3	A	1	Total	C	N	O	P	0	0
			31	22	1	7	1		
3	B	1	Total	C	N	O	P	0	0
			31	22	1	7	1		
3	B	1	Total	C	N	O	P	0	0
			31	22	1	7	1		
3	B	1	Total	C	N	O	P	0	0
			31	22	1	7	1		

3 Residue-property plots

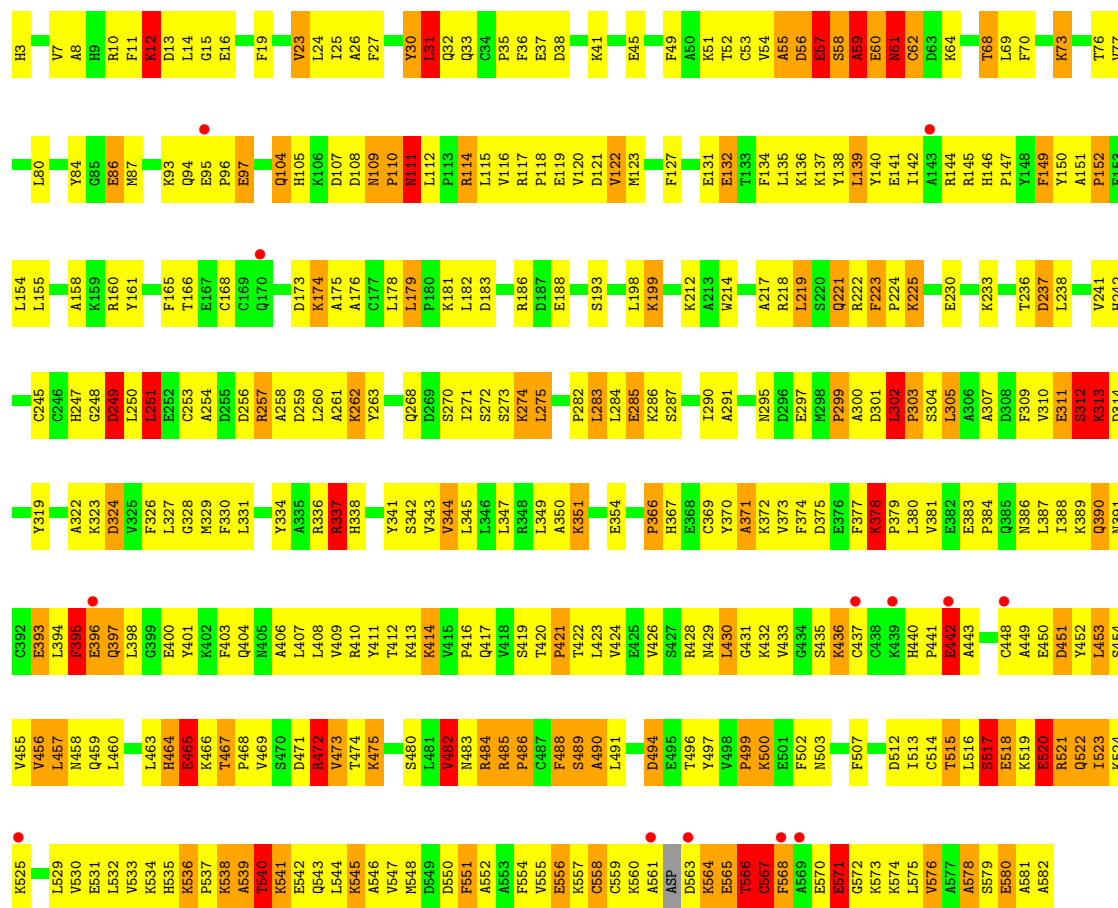
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Albumin



• Molecule 1: Albumin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.26Å 38.47Å 182.46Å 90.00° 104.78° 90.00°	Depositor
Resolution (Å)	47.63 – 3.03 47.63 – 3.03	Depositor EDS
% Data completeness (in resolution range)	86.0 (47.63-3.03) 85.9 (47.63-3.03)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.73Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.261 , 0.291 0.261 , 0.291	Depositor DCC
R_{free} test set	2383 reflections (7.51%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9167	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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 51.94 % 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 5.2227e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.00	13/4530 (0.3%)	1.46	78/6141 (1.3%)
1	B	0.97	11/4528 (0.2%)	1.45	72/6134 (1.2%)
All	All	0.99	24/9058 (0.3%)	1.46	150/12275 (1.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	GLN	CA-C	-8.53	1.43	1.53
1	B	311	GLU	CA-C	-8.06	1.42	1.52
1	B	491	LEU	CA-C	-7.85	1.43	1.52
1	A	93	LYS	CA-C	-7.26	1.43	1.52
1	B	30	TYR	CA-C	-6.82	1.43	1.52
1	B	61	ASN	CA-C	-6.76	1.43	1.52
1	A	578	ALA	CA-CB	-6.66	1.42	1.53
1	A	95	GLU	CA-C	-6.11	1.45	1.52
1	A	504	ALA	CA-C	-5.93	1.45	1.52
1	A	223	PHE	CA-CB	-5.91	1.46	1.53
1	A	112	LEU	CA-C	-5.90	1.46	1.52
1	A	508	THR	CA-C	-5.73	1.45	1.52
1	B	60	GLU	CA-C	-5.71	1.45	1.53
1	A	95	GLU	N-CA	-5.65	1.38	1.46
1	B	30	TYR	CB-CG	-5.48	1.39	1.51
1	A	78	ALA	CA-C	-5.40	1.46	1.52
1	B	30	TYR	CA-CB	-5.40	1.44	1.53
1	B	86	GLU	CA-CB	-5.37	1.45	1.53
1	A	325	VAL	N-CA	-5.24	1.40	1.46
1	A	358	GLU	N-CA	-5.16	1.39	1.46
1	B	31	LEU	N-CA	-5.12	1.39	1.46
1	A	498	VAL	N-CA	-5.10	1.40	1.46
1	B	540	THR	CA-C	-5.04	1.46	1.52
1	B	60	GLU	N-CA	-5.03	1.40	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	GLU	N-CA-C	-20.17	87.77	112.38
1	B	567	CYS	N-CA-C	-19.95	89.59	111.14
1	A	94	GLN	N-CA-C	17.95	131.35	108.19
1	B	299	PRO	N-CA-C	16.22	133.67	114.20
1	A	129	ASP	N-CA-C	15.01	131.02	113.01
1	A	497	TYR	N-CA-C	15.00	129.74	110.24
1	A	373	VAL	CB-CA-C	-13.68	94.12	112.04
1	B	251	LEU	N-CA-C	-12.48	97.70	113.43
1	B	108	ASP	CA-C-N	-12.27	108.30	123.15
1	B	108	ASP	C-N-CA	-12.27	108.30	123.15
1	A	323	LYS	N-CA-C	11.84	125.55	111.82
1	A	567	CYS	N-CA-C	-11.83	85.59	110.80
1	B	109	ASN	CA-C-N	11.37	134.05	119.84
1	B	109	ASN	C-N-CA	11.37	134.05	119.84
1	A	313	LYS	N-CA-C	-10.60	93.10	109.85
1	B	567	CYS	CB-CA-C	10.57	127.61	110.90
1	B	482	VAL	N-CA-C	-9.93	102.96	112.29
1	B	443	ALA	N-CA-C	-9.59	102.08	113.88
1	A	568	PHE	N-CA-C	-9.57	96.74	110.24
1	A	493	VAL	N-CA-C	9.54	122.65	108.54
1	A	178	LEU	N-CA-C	9.48	121.38	111.14
1	A	76	THR	N-CA-C	-9.31	102.74	114.56
1	B	62	CYS	N-CA-C	-9.27	101.06	111.82
1	B	55	ALA	N-CA-C	-9.13	102.96	114.56
1	A	302	LEU	CA-C-N	9.01	131.10	119.84
1	A	302	LEU	C-N-CA	9.01	131.10	119.84
1	A	577	ALA	N-CA-C	-8.83	101.33	112.90
1	A	79	THR	N-CA-C	-8.62	103.30	113.21
1	B	465	GLU	N-CA-C	-8.46	102.01	111.82
1	B	263	TYR	N-CA-C	-8.26	102.22	111.14
1	A	130	ASN	N-CA-C	-8.25	93.22	110.80
1	B	456	VAL	N-CA-C	-8.16	104.54	111.56
1	B	566	THR	CA-C-N	-8.13	109.39	120.44
1	B	566	THR	C-N-CA	-8.13	109.39	120.44
1	B	249	ASP	N-CA-C	-8.05	93.65	110.80
1	A	554	PHE	N-CA-C	-7.99	103.66	113.41
1	A	302	LEU	N-CA-C	7.95	123.50	109.58
1	A	263	TYR	N-CA-C	-7.80	101.88	111.40
1	A	504	ALA	N-CA-C	7.72	120.82	111.40
1	A	412	THR	N-CA-C	-7.61	103.84	113.43
1	B	302	LEU	CA-C-N	7.47	129.18	119.84
1	B	302	LEU	C-N-CA	7.47	129.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	VAL	N-CA-C	-7.42	103.23	110.72
1	A	543	GLN	N-CA-C	-7.39	103.31	111.36
1	B	110	PRO	CA-C-N	-7.23	111.88	123.23
1	B	110	PRO	C-N-CA	-7.23	111.88	123.23
1	B	485	ARG	CA-C-N	-7.18	111.02	118.85
1	B	485	ARG	C-N-CA	-7.18	111.02	118.85
1	A	311	GLU	N-CA-C	7.16	118.88	111.14
1	B	565	GLU	N-CA-C	-7.01	95.86	110.80
1	A	161	TYR	N-CA-C	-6.96	103.74	111.82
1	B	559	CYS	N-CA-C	-6.90	103.25	113.61
1	A	503	ASN	N-CA-C	-6.85	95.57	107.49
1	B	223	PHE	CA-C-N	-6.81	112.89	120.45
1	B	223	PHE	C-N-CA	-6.81	112.89	120.45
1	A	325	VAL	N-CA-C	-6.78	103.17	110.23
1	B	520	GLU	CA-C-N	6.74	129.64	120.54
1	B	520	GLU	C-N-CA	6.74	129.64	120.54
1	B	313	LYS	N-CA-C	-6.70	96.52	110.80
1	B	556	GLU	N-CA-C	-6.70	104.37	112.54
1	A	95	GLU	CA-CB-CG	-6.68	100.73	114.10
1	B	23	VAL	CB-CA-C	-6.67	103.16	111.70
1	B	87	MET	N-CA-C	-6.65	103.28	111.33
1	A	134	PHE	N-CA-C	-6.64	102.48	112.04
1	A	459	GLN	N-CA-C	-6.63	103.72	112.34
1	B	111	ASN	N-CA-C	6.61	120.77	107.41
1	A	564	LYS	N-CA-C	-6.60	96.74	110.80
1	B	567	CYS	CA-CB-SG	6.56	129.48	114.40
1	A	74	LEU	N-CA-C	-6.54	104.08	111.14
1	A	154	LEU	N-CA-C	-6.49	104.29	111.82
1	A	360	CYS	N-CA-C	6.46	119.64	111.69
1	A	504	ALA	CA-C-O	-6.45	113.64	120.55
1	A	96	PRO	N-CA-C	-6.45	104.14	113.75
1	A	556	GLU	N-CA-C	-6.45	100.73	111.37
1	A	271	ILE	CB-CA-C	-6.45	105.32	111.44
1	B	312	SER	N-CA-C	-6.42	97.14	110.80
1	A	372	LYS	N-CA-C	6.35	121.24	109.56
1	B	12	LYS	N-CA-C	6.29	118.14	111.28
1	B	467	THR	CA-C-N	6.28	126.65	119.93
1	B	467	THR	C-N-CA	6.28	126.65	119.93
1	A	566	THR	N-CA-C	-6.24	97.52	110.80
1	B	304	SER	N-CA-C	-6.01	99.39	108.52
1	A	555	VAL	N-CA-C	-5.96	105.04	110.82
1	A	406	ALA	N-CA-C	-5.92	103.60	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	LYS	N-CA-C	5.92	119.32	111.75
1	B	565	GLU	CA-C-N	-5.91	110.26	121.54
1	B	565	GLU	C-N-CA	-5.91	110.26	121.54
1	A	581	ALA	N-CA-C	-5.88	94.54	111.00
1	B	566	THR	N-CA-C	5.87	123.31	110.80
1	A	171	ALA	N-CA-C	5.86	117.69	108.96
1	A	438	CYS	N-CA-C	-5.84	105.98	113.23
1	A	57	GLU	CA-C-N	-5.81	113.31	122.79
1	A	57	GLU	C-N-CA	-5.81	113.31	122.79
1	B	110	PRO	N-CA-C	-5.80	100.53	112.47
1	A	363	ALA	N-CA-C	5.78	117.27	108.07
1	B	337	ARG	N-CA-C	-5.73	105.78	112.89
1	A	112	LEU	CB-CA-C	-5.73	100.91	109.56
1	A	400	GLU	N-CA-C	-5.72	104.95	111.07
1	A	131	GLU	N-CA-C	-5.71	106.36	113.38
1	A	552	ALA	O-C-N	5.70	130.17	122.59
1	A	571	GLU	N-CA-C	-5.68	106.30	113.18
1	A	465	GLU	N-CA-C	-5.68	105.07	112.23
1	A	503	ASN	CA-C-N	-5.67	111.23	120.71
1	A	503	ASN	C-N-CA	-5.67	111.23	120.71
1	B	475	LYS	N-CA-C	-5.67	105.01	111.14
1	B	60	GLU	O-C-N	5.62	128.75	121.79
1	A	107	ASP	N-CA-C	5.61	117.45	108.41
1	B	338	HIS	N-CA-C	5.61	118.29	108.75
1	A	437	CYS	N-CA-C	5.61	122.75	110.80
1	A	97	GLU	N-CA-C	5.58	118.29	111.82
1	A	500	LYS	O-C-N	5.55	129.24	122.96
1	B	60	GLU	CA-CB-CG	-5.47	103.15	114.10
1	B	522	GLN	N-CA-C	-5.45	105.42	111.36
1	B	86	GLU	N-CA-CB	-5.45	102.53	110.53
1	A	346	LEU	N-CA-C	-5.44	105.50	111.82
1	A	508	THR	N-CA-C	-5.44	99.21	110.80
1	A	121	ASP	N-CA-C	5.43	116.89	111.07
1	A	90	CYS	N-CA-C	-5.42	105.79	112.90
1	A	579	SER	N-CA-C	-5.41	100.36	109.07
1	B	59	ALA	CA-C-N	-5.40	113.20	121.74
1	B	59	ALA	C-N-CA	-5.40	113.20	121.74
1	B	490	ALA	CA-C-N	-5.38	112.86	121.58
1	B	490	ALA	C-N-CA	-5.38	112.86	121.58
1	A	349	LEU	N-CA-C	-5.38	104.83	111.33
1	A	456	VAL	CB-CA-C	-5.38	104.82	111.70
1	B	225	LYS	N-CA-C	-5.35	106.60	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	PHE	N-CA-C	-5.33	106.72	113.18
1	B	488	PHE	N-CA-C	-5.29	105.42	111.14
1	A	448	CYS	CB-CA-C	5.29	119.19	110.88
1	A	362	ALA	CA-C-N	-5.29	110.03	122.19
1	A	362	ALA	C-N-CA	-5.29	110.03	122.19
1	B	536	LYS	N-CA-C	-5.26	101.37	109.79
1	B	491	LEU	N-CA-C	-5.24	99.28	107.93
1	B	393	GLU	N-CA-C	-5.21	106.77	113.23
1	A	552	ALA	CA-C-N	5.17	131.42	121.54
1	A	552	ALA	C-N-CA	5.17	131.42	121.54
1	A	565	GLU	N-CA-C	5.16	121.57	113.72
1	A	223	PHE	CB-CA-C	-5.13	104.14	110.96
1	B	455	VAL	CA-C-N	-5.13	117.90	123.08
1	B	455	VAL	C-N-CA	-5.13	117.90	123.08
1	B	302	LEU	CA-CB-CG	-5.12	98.39	116.30
1	B	564	LYS	N-CA-C	-5.10	99.94	110.80
1	B	139	LEU	N-CA-C	-5.07	105.64	111.07
1	A	497	TYR	CA-C-O	5.07	126.91	121.44
1	B	414	LYS	CA-CB-CG	-5.05	103.99	114.10
1	B	274	LYS	N-CA-C	-5.05	106.81	112.87
1	A	420	THR	N-CA-C	-5.04	105.59	112.35
1	B	558	CYS	N-CA-C	-5.03	106.99	114.64
1	A	4	LYS	N-CA-C	5.01	119.59	111.37
1	A	287	SER	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4443	0	4212	542	1
1	B	4442	0	4216	528	0
2	A	48	0	81	6	0
2	B	48	0	81	29	0
3	A	93	0	138	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	93	0	138	80	0
All	All	9167	0	8866	1087	1

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 60.

All (1087) 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:B:149:PHE:CE2	3:B:603:LPC:H0A1	1.43	1.54
1:A:485:ARG:HH11	3:A:605:LPC:C0B	1.33	1.40
1:B:149:PHE:CE2	3:B:603:LPC:H0C3	1.58	1.37
1:B:158:ALA:HB1	3:B:603:LPC:CK	1.53	1.36
1:B:149:PHE:CZ	3:B:603:LPC:H0C3	1.61	1.34
1:B:218:ARG:CZ	2:B:601:MYR:H141	1.58	1.32
1:B:149:PHE:CD2	3:B:603:LPC:H0A1	1.67	1.29
1:B:537:PRO:O	1:B:538:LYS:CG	1.77	1.29
1:A:504:ALA:O	1:A:506:THR:N	1.61	1.28
1:B:149:PHE:CE2	3:B:603:LPC:C0A	2.17	1.28
1:A:575:LEU:CA	1:A:578:ALA:HB3	1.63	1.27
1:A:413:LYS:C	1:A:493:VAL:HG22	1.61	1.23
1:A:135:LEU:HB3	3:A:604:LPC:CK	1.69	1.22
1:B:60:GLU:O	1:B:62:CYS:N	1.71	1.22
1:B:149:PHE:CZ	3:B:603:LPC:C0C	2.25	1.19
1:B:149:PHE:CE2	3:B:603:LPC:C0C	2.27	1.17
1:A:94:GLN:O	1:A:98:ARG:N	1.77	1.16
1:B:537:PRO:O	1:B:538:LYS:HG3	1.02	1.16
1:B:383:GLU:OE1	1:B:485:ARG:NH1	1.77	1.15
1:A:575:LEU:HA	1:A:578:ALA:HB3	1.28	1.14
1:A:344:VAL:HG21	3:A:605:LPC:C0A	1.75	1.14
1:B:218:ARG:NE	2:B:601:MYR:H141	1.63	1.12
1:B:383:GLU:CD	1:B:485:ARG:HH12	1.57	1.10
1:A:132:GLU:OE2	1:A:132:GLU:HA	1.48	1.10
1:A:344:VAL:CG2	3:A:605:LPC:H0A1	1.80	1.10
1:B:138:TYR:CD1	3:B:603:LPC:HD1	1.84	1.10
1:B:60:GLU:CG	1:B:61:ASN:H	1.62	1.09
1:B:60:GLU:HG2	1:B:61:ASN:N	1.66	1.09
1:A:506:THR:HG22	1:A:507:PHE:N	1.63	1.09
1:B:158:ALA:CB	3:B:603:LPC:HK2	1.84	1.08
1:B:518:GLU:OE1	1:B:521:ARG:NH1	1.85	1.08
1:A:222:ARG:NH1	1:A:293:VAL:O	1.87	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:O	1:A:293:VAL:HG12	1.52	1.07
1:B:483:ASN:O	1:B:486:PRO:HD2	1.55	1.07
1:A:413:LYS:O	1:A:493:VAL:HG22	1.55	1.06
1:B:570:GLU:HA	1:B:573:LYS:H	1.16	1.06
1:A:135:LEU:HB3	3:A:604:LPC:HK2	1.31	1.06
1:A:485:ARG:NH1	3:A:605:LPC:C0B	2.16	1.06
1:A:485:ARG:HD3	3:A:605:LPC:H0B2	1.34	1.05
1:A:344:VAL:HG21	3:A:605:LPC:H0A1	1.35	1.05
1:B:60:GLU:HG2	1:B:61:ASN:OD1	1.53	1.05
1:B:218:ARG:NE	2:B:601:MYR:C14	2.20	1.04
1:B:485:ARG:HD2	3:B:604:LPC:O5B	1.58	1.02
1:B:291:ALA:HA	2:B:601:MYR:H112	1.39	1.01
1:A:485:ARG:HH11	3:A:605:LPC:H0B2	1.26	1.00
1:B:60:GLU:HG2	1:B:61:ASN:H	0.84	1.00
1:A:553:ALA:HB2	3:A:606:LPC:H0C1	1.42	0.99
1:B:344:VAL:CG2	3:B:604:LPC:H0A1	1.93	0.99
1:A:342:SER:OG	3:A:605:LPC:H0C3	1.61	0.99
1:A:413:LYS:C	1:A:493:VAL:CG2	2.35	0.99
1:A:529:LEU:HD22	3:A:606:LPC:HB1	1.45	0.98
1:B:138:TYR:CE1	3:B:603:LPC:HB2	1.99	0.98
1:A:357:LEU:O	1:A:360:CYS:N	1.94	0.98
1:A:344:VAL:CG2	3:A:605:LPC:C0A	2.38	0.97
1:B:139:LEU:HB2	3:B:603:LPC:HJ1	1.45	0.97
1:A:267:ASN:O	1:A:271:ILE:HG13	1.63	0.97
1:A:158:ALA:HB1	3:A:604:LPC:HJ1	1.45	0.97
1:B:224:PRO:HB3	1:B:336:ARG:HB2	1.42	0.96
1:B:23:VAL:HG22	2:B:602:MYR:C14	1.94	0.96
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.45	0.96
1:B:401:TYR:OH	1:B:525:LYS:HE2	1.64	0.96
1:B:60:GLU:C	1:B:62:CYS:H	1.74	0.95
1:A:149:PHE:CD2	3:A:604:LPC:H0A1	2.01	0.95
1:B:344:VAL:HG23	3:B:604:LPC:H0A1	1.48	0.95
1:B:158:ALA:CB	3:B:603:LPC:CK	2.43	0.95
1:B:158:ALA:HB1	3:B:603:LPC:HK2	0.95	0.94
1:A:95:GLU:HB3	1:A:96:PRO:HD3	1.45	0.94
1:B:41:LYS:O	1:B:45:GLU:HG3	1.67	0.94
1:A:485:ARG:HH11	3:A:605:LPC:H0B1	1.29	0.94
1:B:411:TYR:CE1	3:B:604:LPC:HL1	2.02	0.94
1:B:507:PHE:CE2	3:B:605:LPC:HL2	2.02	0.94
1:B:149:PHE:HE2	3:B:603:LPC:H0C3	1.26	0.93
1:A:313:LYS:O	1:A:314:ASP:HB2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:O	1:B:58:SER:N	2.01	0.93
2:B:601:MYR:C5	2:B:601:MYR:H92	1.98	0.92
1:B:472:ARG:O	1:B:475:LYS:N	2.00	0.92
1:B:114:ARG:HH21	1:B:116:VAL:HA	1.34	0.92
1:A:504:ALA:C	1:A:506:THR:H	1.75	0.92
1:A:390:GLN:HE21	1:A:391:ASN:N	1.67	0.91
1:B:311:GLU:O	1:B:312:SER:C	2.10	0.91
1:B:23:VAL:HG22	2:B:602:MYR:H141	1.50	0.91
1:B:149:PHE:HZ	3:B:603:LPC:C0C	1.78	0.91
1:B:138:TYR:HE1	3:B:603:LPC:HB2	1.36	0.90
1:A:575:LEU:CA	1:A:578:ALA:CB	2.50	0.90
1:B:485:ARG:HD3	3:B:604:LPC:H22	1.54	0.90
1:A:149:PHE:CE2	3:A:604:LPC:H0C3	2.07	0.90
1:B:525:LYS:HE3	3:B:605:LPC:H72	1.53	0.90
1:B:149:PHE:HE2	3:B:603:LPC:C0C	1.78	0.89
1:B:237:ASP:HB3	1:B:260:LEU:HD13	1.52	0.89
1:B:540:THR:HB	1:B:543:GLN:HG3	1.54	0.89
1:B:570:GLU:C	1:B:572:GLY:N	2.16	0.89
2:B:601:MYR:H92	2:B:601:MYR:H52	1.52	0.89
1:B:287:SER:OG	2:B:602:MYR:O1	1.90	0.89
1:A:575:LEU:C	1:A:578:ALA:HB3	1.98	0.89
3:A:605:LPC:C8	3:A:605:LPC:HD2	2.03	0.89
1:A:390:GLN:HE21	1:A:390:GLN:C	1.81	0.88
1:A:504:ALA:C	1:A:506:THR:N	2.29	0.88
1:B:344:VAL:HG23	3:B:604:LPC:C0A	2.03	0.88
1:A:135:LEU:CB	3:A:604:LPC:HK2	2.03	0.88
1:A:565:GLU:HA	1:A:565:GLU:OE2	1.73	0.88
1:B:120:VAL:HG21	1:B:175:ALA:HB2	1.56	0.88
1:A:93:LYS:O	1:A:94:GLN:HG3	1.74	0.88
1:A:553:ALA:N	3:A:606:LPC:H21	1.88	0.87
1:A:362:ALA:O	1:A:363:ALA:HB2	1.74	0.87
1:A:552:ALA:O	1:A:555:VAL:N	2.06	0.87
1:A:575:LEU:HA	1:A:578:ALA:CB	2.05	0.87
1:B:312:SER:C	1:B:313:LYS:O	2.09	0.86
1:A:450:GLU:O	1:A:454:SER:HB3	1.76	0.86
1:B:158:ALA:HB1	3:B:603:LPC:HK1	1.54	0.86
1:B:299:PRO:O	1:B:300:ALA:HB3	1.74	0.86
1:B:485:ARG:O	1:B:485:ARG:HG2	1.74	0.86
1:A:552:ALA:HB1	3:A:606:LPC:H21	1.55	0.85
1:B:459:GLN:O	1:B:463:LEU:HG	1.76	0.85
1:A:387:LEU:O	1:A:391:ASN:HB2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:GLN:HE22	1:B:494:ASP:CG	1.84	0.85
1:A:552:ALA:C	1:A:554:PHE:H	1.82	0.85
1:A:552:ALA:O	1:A:555:VAL:HG12	1.75	0.85
1:B:411:TYR:OH	3:B:604:LPC:HJ1	1.77	0.85
1:B:540:THR:HB	1:B:543:GLN:CG	2.07	0.85
1:A:577:ALA:HA	1:A:580:GLU:OE1	1.76	0.85
1:B:344:VAL:CG2	3:B:604:LPC:C0A	2.54	0.85
1:A:321:GLU:O	1:A:322:ALA:CB	2.25	0.85
1:A:556:GLU:HG3	1:A:557:LYS:N	1.89	0.85
1:A:115:LEU:HD13	1:A:145:ARG:NH1	1.91	0.85
1:B:419:SER:O	1:B:423:LEU:HD12	1.76	0.85
1:B:472:ARG:O	1:B:474:THR:N	2.09	0.84
1:B:311:GLU:O	1:B:313:LYS:N	2.10	0.84
1:B:313:LYS:O	1:B:314:ASP:HB2	1.78	0.84
1:B:540:THR:O	1:B:541:LYS:C	2.21	0.83
1:B:183:ASP:HA	1:B:186:ARG:NH1	1.94	0.83
1:B:518:GLU:O	1:B:522:GLN:HG3	1.78	0.83
1:A:413:LYS:HB3	1:A:493:VAL:HG21	1.60	0.83
1:A:367:HIS:O	1:A:371:ALA:HB2	1.79	0.82
1:A:413:LYS:CB	1:A:493:VAL:HG21	2.09	0.82
1:A:566:THR:CA	1:A:568:PHE:O	2.26	0.82
3:A:605:LPC:HD2	3:A:605:LPC:O8	1.79	0.82
1:B:54:VAL:O	1:B:54:VAL:HG12	1.80	0.82
1:B:395:PHE:CE2	1:B:435:SER:HA	2.14	0.82
1:B:570:GLU:CA	1:B:573:LYS:H	1.92	0.82
1:A:193:SER:HB2	3:A:604:LPC:H0B3	1.62	0.82
1:A:93:LYS:O	1:A:94:GLN:OE1	1.98	0.81
1:B:199:LYS:HE3	1:B:242:HIS:CE1	2.14	0.81
1:B:68:THR:OG1	1:B:95:GLU:OE1	1.97	0.81
1:A:436:LYS:O	1:A:438:CYS:N	2.13	0.81
1:B:543:GLN:OE1	1:B:582:ALA:HB2	1.81	0.80
1:B:248:GLY:O	1:B:249:ASP:HB3	1.81	0.80
1:A:485:ARG:HD3	3:A:605:LPC:C0B	2.10	0.80
1:B:517:SER:O	1:B:521:ARG:HD3	1.80	0.80
1:A:254:ALA:HB1	2:A:602:MYR:H51	1.64	0.80
1:A:485:ARG:NH1	3:A:605:LPC:H0B1	1.91	0.80
1:A:563:ASP:OD1	1:A:564:LYS:O	2.00	0.79
1:A:138:TYR:CE1	3:A:604:LPC:HB2	2.17	0.79
1:B:193:SER:HB2	3:B:603:LPC:H0A2	1.63	0.79
1:B:557:LYS:O	1:B:567:CYS:SG	2.41	0.79
1:B:552:ALA:HB2	3:B:605:LPC:O8	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:O	1:A:322:ALA:HB2	1.83	0.79
1:A:506:THR:HG22	1:A:507:PHE:H	1.45	0.79
1:A:93:LYS:O	1:A:94:GLN:CG	2.31	0.78
1:B:485:ARG:CD	3:B:604:LPC:O5B	2.31	0.78
1:B:149:PHE:CZ	3:B:603:LPC:H0C2	2.18	0.78
1:B:149:PHE:HE2	3:B:603:LPC:N1	1.80	0.78
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.65	0.78
1:B:257:ARG:NH2	1:B:287:SER:OG	2.16	0.78
1:B:60:GLU:HG2	1:B:61:ASN:CG	2.09	0.78
1:B:507:PHE:HE2	3:B:605:LPC:HL2	1.46	0.78
1:B:149:PHE:CE2	3:B:603:LPC:N1	2.52	0.78
1:B:485:ARG:HE	3:B:604:LPC:H0B2	1.49	0.78
3:A:605:LPC:HD2	3:A:605:LPC:H8	1.64	0.77
1:A:319:TYR:CE2	1:A:323:LYS:HD3	2.19	0.77
1:B:401:TYR:OH	1:B:525:LYS:CE	2.33	0.77
1:A:553:ALA:HB2	3:A:606:LPC:C0C	2.14	0.77
1:A:132:GLU:HB3	1:A:133:THR:HG23	1.66	0.77
1:A:373:VAL:O	1:A:376:GLU:N	2.17	0.77
1:B:564:LYS:C	1:B:566:THR:N	2.29	0.77
1:A:95:GLU:HB3	1:A:96:PRO:CD	2.07	0.77
1:A:262:LYS:HB3	1:A:286:LYS:NZ	2.00	0.76
1:B:60:GLU:C	1:B:62:CYS:N	2.35	0.76
1:B:186:ARG:HA	3:B:603:LPC:O5A	1.85	0.76
1:B:219:LEU:HD23	1:B:223:PHE:CE2	2.21	0.76
1:A:529:LEU:HD22	3:A:606:LPC:CB	2.15	0.76
1:A:56:ASP:O	1:A:58:SER:N	2.16	0.76
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.66	0.76
1:A:357:LEU:O	1:A:359:LYS:N	2.18	0.76
1:B:61:ASN:HB3	1:B:64:LYS:HG3	1.65	0.76
1:B:453:LEU:O	1:B:457:LEU:HD22	1.85	0.76
1:B:556:GLU:O	1:B:560:LYS:HB3	1.85	0.76
1:B:436:LYS:NZ	1:B:452:TYR:OH	2.19	0.76
1:B:60:GLU:CG	1:B:61:ASN:OD1	2.30	0.76
1:B:403:PHE:HE2	1:B:431:GLY:HA2	1.50	0.76
1:B:540:THR:O	1:B:543:GLN:N	2.19	0.76
1:B:286:LYS:O	1:B:290:ILE:HG13	1.86	0.76
1:B:436:LYS:NZ	1:B:452:TYR:CZ	2.54	0.75
3:A:605:LPC:CJ	3:A:605:LPC:HF1	2.14	0.75
1:A:574:LYS:C	1:A:578:ALA:HB2	2.12	0.75
1:B:219:LEU:HD23	1:B:223:PHE:HE2	1.51	0.75
1:A:37:GLU:CD	1:A:37:GLU:H	1.95	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LYS:O	1:A:290:ILE:HG13	1.87	0.74
1:B:250:LEU:HD23	1:B:250:LEU:O	1.87	0.74
1:A:135:LEU:HB3	3:A:604:LPC:HK1	1.67	0.74
1:B:563:ASP:OD2	1:B:566:THR:CB	2.36	0.74
1:A:577:ALA:CA	1:A:580:GLU:OE1	2.35	0.74
1:A:460:LEU:HD12	1:A:460:LEU:O	1.87	0.74
1:B:400:GLU:O	1:B:404:GLN:HG3	1.87	0.74
1:B:518:GLU:OE1	1:B:518:GLU:HA	1.87	0.74
1:A:529:LEU:O	1:A:533:VAL:HG23	1.88	0.74
1:B:387:LEU:HD12	1:B:485:ARG:NH2	2.02	0.74
1:B:395:PHE:O	1:B:396:GLU:C	2.30	0.74
1:A:535:HIS:C	1:A:537:PRO:HD3	2.13	0.73
1:A:565:GLU:OE2	1:A:565:GLU:CA	2.34	0.73
1:A:115:LEU:HD13	1:A:145:ARG:CZ	2.19	0.73
1:A:575:LEU:N	1:A:578:ALA:CB	2.52	0.73
1:B:24:LEU:HD23	1:B:139:LEU:HD23	1.71	0.73
1:A:268:GLN:O	1:A:272:SER:O	2.06	0.73
1:B:344:VAL:HG21	3:B:604:LPC:H0A1	1.70	0.73
1:B:351:LYS:HD3	1:B:354:GLU:OE1	1.88	0.73
1:A:95:GLU:CB	1:A:96:PRO:HD3	2.16	0.73
1:A:258:ALA:O	1:A:262:LYS:HG3	1.89	0.72
1:B:60:GLU:OE2	1:B:61:ASN:ND2	2.21	0.72
1:A:539:ALA:HB1	1:A:544:LEU:HD13	1.68	0.72
1:B:115:LEU:HD13	1:B:145:ARG:CZ	2.20	0.72
1:B:558:CYS:SG	1:B:568:PHE:N	2.63	0.72
1:B:140:TYR:CZ	1:B:144:ARG:HD2	2.25	0.72
1:A:231:VAL:O	1:A:235:VAL:HG23	1.89	0.72
1:A:388:ILE:CD1	3:A:605:LPC:H72	2.20	0.72
1:B:502:PHE:O	1:B:502:PHE:CD1	2.43	0.72
1:B:305:LEU:HD23	1:B:305:LEU:N	2.02	0.71
1:A:574:LYS:C	1:A:578:ALA:CB	2.63	0.71
1:A:558:CYS:SG	1:A:568:PHE:N	2.63	0.71
1:B:149:PHE:HZ	3:B:603:LPC:H0C2	1.55	0.71
1:A:504:ALA:O	1:A:506:THR:CA	2.39	0.71
1:B:389:LYS:O	1:B:393:GLU:HG3	1.91	0.71
1:B:560:LYS:O	1:B:560:LYS:HG3	1.90	0.71
1:A:3:HIS:CG	1:A:4:LYS:H	2.09	0.70
1:A:506:THR:CG2	1:A:507:PHE:N	2.37	0.70
1:A:529:LEU:CD2	3:A:606:LPC:OQ1	2.40	0.70
1:B:114:ARG:NH2	1:B:116:VAL:HA	2.04	0.70
1:B:258:ALA:O	1:B:262:LYS:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:THR:HA	1:A:568:PHE:O	1.92	0.70
1:B:23:VAL:HG22	2:B:602:MYR:C13	2.21	0.70
1:B:482:VAL:O	1:B:482:VAL:CG1	2.40	0.70
1:A:351:LYS:HE3	1:A:354:GLU:OE1	1.92	0.69
1:B:390:GLN:O	1:B:394:LEU:HD23	1.92	0.69
1:A:373:VAL:O	1:A:375:ASP:N	2.26	0.69
1:B:551:PHE:HD1	3:B:605:LPC:HO8	1.40	0.69
1:A:135:LEU:CB	3:A:604:LPC:CK	2.61	0.69
1:B:139:LEU:HB2	3:B:603:LPC:CJ	2.22	0.69
1:B:410:ARG:O	1:B:414:LYS:HG3	1.92	0.69
1:B:33:GLN:HG2	1:B:84:TYR:CE1	2.28	0.69
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.74	0.69
1:A:428:ARG:O	1:A:431:GLY:N	2.26	0.69
1:A:545:LYS:O	1:A:545:LYS:HD3	1.93	0.69
1:A:381:VAL:CG1	1:A:385:GLN:NE2	2.56	0.69
1:B:507:PHE:CE2	3:B:605:LPC:CL	2.75	0.69
1:B:249:ASP:OD1	1:B:249:ASP:C	2.35	0.69
1:A:390:GLN:C	1:A:390:GLN:NE2	2.51	0.69
1:B:107:ASP:OD2	1:B:110:PRO:HA	1.93	0.69
1:B:120:VAL:HG21	1:B:175:ALA:CB	2.22	0.69
1:B:115:LEU:HD13	1:B:145:ARG:NH1	2.07	0.68
1:A:135:LEU:HB3	3:A:604:LPC:CL	2.24	0.68
1:A:552:ALA:C	1:A:554:PHE:N	2.51	0.68
1:A:552:ALA:CB	3:A:606:LPC:H21	2.22	0.68
1:A:86:GLU:O	1:A:89:ASP:HB2	1.93	0.68
1:A:471:ASP:O	1:A:475:LYS:N	2.26	0.68
1:B:149:PHE:HE2	3:B:603:LPC:C2	2.06	0.68
1:A:129:ASP:O	1:A:130:ASN:HB2	1.93	0.68
1:A:344:VAL:CG2	3:A:605:LPC:H0A2	2.24	0.68
1:A:566:THR:C	1:A:568:PHE:O	2.36	0.68
1:B:73:LYS:O	1:B:73:LYS:HG3	1.94	0.67
1:B:222:ARG:HD3	1:B:295:ASN:OD1	1.94	0.67
1:A:257:ARG:O	1:A:261:ALA:HB2	1.94	0.67
1:A:575:LEU:N	1:A:578:ALA:HB3	2.08	0.67
1:A:167:GLU:O	1:A:167:GLU:HG2	1.94	0.67
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.30	0.67
1:B:525:LYS:HE3	3:B:605:LPC:C7	2.24	0.67
1:A:132:GLU:OE2	1:A:132:GLU:CA	2.35	0.67
1:B:420:THR:OG1	1:B:534:LYS:HE3	1.95	0.67
1:A:94:GLN:O	1:A:95:GLU:C	2.37	0.67
1:A:555:VAL:HG13	1:A:556:GLU:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:OE2	1:B:61:ASN:OD1	2.12	0.67
1:B:149:PHE:HE2	3:B:603:LPC:C0A	1.89	0.67
1:A:225:LYS:HD3	1:A:297:GLU:O	1.95	0.66
1:A:575:LEU:O	1:A:579:SER:N	2.28	0.66
1:B:312:SER:O	1:B:313:LYS:O	2.14	0.66
1:A:56:ASP:O	1:A:56:ASP:CG	2.38	0.66
1:A:341:TYR:CD2	1:A:345:LEU:HD23	2.30	0.66
1:B:183:ASP:HA	1:B:186:ARG:HH12	1.59	0.66
1:A:115:LEU:HD13	1:A:145:ARG:HH12	1.59	0.66
1:A:222:ARG:C	1:A:224:PRO:HD3	2.21	0.66
1:A:541:LYS:C	1:A:542:GLU:HG2	2.20	0.66
1:B:56:ASP:O	1:B:56:ASP:CG	2.37	0.66
1:B:60:GLU:OE2	1:B:61:ASN:CG	2.38	0.66
1:A:388:ILE:HD13	3:A:605:LPC:H72	1.78	0.66
1:A:507:PHE:HB3	3:A:606:LPC:HI1	1.76	0.66
1:A:373:VAL:C	1:A:375:ASP:N	2.52	0.66
1:A:458:ASN:C	1:A:460:LEU:N	2.51	0.66
1:B:520:GLU:O	1:B:523:ILE:HB	1.95	0.66
1:B:564:LYS:O	1:B:565:GLU:C	2.39	0.66
1:A:298:MET:HE3	1:A:337:ARG:HA	1.78	0.66
1:B:417:GLN:O	1:B:469:VAL:HG11	1.96	0.65
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.79	0.65
1:A:78:ALA:C	1:A:80:LEU:H	2.04	0.65
1:A:311:GLU:O	1:A:312:SER:O	2.14	0.65
1:A:414:LYS:N	1:A:493:VAL:CG2	2.59	0.65
1:B:391:ASN:O	1:B:394:LEU:HB2	1.96	0.65
1:B:570:GLU:HA	1:B:573:LYS:N	2.00	0.65
1:A:171:ALA:O	1:A:172:ALA:O	2.15	0.65
1:B:150:TYR:O	1:B:151:ALA:C	2.34	0.65
1:B:507:PHE:CD2	3:B:605:LPC:HL2	2.31	0.65
1:B:56:ASP:O	1:B:56:ASP:OD1	2.15	0.65
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.62	0.65
1:A:411:TYR:CD1	3:A:605:LPC:HL1	2.32	0.64
1:B:570:GLU:C	1:B:572:GLY:H	1.96	0.64
1:A:428:ARG:O	1:A:429:ASN:C	2.39	0.64
1:B:138:TYR:CG	3:B:603:LPC:HD1	2.31	0.64
1:B:480:SER:OG	1:B:483:ASN:HB2	1.98	0.64
1:A:93:LYS:O	1:A:94:GLN:CD	2.41	0.64
1:A:285:GLU:O	1:A:286:LYS:C	2.40	0.64
1:A:290:ILE:O	1:A:293:VAL:CG1	2.39	0.64
1:A:373:VAL:O	1:A:374:PHE:C	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:THR:N	1:A:421:PRO:HD2	2.13	0.64
1:B:138:TYR:CE1	3:B:603:LPC:CB	2.79	0.64
1:A:552:ALA:HB1	3:A:606:LPC:C2	2.28	0.64
1:B:507:PHE:CE2	3:B:605:LPC:CM	2.80	0.64
1:A:112:LEU:HD12	1:A:145:ARG:HG2	1.78	0.64
1:A:190:LYS:C	1:A:192:SER:H	2.05	0.64
1:A:553:ALA:HA	1:A:556:GLU:HB3	1.80	0.64
1:A:39:HIS:HA	1:A:42:LEU:HD12	1.80	0.64
1:B:33:GLN:HG2	1:B:84:TYR:HE1	1.62	0.64
1:A:22:LEU:HD22	1:A:151:ALA:HB1	1.80	0.64
1:B:407:LEU:HD13	1:B:430:LEU:HB3	1.80	0.64
1:B:543:GLN:O	1:B:547:VAL:HG23	1.98	0.64
1:A:260:LEU:O	1:A:264:ILE:HG13	1.97	0.64
1:B:517:SER:O	1:B:521:ARG:CD	2.45	0.64
1:A:411:TYR:CE1	3:A:605:LPC:HL1	2.33	0.63
3:A:605:LPC:CJ	3:A:605:LPC:CF	2.75	0.63
1:B:218:ARG:NE	2:B:601:MYR:H143	2.12	0.63
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.26	0.63
1:A:488:PHE:C	1:A:490:ALA:H	2.06	0.63
1:B:499:PRO:HB3	1:B:535:HIS:O	1.98	0.63
1:B:94:GLN:C	1:B:96:PRO:HD2	2.23	0.63
1:B:344:VAL:HG21	3:B:604:LPC:C0A	2.26	0.63
1:A:485:ARG:HH11	3:A:605:LPC:H0B3	1.52	0.63
1:A:456:VAL:C	1:A:458:ASN:H	2.07	0.62
1:B:45:GLU:OE2	1:B:73:LYS:NZ	2.31	0.62
1:A:526:GLN:O	1:A:529:LEU:HB3	1.98	0.62
1:A:95:GLU:O	1:A:96:PRO:C	2.42	0.62
1:A:344:VAL:HG23	3:A:605:LPC:C0A	2.30	0.62
1:A:499:PRO:HB3	1:A:535:HIS:O	1.99	0.62
1:B:387:LEU:HD12	1:B:485:ARG:HH22	1.61	0.62
1:A:74:LEU:C	1:A:76:THR:H	2.05	0.62
1:B:400:GLU:O	1:B:400:GLU:HG2	1.99	0.62
1:B:466:LYS:C	1:B:467:THR:OG1	2.40	0.62
1:B:310:VAL:HG12	1:B:310:VAL:O	1.98	0.62
1:A:158:ALA:HB1	3:A:604:LPC:CJ	2.25	0.61
1:B:575:LEU:CA	1:B:578:ALA:HB3	2.29	0.61
1:B:387:LEU:O	1:B:391:ASN:HB2	1.99	0.61
1:B:424:VAL:O	1:B:428:ARG:HG3	1.99	0.61
1:A:577:ALA:C	1:A:580:GLU:OE1	2.44	0.61
1:B:351:LYS:HD2	1:B:351:LYS:O	2.01	0.61
1:A:556:GLU:O	1:A:557:LYS:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:PHE:HB3	1:B:271:ILE:O	2.00	0.61
1:A:579:SER:O	1:A:580:GLU:CG	2.49	0.61
1:B:537:PRO:O	1:B:537:PRO:CG	2.46	0.61
1:B:395:PHE:HZ	1:B:435:SER:HB2	1.65	0.61
1:B:23:VAL:HG22	2:B:602:MYR:H132	1.83	0.61
1:B:420:THR:N	1:B:421:PRO:HD2	2.14	0.61
1:B:448:CYS:O	1:B:449:ALA:C	2.44	0.61
1:B:579:SER:O	1:B:581:ALA:N	2.34	0.61
1:B:507:PHE:CE2	3:B:605:LPC:HM2	2.36	0.60
1:A:535:HIS:O	1:A:537:PRO:HD3	2.00	0.60
1:A:566:THR:O	1:A:567:CYS:O	2.20	0.60
1:B:218:ARG:CZ	2:B:601:MYR:C14	2.52	0.60
1:B:140:TYR:CE1	1:B:144:ARG:HD2	2.36	0.60
1:B:387:LEU:CD1	1:B:485:ARG:NH2	2.64	0.60
1:A:94:GLN:O	1:A:95:GLU:O	2.20	0.60
1:A:249:ASP:OD1	1:A:249:ASP:O	2.18	0.60
1:A:388:ILE:CD1	3:A:605:LPC:C7	2.79	0.60
1:B:570:GLU:O	1:B:574:LYS:N	2.32	0.60
1:A:51:LYS:O	1:A:54:VAL:HG12	2.00	0.60
1:A:53:CYS:C	1:A:55:ALA:H	2.10	0.60
1:B:301:ASP:O	1:B:302:LEU:C	2.44	0.60
1:B:56:ASP:O	1:B:57:GLU:C	2.44	0.60
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.82	0.60
1:B:579:SER:C	1:B:581:ALA:N	2.60	0.60
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.83	0.60
1:A:266:GLU:C	1:A:267:ASN:OD1	2.45	0.60
1:A:407:LEU:HD13	1:A:430:LEU:HB3	1.84	0.60
1:B:467:THR:HG22	1:B:467:THR:O	2.02	0.60
1:B:557:LYS:O	1:B:557:LYS:CG	2.50	0.59
1:A:115:LEU:CD1	1:A:145:ARG:HH12	2.15	0.59
1:A:281:LYS:HD3	1:A:285:GLU:OE1	2.03	0.59
1:A:417:GLN:HB3	1:A:469:VAL:HG12	1.82	0.59
1:A:567:CYS:O	1:A:568:PHE:C	2.45	0.59
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.84	0.59
1:B:517:SER:OG	1:B:518:GLU:N	2.34	0.59
1:B:578:ALA:C	1:B:580:GLU:H	2.09	0.59
1:B:19:PHE:O	1:B:23:VAL:HG23	2.03	0.59
1:B:437:CYS:HA	1:B:440:HIS:HD2	1.67	0.59
1:B:471:ASP:O	1:B:472:ARG:O	2.19	0.59
1:B:532:LEU:C	1:B:532:LEU:HD23	2.27	0.59
1:A:95:GLU:CB	1:A:96:PRO:CD	2.72	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HG2	1:B:222:ARG:NH1	2.18	0.59
1:B:420:THR:H	1:B:421:PRO:HD2	1.67	0.59
3:A:605:LPC:HF1	3:A:605:LPC:HJ1	1.84	0.59
1:A:313:LYS:O	1:A:314:ASP:CB	2.44	0.59
1:B:472:ARG:O	1:B:473:VAL:C	2.46	0.59
1:A:489:SER:N	3:A:605:LPC:HH2	2.18	0.59
1:B:450:GLU:O	1:B:454:SER:HB3	2.02	0.59
1:A:363:ALA:O	1:A:364:ALA:C	2.45	0.58
1:A:522:GLN:O	1:A:526:GLN:HG3	2.03	0.58
1:B:212:LYS:HD3	2:B:606:MYR:H143	1.85	0.58
1:B:540:THR:H	1:B:543:GLN:HB2	1.66	0.58
1:B:198:LEU:HD12	1:B:198:LEU:O	2.04	0.58
1:B:395:PHE:HE2	1:B:435:SER:HA	1.64	0.58
1:A:119:GLU:O	1:A:121:ASP:N	2.35	0.58
1:A:499:PRO:HG3	1:A:537:PRO:HG2	1.86	0.58
1:A:554:PHE:O	1:A:557:LYS:HB3	2.03	0.58
1:A:573:LYS:C	1:A:575:LEU:H	2.11	0.58
1:A:76:THR:C	1:A:77:VAL:O	2.45	0.58
1:A:94:GLN:HA	1:A:98:ARG:HB2	1.86	0.58
1:A:437:CYS:SG	1:A:448:CYS:C	2.87	0.58
1:A:503:ASN:C	1:A:503:ASN:OD1	2.43	0.58
1:A:149:PHE:HD2	1:A:154:LEU:CD1	2.17	0.58
1:B:173:ASP:O	1:B:174:LYS:C	2.47	0.58
1:B:502:PHE:HD2	1:B:535:HIS:NE2	2.01	0.58
1:A:485:ARG:HH21	1:A:489:SER:CB	2.17	0.58
1:A:552:ALA:O	1:A:554:PHE:N	2.35	0.58
1:B:426:VAL:HG21	1:B:460:LEU:HD13	1.84	0.58
1:A:30:TYR:CD1	1:A:106:LYS:HE3	2.39	0.58
1:B:507:PHE:HE2	3:B:605:LPC:CL	2.13	0.58
1:A:115:LEU:HD13	1:A:145:ARG:NH2	2.18	0.58
1:B:155:LEU:O	1:B:158:ALA:HB3	2.04	0.58
1:A:489:SER:CA	3:A:605:LPC:HH2	2.33	0.58
1:B:319:TYR:CE2	1:B:323:LYS:HD3	2.39	0.58
1:B:575:LEU:O	1:B:579:SER:N	2.37	0.58
1:A:95:GLU:C	1:A:95:GLU:OE2	2.46	0.57
1:A:119:GLU:O	1:A:120:VAL:C	2.47	0.57
1:A:293:VAL:HG22	1:A:294:GLU:N	2.19	0.57
1:A:370:TYR:C	1:A:372:LYS:N	2.58	0.57
1:B:218:ARG:NH1	2:B:601:MYR:H141	2.12	0.57
1:B:403:PHE:CE2	1:B:431:GLY:HA2	2.37	0.57
1:A:219:LEU:HD23	1:A:223:PHE:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:NE	3:B:604:LPC:H0B2	2.16	0.57
1:B:572:GLY:O	1:B:576:VAL:HG23	2.05	0.57
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.36	0.57
1:A:545:LYS:HD3	1:A:545:LYS:C	2.30	0.57
1:B:10:ARG:O	1:B:14:LEU:HB2	2.04	0.57
1:B:138:TYR:CE1	3:B:603:LPC:HD1	2.38	0.57
1:A:413:LYS:CB	1:A:493:VAL:CG2	2.80	0.57
1:B:158:ALA:CB	3:B:603:LPC:HK1	2.19	0.57
1:B:396:GLU:O	1:B:397:GLN:C	2.43	0.57
1:A:319:TYR:O	1:A:323:LYS:HG2	2.05	0.57
1:B:564:LYS:C	1:B:566:THR:H	2.13	0.57
1:A:90:CYS:O	1:A:93:LYS:HB2	2.05	0.57
1:A:540:THR:O	1:A:544:LEU:HB2	2.04	0.57
1:B:466:LYS:C	1:B:467:THR:HG1	2.11	0.57
1:A:331:LEU:HD11	1:A:347:LEU:HD23	1.86	0.57
1:B:312:SER:O	1:B:313:LYS:C	2.44	0.57
1:B:350:ALA:CB	2:B:606:MYR:H52	2.35	0.57
1:A:284:LEU:O	1:A:284:LEU:HD23	2.05	0.57
1:B:537:PRO:O	1:B:538:LYS:CB	2.45	0.57
1:B:551:PHE:CD1	1:B:551:PHE:C	2.82	0.57
1:B:37:GLU:CD	1:B:37:GLU:H	2.13	0.56
1:A:344:VAL:HG21	3:A:605:LPC:H0A2	1.80	0.56
1:B:247:HIS:CG	1:B:247:HIS:O	2.57	0.56
1:B:442:GLU:OE1	1:B:442:GLU:N	2.37	0.56
1:A:414:LYS:HA	1:A:493:VAL:HA	1.86	0.56
1:A:493:VAL:HG12	1:A:493:VAL:O	2.05	0.56
1:B:517:SER:O	1:B:521:ARG:HB2	2.04	0.56
1:B:540:THR:HB	1:B:543:GLN:HG2	1.86	0.56
1:A:138:TYR:CD1	3:A:604:LPC:HB2	2.40	0.56
1:A:388:ILE:HD11	3:A:605:LPC:H72	1.87	0.56
1:A:457:LEU:HD11	3:A:605:LPC:HK1	1.88	0.56
1:B:482:VAL:O	1:B:482:VAL:HG13	2.06	0.56
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.34	0.56
1:A:345:LEU:HD11	1:A:381:VAL:HA	1.88	0.56
1:A:556:GLU:CG	1:A:557:LYS:N	2.64	0.56
1:A:576:VAL:O	3:A:606:LPC:HN2	2.05	0.56
1:B:158:ALA:CA	3:B:603:LPC:HK1	2.35	0.56
1:A:160:ARG:NH2	1:A:188:GLU:OE2	2.38	0.56
1:A:357:LEU:O	1:A:358:GLU:C	2.48	0.56
1:B:94:GLN:HB3	1:B:96:PRO:HD2	1.88	0.56
1:B:273:SER:C	1:B:275:LEU:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:GLN:OE1	1:B:582:ALA:CB	2.53	0.56
1:A:418:VAL:HG21	1:A:423:LEU:HD21	1.87	0.56
1:B:564:LYS:O	1:B:566:THR:N	2.37	0.56
1:A:85:GLY:O	1:A:86:GLU:C	2.49	0.56
1:A:324:ASP:O	1:A:325:VAL:C	2.47	0.56
1:A:458:ASN:O	1:A:461:CYS:N	2.39	0.56
1:B:30:TYR:HB3	1:B:31:LEU:HD13	1.88	0.56
1:B:465:GLU:C	1:B:467:THR:H	2.14	0.56
1:B:578:ALA:C	1:B:580:GLU:N	2.64	0.56
1:B:260:LEU:HD23	2:B:601:MYR:H72	1.88	0.55
1:B:219:LEU:CD2	1:B:223:PHE:HE2	2.19	0.55
1:B:299:PRO:O	1:B:300:ALA:CB	2.42	0.55
1:B:310:VAL:O	1:B:310:VAL:CG1	2.55	0.55
1:A:80:LEU:O	1:A:84:TYR:HB2	2.07	0.55
1:A:357:LEU:C	1:A:359:LYS:N	2.64	0.55
1:A:555:VAL:CG1	1:A:556:GLU:N	2.69	0.55
1:B:539:ALA:HB3	1:B:544:LEU:HD11	1.88	0.55
1:A:249:ASP:O	1:A:251:LEU:N	2.39	0.55
1:B:36:PHE:HZ	1:B:136:LYS:HB2	1.72	0.55
1:B:561:ALA:O	1:B:563:ASP:O	2.25	0.55
1:A:381:VAL:HG12	1:A:385:GLN:NE2	2.21	0.55
1:A:555:VAL:O	1:A:556:GLU:C	2.46	0.55
1:B:127:PHE:O	1:B:131:GLU:HB2	2.07	0.55
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.88	0.55
1:A:552:ALA:C	3:A:606:LPC:H21	2.31	0.55
1:A:529:LEU:HD22	3:A:606:LPC:OQ1	2.07	0.55
1:A:575:LEU:N	1:A:578:ALA:HB2	2.20	0.55
1:B:152:PRO:O	1:B:155:LEU:HB3	2.06	0.55
1:A:15:GLY:O	1:A:16:GLU:C	2.50	0.55
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.87	0.55
1:A:273:SER:O	1:A:275:LEU:N	2.40	0.55
1:A:424:VAL:O	1:A:428:ARG:HG3	2.06	0.55
1:B:146:HIS:CG	3:B:603:LPC:H0A3	2.42	0.55
1:B:411:TYR:CZ	3:B:604:LPC:HJ1	2.42	0.55
1:B:560:LYS:O	1:B:560:LYS:CG	2.55	0.55
1:A:565:GLU:CD	1:A:565:GLU:O	2.50	0.54
1:A:78:ALA:C	1:A:80:LEU:N	2.64	0.54
1:A:262:LYS:HB3	1:A:286:LYS:HZ2	1.72	0.54
1:B:199:LYS:HE3	1:B:242:HIS:HE1	1.68	0.54
1:B:219:LEU:HD11	1:B:238:LEU:HD22	1.90	0.54
1:B:370:TYR:O	1:B:372:LYS:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:O	1:B:546:ALA:N	2.39	0.54
1:B:49:PHE:O	1:B:52:THR:HB	2.07	0.54
1:B:257:ARG:NH2	2:B:602:MYR:O1	2.36	0.54
1:B:537:PRO:O	1:B:537:PRO:CD	2.54	0.54
1:A:274:LYS:HE3	1:A:296:ASP:HA	1.87	0.54
1:B:27:PHE:CE1	1:B:70:PHE:HE1	2.26	0.54
1:B:512:ASP:OD1	1:B:513:ILE:N	2.40	0.54
1:A:350:ALA:HB3	2:A:601:MYR:H71	1.89	0.54
1:A:504:ALA:O	1:A:505:GLU:C	2.41	0.54
1:A:390:GLN:HE21	1:A:391:ASN:CA	2.20	0.54
1:A:564:LYS:O	1:A:565:GLU:HB3	2.06	0.54
1:A:370:TYR:C	1:A:370:TYR:CD1	2.86	0.54
1:A:580:GLU:O	1:A:581:ALA:HB2	2.07	0.54
1:A:93:LYS:C	1:A:94:GLN:OE1	2.51	0.54
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.89	0.54
1:A:357:LEU:N	1:A:357:LEU:HD23	2.21	0.54
1:A:415:VAL:O	1:A:418:VAL:HG22	2.07	0.54
1:A:579:SER:O	1:A:580:GLU:CB	2.56	0.53
1:B:149:PHE:CD2	1:B:154:LEU:HD13	2.43	0.53
1:A:324:ASP:OD1	1:A:324:ASP:N	2.40	0.53
1:B:351:LYS:CE	1:B:354:GLU:OE1	2.56	0.53
1:A:305:LEU:HD21	1:A:333:GLU:CB	2.38	0.53
1:B:95:GLU:N	1:B:96:PRO:HD2	2.23	0.53
1:B:412:THR:HA	1:B:423:LEU:HD22	1.90	0.53
1:B:466:LYS:O	1:B:467:THR:OG1	2.26	0.53
1:A:388:ILE:HD13	3:A:605:LPC:C7	2.37	0.53
1:A:494:ASP:O	1:A:494:ASP:OD1	2.26	0.53
1:B:68:THR:HG22	1:B:69:LEU:N	2.23	0.53
1:A:22:LEU:CD2	1:A:151:ALA:HB1	2.38	0.53
1:B:41:LYS:O	1:B:45:GLU:CG	2.50	0.53
1:B:114:ARG:O	1:B:114:ARG:HG3	2.09	0.53
1:B:581:ALA:O	1:B:582:ALA:C	2.50	0.53
1:A:149:PHE:CE1	1:A:196:GLN:OE1	2.62	0.53
1:A:484:ARG:O	1:A:488:PHE:HD2	1.92	0.53
1:B:575:LEU:HA	1:B:578:ALA:HB3	1.89	0.53
1:A:414:LYS:HG2	1:A:493:VAL:HG23	1.91	0.53
1:A:432:LYS:O	1:A:436:LYS:N	2.35	0.53
1:A:529:LEU:HD22	3:A:606:LPC:CA	2.38	0.53
1:B:571:GLU:HA	1:B:571:GLU:OE1	2.09	0.53
1:A:458:ASN:C	1:A:458:ASN:OD1	2.51	0.53
1:A:485:ARG:O	1:A:486:PRO:C	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:O	1:A:60:GLU:C	2.51	0.53
1:B:13:ASP:OD1	1:B:13:ASP:C	2.52	0.53
1:B:344:VAL:HG23	3:B:604:LPC:H0A2	1.90	0.53
1:B:452:TYR:O	1:B:454:SER:N	2.41	0.53
1:A:370:TYR:C	1:A:372:LYS:H	2.17	0.53
1:B:218:ARG:CD	2:B:601:MYR:C14	2.87	0.53
1:B:253:CYS:O	1:B:257:ARG:HG3	2.09	0.53
1:B:291:ALA:CA	2:B:601:MYR:H112	2.25	0.53
1:B:539:ALA:CB	1:B:544:LEU:CD1	2.87	0.53
1:A:96:PRO:HD2	1:A:97:GLU:H	1.74	0.52
1:B:429:ASN:O	1:B:432:LYS:HB2	2.09	0.52
1:B:485:ARG:NE	3:B:604:LPC:C0B	2.72	0.52
1:A:21:ALA:O	1:A:25:ILE:HG13	2.09	0.52
1:B:8:ALA:O	1:B:12:LYS:HB2	2.09	0.52
1:B:284:LEU:HA	2:B:602:MYR:H41	1.91	0.52
1:A:381:VAL:HG13	1:A:385:GLN:NE2	2.23	0.52
1:A:566:THR:HA	1:A:569:ALA:HB3	1.91	0.52
1:B:15:GLY:O	1:B:16:GLU:C	2.53	0.52
1:B:302:LEU:HB3	1:B:337:ARG:NH1	2.24	0.52
1:A:15:GLY:O	1:A:17:GLU:N	2.43	0.52
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.39	0.52
1:A:485:ARG:CD	3:A:605:LPC:H0B2	2.24	0.52
1:B:500:LYS:H	1:B:535:HIS:HA	1.75	0.52
1:A:149:PHE:HD2	1:A:154:LEU:HD13	1.74	0.52
1:A:299:PRO:O	1:A:301:ASP:N	2.38	0.52
1:A:413:LYS:HB3	1:A:493:VAL:CG2	2.33	0.52
1:A:453:LEU:O	1:A:457:LEU:HB2	2.09	0.52
1:A:94:GLN:O	1:A:97:GLU:N	2.43	0.52
1:A:441:PRO:O	1:A:442:GLU:C	2.53	0.52
1:B:135:LEU:HB3	3:B:603:LPC:HL1	1.92	0.52
1:B:261:ALA:HB2	1:B:287:SER:HB3	1.92	0.52
1:B:419:SER:O	1:B:423:LEU:CD1	2.54	0.52
1:B:515:THR:O	1:B:515:THR:OG1	2.20	0.52
1:A:342:SER:HG	3:A:605:LPC:H0C3	1.71	0.51
1:A:471:ASP:O	1:A:474:THR:N	2.43	0.51
1:B:250:LEU:O	1:B:250:LEU:CD2	2.57	0.51
1:B:544:LEU:C	1:B:546:ALA:N	2.67	0.51
1:B:351:LYS:CD	1:B:354:GLU:OE1	2.57	0.51
1:B:387:LEU:CD1	1:B:485:ARG:HH22	2.23	0.51
1:B:552:ALA:HB1	3:B:605:LPC:O5A	2.10	0.51
1:B:31:LEU:N	1:B:31:LEU:CD1	2.71	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:CYS:C	1:B:55:ALA:H	2.18	0.51
1:B:237:ASP:CB	1:B:260:LEU:HD13	2.34	0.51
1:A:51:LYS:HA	1:A:54:VAL:HG12	1.92	0.51
1:A:110:PRO:HG3	1:A:145:ARG:HA	1.91	0.51
1:A:273:SER:C	1:A:275:LEU:H	2.17	0.51
1:A:458:ASN:C	1:A:460:LEU:H	2.16	0.51
1:A:464:HIS:CE1	1:A:474:THR:OG1	2.63	0.51
1:A:540:THR:C	1:A:542:GLU:H	2.17	0.51
1:B:149:PHE:HZ	3:B:603:LPC:H0C3	1.36	0.51
1:B:341:TYR:CG	1:B:345:LEU:HD23	2.46	0.51
1:B:350:ALA:HB3	2:B:606:MYR:H52	1.92	0.51
1:A:464:HIS:HE1	1:A:474:THR:OG1	1.92	0.51
1:A:552:ALA:HB1	3:A:606:LPC:H0B1	1.92	0.51
1:B:579:SER:C	1:B:581:ALA:H	2.17	0.51
1:A:413:LYS:HB2	1:A:493:VAL:HG21	1.89	0.51
1:B:299:PRO:HG2	1:B:302:LEU:HD21	1.93	0.51
1:B:389:LYS:O	1:B:393:GLU:CG	2.58	0.51
1:A:3:HIS:CG	1:A:4:LYS:N	2.76	0.51
1:A:131:GLU:O	1:A:132:GLU:C	2.53	0.51
1:A:267:ASN:O	1:A:271:ILE:CG1	2.50	0.51
1:A:576:VAL:HA	3:A:606:LPC:HL1	1.92	0.51
1:B:230:GLU:OE1	1:B:230:GLU:HA	2.11	0.51
1:B:467:THR:N	1:B:468:PRO:HD3	2.25	0.51
1:A:539:ALA:HB1	1:A:544:LEU:CD1	2.37	0.51
1:B:160:ARG:NH1	1:B:188:GLU:OE1	2.44	0.51
1:B:548:MET:C	1:B:550:ASP:N	2.68	0.51
1:A:112:LEU:CD1	1:A:145:ARG:HG2	2.41	0.51
1:A:258:ALA:O	1:A:262:LYS:CG	2.59	0.51
1:A:56:ASP:OD1	1:A:56:ASP:C	2.54	0.50
1:A:95:GLU:OE2	1:A:95:GLU:CA	2.49	0.50
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.93	0.50
1:A:457:LEU:HD12	1:A:460:LEU:HD23	1.92	0.50
1:A:540:THR:HG22	1:A:541:LYS:N	2.24	0.50
1:B:33:GLN:HB2	1:B:84:TYR:CZ	2.46	0.50
1:A:127:PHE:C	1:A:129:ASP:N	2.66	0.50
1:B:58:SER:C	1:B:59:ALA:O	2.54	0.50
1:A:90:CYS:HA	1:A:93:LYS:HD2	1.92	0.50
1:A:165:PHE:O	1:A:169:CYS:HB2	2.12	0.50
1:A:485:ARG:HH21	1:A:489:SER:HB2	1.76	0.50
1:B:138:TYR:CD1	3:B:603:LPC:CB	2.94	0.50
1:B:459:GLN:O	1:B:459:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:O	1:A:303:PRO:O	2.28	0.50
1:A:420:THR:H	1:A:421:PRO:HD2	1.77	0.50
1:B:104:GLN:C	1:B:105:HIS:CD2	2.89	0.50
1:A:311:GLU:O	1:A:312:SER:C	2.49	0.50
1:A:461:CYS:O	1:A:464:HIS:N	2.40	0.50
1:A:565:GLU:O	1:A:565:GLU:CG	2.59	0.50
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.30	0.50
2:B:601:MYR:H92	2:B:601:MYR:H51	1.91	0.50
1:A:138:TYR:O	1:A:142:ILE:HG12	2.12	0.50
1:A:401:TYR:CE1	1:A:522:GLN:HB3	2.47	0.50
1:A:418:VAL:CG2	1:A:423:LEU:HD21	2.42	0.50
1:A:436:LYS:CG	1:A:437:CYS:H	2.24	0.50
1:A:525:LYS:NZ	3:A:606:LPC:O5A	2.28	0.50
1:B:60:GLU:CD	1:B:61:ASN:OD1	2.55	0.50
1:B:104:GLN:C	1:B:105:HIS:HD2	2.20	0.50
1:A:507:PHE:HA	1:A:509:PHE:CZ	2.47	0.50
1:B:35:PRO:HG2	1:B:38:ASP:HB2	1.94	0.50
1:B:570:GLU:O	1:B:573:LYS:N	2.45	0.50
1:A:138:TYR:CG	3:A:604:LPC:HD1	2.47	0.49
1:A:529:LEU:HD23	3:A:606:LPC:OQ1	2.11	0.49
1:A:575:LEU:O	1:A:578:ALA:HB3	2.12	0.49
1:A:579:SER:O	1:A:580:GLU:OE1	2.30	0.49
1:B:116:VAL:HG23	1:B:116:VAL:O	2.12	0.49
1:B:420:THR:O	1:B:422:THR:N	2.45	0.49
1:A:30:TYR:CE1	1:A:106:LYS:NZ	2.77	0.49
1:A:66:LEU:HA	1:A:69:LEU:HD12	1.94	0.49
1:B:540:THR:O	1:B:542:GLU:N	2.45	0.49
1:A:485:ARG:HD3	3:A:605:LPC:H22	1.93	0.49
1:B:96:PRO:HG2	1:B:97:GLU:HG2	1.93	0.49
1:A:135:LEU:HB3	3:A:604:LPC:HL1	1.94	0.49
1:A:404:GLN:NE2	1:A:428:ARG:HB3	2.27	0.49
1:A:485:ARG:NH1	3:A:605:LPC:H0B3	2.17	0.49
1:A:360:CYS:SG	1:A:370:TYR:HB3	2.52	0.49
1:A:258:ALA:O	1:A:261:ALA:HB3	2.13	0.49
1:A:373:VAL:C	1:A:375:ASP:H	2.19	0.49
1:A:34:CYS:O	1:A:140:TYR:OH	2.30	0.49
1:B:111:ASN:ND2	1:B:111:ASN:N	2.60	0.49
1:A:135:LEU:CD1	1:A:162:LYS:HG3	2.42	0.49
1:A:414:LYS:N	1:A:493:VAL:HG23	2.27	0.49
1:B:24:LEU:CD2	1:B:139:LEU:HD23	2.41	0.49
1:B:114:ARG:HE	1:B:116:VAL:HG12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:SER:O	1:B:483:ASN:N	2.37	0.49
1:B:579:SER:O	1:B:580:GLU:C	2.54	0.49
1:A:135:LEU:C	3:A:604:LPC:HK1	2.37	0.49
1:A:284:LEU:HD23	1:A:284:LEU:C	2.38	0.49
1:A:509:PHE:HB3	1:A:513:ILE:HD13	1.94	0.49
1:B:464:HIS:ND1	1:B:464:HIS:C	2.71	0.49
1:A:3:HIS:CD2	1:A:4:LYS:H	2.30	0.49
1:B:456:VAL:O	1:B:457:LEU:C	2.55	0.49
1:A:150:TYR:OH	2:A:602:MYR:O2	2.29	0.48
1:A:381:VAL:CG1	1:A:385:GLN:HE22	2.26	0.48
1:A:407:LEU:HB3	1:A:411:TYR:HE2	1.78	0.48
1:A:407:LEU:O	1:A:411:TYR:CD2	2.66	0.48
1:B:178:LEU:O	1:B:181:LYS:HB3	2.13	0.48
1:B:322:ALA:O	1:B:323:LYS:C	2.56	0.48
1:A:381:VAL:HG13	1:A:385:GLN:HE21	1.77	0.48
1:A:456:VAL:O	1:A:458:ASN:N	2.42	0.48
1:B:417:GLN:O	1:B:469:VAL:CG1	2.60	0.48
1:A:49:PHE:O	1:A:52:THR:HB	2.13	0.48
1:A:53:CYS:C	1:A:55:ALA:N	2.71	0.48
1:A:266:GLU:O	1:A:267:ASN:OD1	2.31	0.48
1:A:319:TYR:CZ	1:A:323:LYS:HD3	2.48	0.48
1:A:436:LYS:CG	1:A:437:CYS:N	2.73	0.48
1:A:501:GLU:O	1:A:502:PHE:C	2.56	0.48
1:B:254:ALA:HB1	2:B:602:MYR:H52	1.93	0.48
1:B:384:PRO:O	1:B:388:ILE:HG12	2.14	0.48
1:A:495:GLU:OE1	1:A:495:GLU:HA	2.10	0.48
1:B:538:LYS:O	1:B:539:ALA:O	2.31	0.48
1:A:158:ALA:CB	3:A:604:LPC:HJ1	2.30	0.48
1:A:274:LYS:CE	1:A:296:ASP:HA	2.44	0.48
1:A:287:SER:OG	2:A:602:MYR:O1	2.15	0.48
1:A:435:SER:O	1:A:436:LYS:O	2.30	0.48
1:A:456:VAL:C	1:A:458:ASN:N	2.72	0.48
1:B:152:PRO:O	1:B:155:LEU:N	2.46	0.48
1:B:217:ALA:O	1:B:221:GLN:HG2	2.14	0.48
1:B:302:LEU:CD1	1:B:302:LEU:H	2.20	0.48
1:B:539:ALA:CB	1:B:544:LEU:HD11	2.43	0.48
1:A:157:PHE:O	1:A:160:ARG:HB2	2.14	0.48
1:A:485:ARG:CB	1:A:486:PRO:HD3	2.42	0.48
1:A:552:ALA:HB3	1:A:553:ALA:H	1.12	0.48
1:B:483:ASN:O	1:B:486:PRO:CD	2.44	0.48
1:A:150:TYR:O	1:A:151:ALA:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:CA	1:A:493:VAL:HG23	2.44	0.48
1:A:414:LYS:O	1:A:415:VAL:HG13	2.13	0.48
1:B:513:ILE:HA	1:B:516:LEU:HD12	1.95	0.48
1:A:275:LEU:HD21	1:A:290:ILE:HG23	1.96	0.48
1:B:257:ARG:HH21	1:B:287:SER:HG	1.57	0.48
1:B:302:LEU:CB	1:B:337:ARG:NH1	2.77	0.48
1:A:404:GLN:HG2	1:A:428:ARG:HA	1.95	0.48
1:B:114:ARG:HH21	1:B:116:VAL:CA	2.17	0.48
1:B:233:LYS:HD3	1:B:233:LYS:C	2.39	0.48
1:B:247:HIS:O	1:B:247:HIS:ND1	2.47	0.48
1:B:465:GLU:C	1:B:465:GLU:CD	2.80	0.48
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.95	0.48
1:A:345:LEU:O	1:A:349:LEU:HG	2.14	0.48
1:B:225:LYS:HE3	1:B:297:GLU:O	2.14	0.48
1:B:268:GLN:C	1:B:270:SER:H	2.22	0.48
1:B:53:CYS:O	1:B:57:GLU:N	2.47	0.47
1:B:112:LEU:N	1:B:112:LEU:HD12	2.29	0.47
1:A:76:THR:O	1:A:77:VAL:O	2.32	0.47
1:A:219:LEU:HD23	1:A:223:PHE:CE2	2.48	0.47
1:A:485:ARG:HB3	1:A:486:PRO:CD	2.38	0.47
1:A:114:ARG:HG3	1:A:114:ARG:O	2.13	0.47
1:A:237:ASP:O	1:A:238:LEU:C	2.57	0.47
1:B:33:GLN:HB2	1:B:84:TYR:OH	2.13	0.47
1:B:407:LEU:HD22	1:B:411:TYR:HE2	1.79	0.47
1:B:416:PRO:HG2	1:B:497:TYR:CD2	2.49	0.47
1:B:564:LYS:O	1:B:566:THR:CB	2.62	0.47
1:B:570:GLU:C	1:B:573:LYS:N	2.72	0.47
1:A:152:PRO:O	1:A:155:LEU:HB3	2.15	0.47
1:B:23:VAL:CG2	2:B:602:MYR:H132	2.44	0.47
1:B:30:TYR:CD1	1:B:30:TYR:N	2.79	0.47
1:B:218:ARG:HA	1:B:221:GLN:OE1	2.14	0.47
1:B:483:ASN:O	1:B:485:ARG:N	2.47	0.47
1:A:128:HIS:ND1	1:A:128:HIS:C	2.72	0.47
1:A:149:PHE:CE2	3:A:604:LPC:C0C	2.90	0.47
1:B:60:GLU:CG	1:B:61:ASN:CG	2.84	0.47
1:B:150:TYR:CE2	1:B:152:PRO:HB2	2.49	0.47
1:B:513:ILE:HA	1:B:516:LEU:CD1	2.45	0.47
1:B:570:GLU:C	1:B:573:LYS:H	2.22	0.47
1:A:127:PHE:C	1:A:129:ASP:H	2.20	0.47
1:A:345:LEU:HD13	1:A:384:PRO:HG3	1.96	0.47
1:A:499:PRO:HG3	1:A:537:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LEU:O	1:A:576:VAL:C	2.56	0.47
1:B:273:SER:C	1:B:275:LEU:N	2.69	0.47
1:A:52:THR:HG22	1:A:59:ALA:CB	2.44	0.47
1:A:150:TYR:H	1:A:196:GLN:HE22	1.62	0.47
1:A:174:LYS:O	1:A:175:ALA:C	2.57	0.47
1:A:452:TYR:O	1:A:453:LEU:C	2.56	0.47
1:A:551:PHE:O	1:A:551:PHE:CD1	2.67	0.47
1:B:324:ASP:OD1	1:B:324:ASP:N	2.48	0.47
1:B:411:TYR:CD1	3:B:604:LPC:HL1	2.49	0.47
1:B:557:LYS:C	1:B:567:CYS:SG	2.97	0.47
1:A:10:ARG:NH1	2:A:602:MYR:H62	2.29	0.47
1:A:76:THR:O	1:A:77:VAL:C	2.58	0.47
1:A:344:VAL:HG23	3:A:605:LPC:H0A2	1.92	0.47
1:A:553:ALA:CB	3:A:606:LPC:C0C	2.91	0.47
1:B:395:PHE:O	1:B:397:GLN:N	2.48	0.47
1:B:465:GLU:C	1:B:467:THR:N	2.71	0.47
1:A:87:MET:C	1:A:89:ASP:N	2.69	0.47
1:A:222:ARG:HD3	2:A:603:MYR:H141	1.96	0.47
1:A:577:ALA:O	1:A:580:GLU:OE1	2.33	0.47
1:A:315:VAL:HG13	1:A:316:CYS:H	1.79	0.47
1:A:506:THR:CG2	1:A:507:PHE:H	2.16	0.47
1:B:250:LEU:HA	1:B:253:CYS:HB3	1.97	0.47
1:A:398:LEU:HB3	1:A:402:LYS:CB	2.44	0.46
1:A:403:PHE:O	1:A:404:GLN:C	2.58	0.46
3:B:604:LPC:H0C1	3:B:604:LPC:H31	1.49	0.46
1:A:183:ASP:O	1:A:186:ARG:HB3	2.15	0.46
1:A:292:GLU:C	1:A:293:VAL:O	2.58	0.46
1:A:485:ARG:NH1	3:A:605:LPC:H0B2	2.08	0.46
1:B:404:GLN:NE2	1:B:428:ARG:HA	2.30	0.46
1:B:299:PRO:HB2	1:B:302:LEU:HD11	1.97	0.46
1:A:290:ILE:C	1:A:292:GLU:H	2.23	0.46
1:B:250:LEU:O	1:B:250:LEU:CG	2.63	0.46
1:A:61:ASN:O	1:A:64:LYS:HG2	2.15	0.46
1:A:138:TYR:CD1	3:A:604:LPC:HD1	2.50	0.46
1:A:178:LEU:CD1	1:A:182:LEU:HG	2.45	0.46
1:A:378:LYS:HG2	1:A:382:GLU:OE2	2.14	0.46
1:A:488:PHE:C	1:A:490:ALA:N	2.68	0.46
1:B:142:ILE:HD11	3:B:603:LPC:H8	1.98	0.46
1:B:272:SER:OG	1:B:273:SER:N	2.49	0.46
1:B:282:PRO:O	1:B:283:LEU:C	2.58	0.46
1:A:348:ARG:O	1:A:349:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:606:LPC:H32	3:A:606:LPC:H0B2	1.64	0.46
1:B:31:LEU:HD13	1:B:31:LEU:N	2.30	0.46
1:B:109:ASN:HA	1:B:110:PRO:HD2	1.34	0.46
1:B:151:ALA:O	1:B:152:PRO:C	2.58	0.46
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.55	0.46
1:B:37:GLU:CD	1:B:37:GLU:N	2.74	0.46
1:B:390:GLN:HE21	1:B:390:GLN:HA	1.81	0.46
1:B:551:PHE:CZ	1:B:555:VAL:HG21	2.50	0.46
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.66	0.46
1:A:293:VAL:CG2	1:A:294:GLU:N	2.79	0.46
1:B:345:LEU:O	1:B:349:LEU:HG	2.16	0.46
1:B:551:PHE:CD1	1:B:552:ALA:N	2.84	0.46
1:A:290:ILE:C	1:A:292:GLU:N	2.68	0.46
1:A:414:LYS:HA	1:A:493:VAL:HG23	1.97	0.46
1:A:452:TYR:O	1:A:455:VAL:HG23	2.16	0.46
1:B:218:ARG:HE	2:B:601:MYR:H143	1.81	0.46
1:B:539:ALA:HB3	1:B:544:LEU:CD1	2.46	0.45
1:A:412:THR:O	1:A:416:PRO:HG3	2.16	0.45
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.76	0.45
1:B:137:LYS:O	1:B:141:GLU:HG2	2.16	0.45
1:B:149:PHE:HE2	3:B:603:LPC:H21	1.79	0.45
1:A:13:ASP:OD2	1:A:283:LEU:HD23	2.15	0.45
1:B:14:LEU:HD21	2:B:602:MYR:H91	1.99	0.45
1:B:173:ASP:HB2	1:B:176:ALA:HB3	1.98	0.45
1:B:319:TYR:HE1	1:B:327:LEU:HD11	1.81	0.45
1:A:139:LEU:HD13	3:A:604:LPC:HJ2	1.97	0.45
1:A:153:GLU:HG2	1:A:157:PHE:HE2	1.82	0.45
1:B:513:ILE:HD12	1:B:514:CYS:N	2.31	0.45
1:A:178:LEU:O	1:A:179:LEU:C	2.58	0.45
1:B:291:ALA:HB2	2:B:601:MYR:H51	1.99	0.45
1:B:367:HIS:O	1:B:371:ALA:HB2	2.15	0.45
1:B:401:TYR:CD2	3:B:605:LPC:H0B3	2.52	0.45
1:A:74:LEU:C	1:A:76:THR:N	2.70	0.45
1:A:127:PHE:O	1:A:129:ASP:N	2.50	0.45
1:A:398:LEU:HB3	1:A:402:LYS:HB3	1.99	0.45
1:B:60:GLU:O	1:B:62:CYS:CB	2.64	0.45
1:B:68:THR:CB	1:B:95:GLU:OE1	2.64	0.45
1:B:11:PHE:CZ	1:B:51:LYS:HE3	2.52	0.45
1:B:25:ILE:O	1:B:26:ALA:C	2.58	0.45
1:B:426:VAL:O	1:B:430:LEU:HB2	2.17	0.45
1:A:509:PHE:CD1	1:A:509:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:TYR:O	1:B:337:ARG:HB3	2.16	0.45
1:B:390:GLN:HE21	1:B:390:GLN:CA	2.30	0.45
1:B:530:VAL:O	1:B:531:GLU:C	2.58	0.45
1:A:42:LEU:O	1:A:46:VAL:HG23	2.17	0.45
1:A:149:PHE:HE1	1:A:196:GLN:OE1	1.99	0.45
1:B:142:ILE:CD1	3:B:603:LPC:H8	2.47	0.45
1:B:396:GLU:O	1:B:397:GLN:O	2.34	0.45
1:B:523:ILE:HG22	1:B:524:LYS:N	2.32	0.45
1:A:543:GLN:O	1:A:547:VAL:HG23	2.17	0.45
1:B:105:HIS:CD2	1:B:105:HIS:N	2.85	0.45
1:B:175:ALA:O	1:B:179:LEU:HB2	2.16	0.45
1:B:344:VAL:HG12	1:B:482:VAL:HG22	1.98	0.45
1:B:377:PHE:O	1:B:378:LYS:C	2.60	0.45
1:B:383:GLU:CD	1:B:485:ARG:NH1	2.42	0.45
1:B:420:THR:HB	1:B:421:PRO:CD	2.47	0.45
1:A:262:LYS:HE3	1:A:262:LYS:HB2	1.37	0.44
1:A:395:PHE:O	1:A:395:PHE:CG	2.70	0.44
1:A:410:ARG:O	1:A:414:LYS:HG3	2.17	0.44
1:A:472:ARG:HB3	1:A:491:LEU:HD21	1.99	0.44
1:A:495:GLU:O	1:A:496:THR:C	2.60	0.44
3:A:605:LPC:CF	3:A:605:LPC:HJ2	2.46	0.44
1:B:390:GLN:O	1:B:394:LEU:CD2	2.61	0.44
1:A:36:PHE:HB3	1:A:37:GLU:OE2	2.18	0.44
1:A:132:GLU:O	1:A:136:LYS:HG2	2.17	0.44
1:A:370:TYR:O	1:A:372:LYS:N	2.50	0.44
1:B:77:VAL:O	1:B:80:LEU:HB2	2.17	0.44
1:B:182:LEU:O	1:B:183:ASP:C	2.59	0.44
1:A:556:GLU:O	1:A:560:LYS:CB	2.66	0.44
1:B:56:ASP:OD1	1:B:56:ASP:C	2.58	0.44
1:B:217:ALA:O	1:B:221:GLN:CG	2.65	0.44
1:B:381:VAL:O	1:B:384:PRO:HD2	2.16	0.44
1:A:190:LYS:C	1:A:192:SER:N	2.70	0.44
1:A:257:ARG:HE	1:A:257:ARG:HB3	1.50	0.44
1:A:426:VAL:HG21	1:A:460:LEU:HB2	1.99	0.44
1:B:554:PHE:CE1	1:B:568:PHE:HA	2.52	0.44
1:A:149:PHE:CG	3:A:604:LPC:H0A1	2.49	0.44
1:A:499:PRO:HG3	1:A:537:PRO:HD2	1.99	0.44
1:B:61:ASN:HB3	1:B:64:LYS:CG	2.44	0.44
1:A:10:ARG:O	1:A:14:LEU:HB2	2.18	0.44
1:A:460:LEU:HD12	1:A:460:LEU:C	2.43	0.44
1:A:504:ALA:O	1:A:506:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:THR:HG22	1:A:507:PHE:CG	2.52	0.44
1:B:302:LEU:HA	1:B:303:PRO:HD3	1.51	0.44
1:B:544:LEU:O	1:B:545:LYS:C	2.61	0.44
1:A:333:GLU:HA	1:A:333:GLU:OE1	2.18	0.44
1:B:552:ALA:CB	3:B:605:LPC:O8	2.61	0.44
1:A:135:LEU:HD22	3:A:604:LPC:HK2	1.99	0.44
1:A:238:LEU:O	1:A:241:VAL:N	2.51	0.44
1:A:414:LYS:N	1:A:493:VAL:HG22	2.20	0.44
1:B:386:ASN:O	1:B:390:GLN:HB2	2.17	0.44
1:A:30:TYR:CD1	1:A:106:LYS:CE	3.01	0.44
1:A:457:LEU:CD1	3:A:605:LPC:HK1	2.48	0.44
1:A:458:ASN:O	1:A:459:GLN:C	2.61	0.44
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.76	0.44
1:B:302:LEU:H	1:B:302:LEU:HD12	1.82	0.44
1:B:342:SER:OG	3:B:604:LPC:H0C3	2.18	0.44
1:A:408:LEU:HD13	1:A:427:SER:OG	2.17	0.43
1:A:558:CYS:C	1:A:560:LYS:H	2.25	0.43
1:A:579:SER:O	1:A:580:GLU:HG3	2.18	0.43
1:B:537:PRO:O	1:B:537:PRO:HG2	2.18	0.43
3:B:605:LPC:H0C1	3:B:605:LPC:O5B	2.18	0.43
1:A:155:LEU:HD23	1:A:284:LEU:HD11	1.99	0.43
1:A:298:MET:CE	1:A:337:ARG:HA	2.46	0.43
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.99	0.43
1:B:467:THR:O	1:B:469:VAL:HG23	2.19	0.43
1:B:519:LYS:O	1:B:523:ILE:HD13	2.18	0.43
1:A:418:VAL:HG23	1:A:423:LEU:CG	2.48	0.43
3:A:606:LPC:HG1	3:A:606:LPC:HJ1	1.29	0.43
1:B:123:MET:HE1	1:B:182:LEU:CD1	2.49	0.43
1:B:403:PHE:O	1:B:406:ALA:HB3	2.17	0.43
1:A:95:GLU:O	1:A:95:GLU:OE2	2.36	0.43
1:A:357:LEU:HB2	1:A:358:GLU:H	1.39	0.43
1:A:387:LEU:HD11	1:A:489:SER:OG	2.18	0.43
1:A:404:GLN:O	1:A:407:LEU:N	2.52	0.43
1:B:199:LYS:CE	1:B:242:HIS:CE1	2.94	0.43
1:A:420:THR:N	1:A:421:PRO:CD	2.80	0.43
1:B:31:LEU:HA	1:B:31:LEU:HD12	1.71	0.43
1:B:275:LEU:HD11	1:B:290:ILE:HG23	2.01	0.43
1:B:347:LEU:HB3	1:B:482:VAL:HG21	2.01	0.43
3:B:605:LPC:O5B	3:B:605:LPC:C0C	2.66	0.43
1:A:125:THR:O	1:A:129:ASP:HB2	2.19	0.43
1:A:494:ASP:OD1	1:A:494:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ASP:O	1:B:147:PRO:HG3	2.18	0.43
1:B:519:LYS:O	1:B:523:ILE:N	2.44	0.43
1:A:499:PRO:HG3	1:A:537:PRO:CG	2.48	0.43
1:B:150:TYR:O	1:B:151:ALA:O	2.37	0.43
1:B:179:LEU:C	1:B:181:LYS:H	2.26	0.43
1:B:285:GLU:O	1:B:286:LYS:C	2.61	0.43
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.79	0.43
1:A:44:ASN:C	1:A:46:VAL:N	2.74	0.43
1:A:386:ASN:O	1:A:390:GLN:HG3	2.19	0.43
1:A:506:THR:O	1:A:508:THR:N	2.52	0.43
1:B:452:TYR:C	1:B:454:SER:N	2.77	0.43
1:B:471:ASP:O	1:B:472:ARG:C	2.62	0.43
1:A:33:GLN:HB2	1:A:84:TYR:CZ	2.53	0.43
1:A:288:HIS:O	1:A:289:CYS:C	2.62	0.43
1:B:430:LEU:HD11	1:B:453:LEU:CD1	2.49	0.43
1:A:25:ILE:HD11	1:A:139:LEU:HD21	2.01	0.43
1:A:253:CYS:O	1:A:257:ARG:HG3	2.19	0.43
1:A:321:GLU:O	1:A:322:ALA:HB3	2.14	0.43
1:B:326:PHE:C	1:B:328:GLY:N	2.76	0.43
1:B:370:TYR:C	1:B:372:LYS:H	2.27	0.43
1:A:101:CYS:O	1:A:105:HIS:HD2	2.02	0.42
1:A:115:LEU:HD21	1:A:141:GLU:HB3	2.01	0.42
1:A:163:ALA:O	1:A:166:THR:HB	2.19	0.42
1:A:234:LEU:HD11	1:A:271:ILE:HD13	2.01	0.42
1:A:398:LEU:H	1:A:398:LEU:HG	1.63	0.42
1:B:14:LEU:HD11	1:B:284:LEU:HD12	2.00	0.42
1:B:119:GLU:HB2	1:B:122:VAL:HG13	2.00	0.42
1:B:161:TYR:O	1:B:165:PHE:CD2	2.72	0.42
1:A:341:TYR:CG	1:A:345:LEU:HD23	2.53	0.42
1:A:408:LEU:HD21	1:A:526:GLN:HB3	2.01	0.42
1:B:30:TYR:O	1:B:32:GLN:N	2.52	0.42
1:B:179:LEU:C	1:B:181:LYS:N	2.77	0.42
1:B:251:LEU:HD22	1:B:251:LEU:HA	1.79	0.42
1:B:351:LYS:HE2	1:B:354:GLU:OE1	2.19	0.42
1:B:548:MET:C	1:B:550:ASP:H	2.26	0.42
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.91	0.42
1:A:408:LEU:HD13	1:A:427:SER:CB	2.49	0.42
1:A:414:LYS:O	1:A:472:ARG:NH2	2.51	0.42
1:A:462:VAL:HA	1:A:465:GLU:HB3	2.01	0.42
1:B:120:VAL:HG11	1:B:175:ALA:N	2.34	0.42
1:B:150:TYR:CG	1:B:152:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ASN:O	1:B:484:ARG:C	2.60	0.42
1:A:311:GLU:C	1:A:312:SER:O	2.62	0.42
1:B:214:TRP:O	1:B:217:ALA:HB3	2.19	0.42
1:B:366:PRO:O	1:B:369:CYS:N	2.52	0.42
1:B:570:GLU:CA	1:B:572:GLY:N	2.80	0.42
1:A:119:GLU:O	1:A:122:VAL:N	2.53	0.42
1:A:414:LYS:HA	1:A:493:VAL:CG2	2.49	0.42
1:B:123:MET:HE1	1:B:182:LEU:HD11	2.01	0.42
1:B:533:VAL:O	1:B:537:PRO:HB3	2.19	0.42
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.71	0.42
1:B:73:LYS:O	1:B:73:LYS:CG	2.66	0.42
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.93	0.42
1:B:378:LYS:HB3	1:B:379:PRO:CD	2.49	0.42
1:A:262:LYS:HB3	1:A:286:LYS:HZ3	1.80	0.42
1:A:319:TYR:CD2	1:A:323:LYS:HD3	2.55	0.42
1:A:412:THR:OG1	1:A:423:LEU:HD13	2.20	0.42
1:A:422:THR:C	1:A:424:VAL:N	2.76	0.42
1:B:305:LEU:O	1:B:309:PHE:HB2	2.18	0.42
1:B:428:ARG:O	1:B:429:ASN:C	2.63	0.42
1:B:454:SER:C	1:B:456:VAL:H	2.27	0.42
1:A:44:ASN:O	1:A:45:GLU:C	2.62	0.42
1:A:195:LYS:HE3	1:A:195:LYS:HB2	1.86	0.42
1:A:205:LYS:HB2	1:A:205:LYS:HE3	1.81	0.42
1:A:262:LYS:HG3	1:A:262:LYS:H	1.59	0.42
1:B:138:TYR:CD1	3:B:603:LPC:CD	2.77	0.42
1:A:388:ILE:HD11	3:A:605:LPC:C7	2.49	0.42
1:B:262:LYS:HB2	1:B:262:LYS:HE2	1.69	0.42
1:B:420:THR:C	1:B:422:THR:N	2.77	0.42
1:A:135:LEU:HD13	3:A:604:LPC:HL1	2.02	0.41
1:A:230:GLU:O	1:A:231:VAL:C	2.63	0.41
1:B:237:ASP:HB3	1:B:260:LEU:CD1	2.38	0.41
3:B:603:LPC:H0B1	3:B:603:LPC:O4	2.20	0.41
1:A:529:LEU:O	1:A:529:LEU:HD12	2.19	0.41
1:A:93:LYS:C	1:A:94:GLN:CG	2.93	0.41
1:A:149:PHE:HE2	3:A:604:LPC:H0C3	1.75	0.41
1:A:234:LEU:HD11	1:A:271:ILE:HG23	2.03	0.41
1:A:407:LEU:HB3	1:A:411:TYR:CE2	2.54	0.41
1:A:435:SER:C	1:A:436:LYS:O	2.63	0.41
1:B:141:GLU:OE1	1:B:144:ARG:NH1	2.53	0.41
1:A:149:PHE:HD2	1:A:154:LEU:HD12	1.85	0.41
1:A:485:ARG:CD	3:A:605:LPC:O5B	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:C	1:A:121:ASP:N	2.77	0.41
1:A:215:ALA:O	1:A:219:LEU:HB2	2.21	0.41
1:A:223:PHE:N	1:A:224:PRO:HD3	2.34	0.41
1:A:293:VAL:HG22	1:A:294:GLU:H	1.86	0.41
1:B:409:VAL:O	1:B:410:ARG:C	2.63	0.41
1:B:570:GLU:CA	1:B:572:GLY:H	2.33	0.41
1:A:238:LEU:O	1:A:241:VAL:HB	2.20	0.41
1:A:292:GLU:O	1:A:293:VAL:O	2.39	0.41
1:A:418:VAL:HG23	1:A:423:LEU:HD11	2.03	0.41
1:B:241:VAL:HG22	1:B:256:ASP:HB3	2.03	0.41
1:B:458:ASN:HB2	1:B:484:ARG:HH12	1.85	0.41
1:B:464:HIS:O	1:B:464:HIS:CG	2.72	0.41
1:A:11:PHE:CZ	1:A:51:LYS:HE3	2.55	0.41
1:A:215:ALA:HB3	1:A:235:VAL:HG13	2.01	0.41
1:A:305:LEU:CD2	1:A:333:GLU:CB	2.98	0.41
1:B:23:VAL:CG2	2:B:602:MYR:H141	2.34	0.41
1:B:117:ARG:NH2	1:B:186:ARG:NH1	2.69	0.41
1:B:370:TYR:C	1:B:372:LYS:N	2.77	0.41
1:B:401:TYR:CE2	3:B:605:LPC:H0B3	2.55	0.41
1:B:412:THR:O	1:B:413:LYS:C	2.63	0.41
1:B:420:THR:N	1:B:421:PRO:CD	2.84	0.41
1:B:529:LEU:O	1:B:532:LEU:HB3	2.21	0.41
1:A:558:CYS:SG	1:A:567:CYS:C	3.04	0.41
1:B:10:ARG:O	1:B:11:PHE:C	2.64	0.41
1:B:118:PRO:HG2	1:B:123:MET:HG3	2.03	0.41
1:B:343:VAL:N	1:B:450:GLU:OE1	2.49	0.41
1:B:520:GLU:O	1:B:523:ILE:CB	2.66	0.41
1:A:96:PRO:CD	1:A:97:GLU:H	2.31	0.41
1:A:127:PHE:O	1:A:131:GLU:HG3	2.20	0.41
1:A:262:LYS:HA	1:A:265:CYS:HB2	2.03	0.41
1:A:452:TYR:O	1:A:455:VAL:CG2	2.69	0.41
1:A:540:THR:C	1:A:542:GLU:N	2.79	0.41
1:A:546:ALA:O	1:A:549:ASP:N	2.54	0.41
1:A:573:LYS:C	1:A:575:LEU:N	2.78	0.41
1:B:56:ASP:C	1:B:58:SER:N	2.76	0.41
1:B:131:GLU:O	1:B:134:PHE:HB3	2.21	0.41
1:B:132:GLU:C	1:B:134:PHE:N	2.79	0.41
1:B:154:LEU:HA	1:B:154:LEU:HD12	1.87	0.41
1:B:449:ALA:O	1:B:453:LEU:N	2.53	0.41
1:B:488:PHE:C	1:B:490:ALA:N	2.78	0.41
1:A:155:LEU:O	1:A:159:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLU:H	1:A:520:GLU:HG2	1.63	0.41
1:B:53:CYS:C	1:B:55:ALA:N	2.79	0.41
1:B:422:THR:O	1:B:423:LEU:C	2.64	0.41
1:B:512:ASP:OD1	1:B:513:ILE:HG23	2.21	0.41
3:B:605:LPC:HB2	3:B:605:LPC:H92	1.64	0.41
1:A:85:GLY:O	1:A:88:ALA:N	2.54	0.40
1:A:138:TYR:HE1	3:A:604:LPC:HB2	1.81	0.40
1:B:319:TYR:HE1	1:B:327:LEU:CD1	2.33	0.40
1:A:212:LYS:O	1:A:213:ALA:C	2.64	0.40
1:A:488:PHE:HB3	3:A:605:LPC:HI1	2.03	0.40
1:A:502:PHE:HD1	1:A:503:ASN:N	2.19	0.40
1:B:118:PRO:HB2	1:B:122:VAL:HG21	2.02	0.40
1:B:168:CYS:SG	1:B:178:LEU:N	2.94	0.40
1:B:532:LEU:O	1:B:536:LYS:CG	2.69	0.40
1:A:42:LEU:HD23	1:A:73:LYS:HD3	2.02	0.40
1:A:555:VAL:CG1	1:A:556:GLU:H	2.33	0.40
1:B:151:ALA:H	1:B:250:LEU:HD11	1.86	0.40
1:B:245:CYS:HA	1:B:253:CYS:HB2	2.03	0.40
1:B:373:VAL:HG13	1:B:374:PHE:N	2.37	0.40
1:B:566:THR:O	1:B:567:CYS:C	2.61	0.40
1:B:372:LYS:O	1:B:375:ASP:HB2	2.22	0.40
1:B:485:ARG:O	1:B:489:SER:HB2	2.21	0.40
1:A:124:CYS:O	1:A:127:PHE:HB3	2.22	0.40
1:A:249:ASP:OD1	1:A:252:GLU:N	2.44	0.40
1:A:315:VAL:HG11	1:A:370:TYR:OH	2.22	0.40
1:A:391:ASN:HB3	3:A:605:LPC:H91	2.03	0.40
1:A:572:GLY:C	1:A:574:LYS:N	2.77	0.40
1:B:268:GLN:C	1:B:270:SER:N	2.79	0.40
1:B:329:MET:O	1:B:330:PHE:C	2.62	0.40
1:B:532:LEU:HD12	3:B:605:LPC:HH2	2.03	0.40

All (1) 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:A:396:GLU:O	1:A:497:TYR:OH[1_565]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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	577/580 (100%)	432 (75%)	97 (17%)	48 (8%)	0	2
1	B	575/580 (99%)	443 (77%)	95 (16%)	37 (6%)	1	5
All	All	1152/1160 (99%)	875 (76%)	192 (17%)	85 (7%)	1	3

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	57	GLU
1	A	95	GLU
1	A	120	VAL
1	A	130	ASN
1	A	172	ALA
1	A	250	LEU
1	A	274	LYS
1	A	303	PRO
1	A	312	SER
1	A	322	ALA
1	A	358	GLU
1	A	436	LYS
1	A	437	CYS
1	A	494	ASP
1	A	505	GLU
1	A	552	ALA
1	A	553	ALA
1	A	557	LYS
1	A	569	ALA
1	A	580	GLU
1	B	57	GLU
1	B	61	ASN
1	B	174	LYS
1	B	303	PRO

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Mol	Chain	Res	Type
1	B	313	LYS
1	B	395	PHE
1	B	472	ARG
1	B	473	VAL
1	B	484	ARG
1	B	538	LYS
1	B	539	ALA
1	B	576	VAL
1	A	293	VAL
1	A	364	ALA
1	A	374	PHE
1	A	457	LEU
1	B	59	ALA
1	B	453	LEU
1	B	517	SER
1	B	541	LYS
1	B	545	LYS
1	A	128	HIS
1	A	174	LYS
1	A	506	THR
1	A	558	CYS
1	A	566	THR
1	B	312	SER
1	B	371	ALA
1	B	397	GLN
1	B	451	ASP
1	B	494	ASP
1	B	499	PRO
1	B	503	ASN
1	A	75	CYS
1	A	150	TYR
1	A	191	ALA
1	A	286	LYS
1	A	300	ALA
1	A	405	ASN
1	A	511	ALA
1	A	562	ASP
1	B	56	ASP
1	B	307	ALA
1	B	441	PRO
1	B	580	GLU
1	A	17	GLU

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Mol	Chain	Res	Type
1	A	86	GLU
1	A	321	GLU
1	A	357	LEU
1	A	507	PHE
1	A	560	LYS
1	B	366	PRO
1	B	566	THR
1	B	578	ALA
1	B	152	PRO
1	B	396	GLU
1	B	442	GLU
1	B	568	PHE
1	A	77	VAL
1	A	576	VAL
1	B	378	LYS
1	B	421	PRO
1	A	469	VAL
1	A	499	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	462/508 (91%)	385 (83%)	77 (17%)	2	10
1	B	461/508 (91%)	390 (85%)	71 (15%)	2	12
All	All	923/1016 (91%)	775 (84%)	148 (16%)	2	11

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	13	ASP
1	A	31	LEU
1	A	64	LYS
1	A	68	THR

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Mol	Chain	Res	Type
1	A	73	LYS
1	A	76	THR
1	A	86	GLU
1	A	93	LYS
1	A	94	GLN
1	A	95	GLU
1	A	99	ASN
1	A	115	LEU
1	A	122	VAL
1	A	123	MET
1	A	128	HIS
1	A	129	ASP
1	A	132	GLU
1	A	179	LEU
1	A	188	GLU
1	A	222	ARG
1	A	225	LYS
1	A	236	THR
1	A	238	LEU
1	A	249	ASP
1	A	262	LYS
1	A	264	ILE
1	A	270	SER
1	A	271	ILE
1	A	274	LYS
1	A	283	LEU
1	A	285	GLU
1	A	315	VAL
1	A	324	ASP
1	A	331	LEU
1	A	348	ARG
1	A	351	LYS
1	A	365	ASP
1	A	373	VAL
1	A	380	LEU
1	A	382	GLU
1	A	387	LEU
1	A	390	GLN
1	A	391	ASN
1	A	393	GLU
1	A	398	LEU
1	A	418	VAL

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Mol	Chain	Res	Type
1	A	419	SER
1	A	425	GLU
1	A	430	LEU
1	A	454	SER
1	A	455	VAL
1	A	459	GLN
1	A	460	LEU
1	A	468	PRO
1	A	471	ASP
1	A	472	ARG
1	A	475	LYS
1	A	478	THR
1	A	485	ARG
1	A	493	VAL
1	A	498	VAL
1	A	500	LYS
1	A	503	ASN
1	A	506	THR
1	A	508	THR
1	A	512	ASP
1	A	515	THR
1	A	520	GLU
1	A	529	LEU
1	A	544	LEU
1	A	545	LYS
1	A	556	GLU
1	A	565	GLU
1	A	571	GLU
1	A	574	LYS
1	A	580	GLU
1	B	3	HIS
1	B	7	VAL
1	B	12	LYS
1	B	31	LEU
1	B	57	GLU
1	B	58	SER
1	B	68	THR
1	B	73	LYS
1	B	76	THR
1	B	86	GLU
1	B	93	LYS
1	B	97	GLU

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Mol	Chain	Res	Type
1	B	104	GLN
1	B	111	ASN
1	B	114	ARG
1	B	121	ASP
1	B	122	VAL
1	B	132	GLU
1	B	149	PHE
1	B	166	THR
1	B	179	LEU
1	B	199	LYS
1	B	219	LEU
1	B	221	GLN
1	B	236	THR
1	B	237	ASP
1	B	249	ASP
1	B	251	LEU
1	B	257	ARG
1	B	259	ASP
1	B	262	LYS
1	B	274	LYS
1	B	275	LEU
1	B	283	LEU
1	B	285	GLU
1	B	302	LEU
1	B	305	LEU
1	B	312	SER
1	B	324	ASP
1	B	331	LEU
1	B	337	ARG
1	B	344	VAL
1	B	351	LYS
1	B	378	LYS
1	B	380	LEU
1	B	390	GLN
1	B	395	PHE
1	B	398	LEU
1	B	430	LEU
1	B	436	LYS
1	B	442	GLU
1	B	451	ASP
1	B	457	LEU
1	B	464	HIS

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Mol	Chain	Res	Type
1	B	465	GLU
1	B	472	ARG
1	B	482	VAL
1	B	486	PRO
1	B	489	SER
1	B	496	THR
1	B	500	LYS
1	B	515	THR
1	B	517	SER
1	B	518	GLU
1	B	520	GLU
1	B	521	ARG
1	B	523	ILE
1	B	540	THR
1	B	551	PHE
1	B	567	CYS
1	B	571	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	3	HIS
1	A	18	ASN
1	A	105	HIS
1	A	146	HIS
1	A	318	ASN
1	A	385	GLN
1	A	390	GLN
1	A	440	HIS
1	A	459	GLN
1	A	464	HIS
1	A	522	GLN
1	B	39	HIS
1	B	94	GLN
1	B	99	ASN
1	B	104	GLN
1	B	105	HIS
1	B	111	ASN
1	B	128	HIS
1	B	146	HIS
1	B	242	HIS
1	B	318	ASN

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Mol	Chain	Res	Type
1	B	390	GLN
1	B	417	GLN
1	B	440	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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$
3	LPC	A	604	-	30,30,30	0.96	4 (13%)	35,37,37	1.24	3 (8%)
2	MYR	B	606	-	15,15,15	0.53	0	15,15,15	1.21	2 (13%)
3	LPC	A	605	-	30,30,30	1.00	1 (3%)	35,37,37	0.93	2 (5%)
2	MYR	B	601	-	15,15,15	0.67	1 (6%)	15,15,15	0.89	0
2	MYR	A	601	-	15,15,15	0.55	0	15,15,15	1.08	1 (6%)
2	MYR	A	603	-	15,15,15	0.55	0	15,15,15	0.97	1 (6%)
2	MYR	A	602	-	15,15,15	0.70	0	15,15,15	2.02	5 (33%)
3	LPC	A	606	-	30,30,30	1.02	1 (3%)	35,37,37	0.97	2 (5%)
3	LPC	B	603	-	30,30,30	1.23	1 (3%)	35,37,37	0.95	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LPC	B	605	-	30,30,30	1.08	3 (10%)	35,37,37	2.53	13 (37%)
3	LPC	B	604	-	30,30,30	1.13	2 (6%)	35,37,37	0.97	2 (5%)
2	MYR	B	602	-	15,15,15	0.94	1 (6%)	15,15,15	1.61	2 (13%)

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
3	LPC	A	604	-	-	16/32/32/32	-
2	MYR	B	606	-	-	6/13/13/13	-
3	LPC	A	605	-	-	22/32/32/32	-
2	MYR	B	601	-	-	6/13/13/13	-
2	MYR	A	601	-	-	7/13/13/13	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	A	602	-	-	2/13/13/13	-
3	LPC	A	606	-	-	21/32/32/32	-
3	LPC	B	603	-	-	17/32/32/32	-
3	LPC	B	605	-	-	18/32/32/32	-
3	LPC	B	604	-	-	21/32/32/32	-
2	MYR	B	602	-	-	10/13/13/13	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	LPC	OQ2-CA	5.71	1.50	1.33
3	B	604	LPC	OQ2-CA	4.93	1.47	1.33
3	A	605	LPC	OQ2-CA	4.49	1.46	1.33
3	A	606	LPC	OQ2-CA	4.43	1.46	1.33
2	B	602	MYR	O1-C1	3.15	1.32	1.22
3	A	604	LPC	OQ2-CA	3.07	1.42	1.33
3	B	605	LPC	C2-C3	2.21	1.58	1.51
3	B	604	LPC	OQ2-C9	-2.18	1.40	1.45
3	A	604	LPC	P5-O5B	2.17	1.58	1.50
3	B	605	LPC	C9-C8	-2.09	1.44	1.51
3	B	605	LPC	P5-O4	2.07	1.67	1.59
3	A	604	LPC	P5-O4	2.06	1.67	1.59
3	A	604	LPC	OQ2-C9	-2.06	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	MYR	O2-C1	-2.03	1.24	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	LPC	C0C-N1-C2	-5.26	89.00	109.91
3	B	605	LPC	C0B-N1-C2	-5.09	89.67	109.91
3	B	605	LPC	C0A-N1-C2	-4.96	90.21	109.91
3	B	605	LPC	C0C-N1-C0B	4.84	121.69	108.98
3	B	605	LPC	CG-CF-CE	-4.81	90.08	114.37
2	B	602	MYR	C3-C2-C1	-4.50	102.77	114.51
3	B	605	LPC	C0C-N1-C0A	4.16	119.89	108.98
3	B	605	LPC	CC-CB-CA	-3.63	100.41	113.69
3	B	605	LPC	C0B-N1-C0A	3.59	118.40	108.98
2	A	602	MYR	C5-C4-C3	-3.53	96.52	114.37
3	B	605	LPC	C3-C2-N1	3.18	126.02	115.82
3	B	604	LPC	OQ2-CA-CB	3.08	121.21	111.83
2	A	602	MYR	C3-C2-C1	-3.06	106.52	114.51
3	A	604	LPC	CH-CG-CF	-3.02	99.08	114.37
2	A	602	MYR	C8-C7-C6	-2.95	99.46	114.37
2	A	601	MYR	C3-C2-C1	-2.78	107.25	114.51
3	A	605	LPC	OQ2-CA-CB	2.73	120.15	111.83
3	B	605	LPC	CE-CD-CC	-2.67	100.89	114.37
3	A	604	LPC	CD-CC-CB	2.67	122.92	113.13
3	B	605	LPC	CI-CH-CG	-2.66	100.91	114.37
3	B	605	LPC	C9-OQ2-CA	-2.65	107.42	117.12
2	A	602	MYR	O2-C1-C2	2.64	122.35	114.00
3	B	603	LPC	OQ2-CA-CB	2.62	119.83	111.83
3	B	605	LPC	OQ2-C9-C8	2.61	118.14	105.85
2	B	602	MYR	C11-C10-C9	-2.61	101.19	114.37
3	B	604	LPC	C3-C2-N1	-2.55	107.65	115.82
3	A	606	LPC	OQ2-CA-CB	2.50	119.45	111.83
2	A	602	MYR	C10-C9-C8	-2.48	101.85	114.37
2	B	606	MYR	C3-C2-C1	-2.45	108.12	114.51
3	B	603	LPC	C9-C8-C7	-2.26	106.15	112.65
2	B	606	MYR	O1-C1-C2	-2.19	116.14	123.09
3	A	605	LPC	C3-C2-N1	-2.16	108.90	115.82
3	A	604	LPC	CF-CE-CD	-2.13	103.62	114.37
2	A	603	MYR	C3-C2-C1	-2.08	109.08	114.51
3	A	606	LPC	O5A-P5-O5B	2.01	121.82	112.44

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	LPC	C3-O4-P5-O5B
3	A	604	LPC	C3-O4-P5-O6
3	A	604	LPC	C7-O6-P5-O4
3	A	605	LPC	N1-C2-C3-O4
3	A	605	LPC	C3-O4-P5-O5B
3	A	605	LPC	C7-O6-P5-O4
3	A	605	LPC	C7-O6-P5-O5A
3	A	605	LPC	C7-O6-P5-O5B
3	A	606	LPC	N1-C2-C3-O4
3	A	606	LPC	C3-O4-P5-O5B
3	A	606	LPC	C3-O4-P5-O6
3	A	606	LPC	C7-O6-P5-O5A
3	A	606	LPC	OQ1-CA-OQ2-C9
3	A	606	LPC	CB-CA-OQ2-C9
3	B	603	LPC	C7-O6-P5-O4
3	B	604	LPC	N1-C2-C3-O4
3	B	604	LPC	C3-O4-P5-O5B
3	B	604	LPC	C7-O6-P5-O4
3	B	604	LPC	C7-O6-P5-O5A
3	B	604	LPC	C7-O6-P5-O5B
3	B	604	LPC	OQ1-CA-OQ2-C9
3	B	605	LPC	C3-O4-P5-O5B
3	B	605	LPC	C3-O4-P5-O6
3	B	605	LPC	C7-O6-P5-O4
3	B	605	LPC	OQ1-CA-OQ2-C9
3	B	605	LPC	CB-CA-OQ2-C9
3	B	604	LPC	CB-CA-OQ2-C9
3	A	605	LPC	CB-CA-OQ2-C9
3	A	605	LPC	OQ1-CA-OQ2-C9
3	A	606	LPC	CG-CH-CI-CJ
3	B	604	LPC	C3-C2-N1-C0C
3	A	604	LPC	C7-C8-C9-OQ2
3	B	605	LPC	C7-C8-C9-OQ2
3	A	606	LPC	O6-C7-C8-O8
2	B	606	MYR	C1-C2-C3-C4
3	A	604	LPC	C3-C2-N1-C0C
2	B	601	MYR	C1-C2-C3-C4
2	B	602	MYR	C1-C2-C3-C4
3	B	604	LPC	CF-CG-CH-CI
3	B	605	LPC	O6-C7-C8-O8
3	A	604	LPC	O8-C8-C9-OQ2
3	A	605	LPC	O8-C8-C9-OQ2

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Mol	Chain	Res	Type	Atoms
3	B	604	LPC	O8-C8-C9-OQ2
3	B	605	LPC	O8-C8-C9-OQ2
2	A	603	MYR	C1-C2-C3-C4
3	B	605	LPC	O6-C7-C8-C9
3	A	604	LPC	C3-C2-N1-C0B
3	B	604	LPC	C3-C2-N1-C0B
3	A	605	LPC	C7-C8-C9-OQ2
3	B	604	LPC	C7-C8-C9-OQ2
3	B	605	LPC	C8-C7-O6-P5
3	A	605	LPC	CI-CJ-CK-CL
3	B	604	LPC	CG-CH-CI-CJ
2	A	603	MYR	C2-C3-C4-C5
2	B	602	MYR	C3-C4-C5-C6
3	B	604	LPC	CB-CC-CD-CE
3	B	605	LPC	CA-CB-CC-CD
3	B	604	LPC	CH-CI-CJ-CK
3	A	606	LPC	CH-CI-CJ-CK
3	B	605	LPC	CI-CJ-CK-CL
3	A	606	LPC	CA-CB-CC-CD
3	A	605	LPC	CF-CG-CH-CI
3	B	605	LPC	CB-CC-CD-CE
3	A	605	LPC	CH-CI-CJ-CK
2	B	602	MYR	C2-C3-C4-C5
3	B	604	LPC	C3-C2-N1-C0A
2	A	603	MYR	C3-C4-C5-C6
2	B	601	MYR	C7-C8-C9-C10
2	B	602	MYR	C6-C7-C8-C9
3	A	605	LPC	CC-CD-CE-CF
3	B	604	LPC	CE-CF-CG-CH
2	A	601	MYR	C7-C8-C9-C10
3	A	604	LPC	CF-CG-CH-CI
3	B	603	LPC	CF-CG-CH-CI
3	B	605	LPC	CF-CG-CH-CI
3	B	603	LPC	CB-CA-OQ2-C9
3	A	605	LPC	CA-CB-CC-CD
3	A	604	LPC	C3-C2-N1-C0A
2	B	602	MYR	C5-C6-C7-C8
2	A	603	MYR	C4-C5-C6-C7
3	A	605	LPC	CD-CE-CF-CG
2	B	601	MYR	C4-C5-C6-C7
2	B	606	MYR	C3-C4-C5-C6
2	B	601	MYR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	601	MYR	C9-C10-C11-C12
3	B	604	LPC	CI-CJ-CK-CL
3	B	603	LPC	OQ1-CA-OQ2-C9
3	B	603	LPC	CB-CC-CD-CE
3	B	603	LPC	CJ-CK-CL-CM
3	A	604	LPC	CB-CA-OQ2-C9
3	B	603	LPC	CI-CJ-CK-CL
2	B	601	MYR	C2-C3-C4-C5
2	A	603	MYR	C11-C10-C9-C8
2	B	602	MYR	C11-C10-C9-C8
3	B	603	LPC	CK-CL-CM-CN
3	A	606	LPC	CF-CG-CH-CI
2	B	606	MYR	C10-C11-C12-C13
2	A	601	MYR	C2-C3-C4-C5
2	A	601	MYR	C11-C10-C9-C8
2	B	602	MYR	C10-C11-C12-C13
3	A	606	LPC	CE-CF-CG-CH
3	A	604	LPC	OQ1-CA-OQ2-C9
3	B	605	LPC	CJ-CK-CL-CM
2	A	603	MYR	C6-C7-C8-C9
3	B	603	LPC	O8-C8-C9-OQ2
3	A	606	LPC	CD-CE-CF-CG
2	B	606	MYR	C6-C7-C8-C9
3	B	604	LPC	CK-CL-CM-CN
2	B	602	MYR	C9-C10-C11-C12
3	B	605	LPC	CK-CL-CM-CN
3	B	604	LPC	CD-CE-CF-CG
3	A	604	LPC	C7-O6-P5-O5B
3	A	606	LPC	C3-O4-P5-O5A
3	A	606	LPC	C7-O6-P5-O4
3	A	606	LPC	C7-O6-P5-O5B
3	B	603	LPC	C3-C2-N1-C0C
3	B	603	LPC	C7-O6-P5-O5B
3	B	605	LPC	C7-O6-P5-O5B
2	B	606	MYR	C5-C6-C7-C8
3	B	603	LPC	C3-C2-N1-C0A
3	B	605	LPC	CG-CH-CI-CJ
2	A	601	MYR	C6-C7-C8-C9
3	A	606	LPC	C8-C7-O6-P5
3	B	603	LPC	CC-CD-CE-CF
2	B	602	MYR	C4-C5-C6-C7
3	B	603	LPC	O6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	606	LPC	CJ-CK-CL-CM
2	A	601	MYR	C5-C6-C7-C8
3	A	605	LPC	C3-C2-N1-C0C
3	B	603	LPC	C3-C2-N1-C0B
3	B	603	LPC	C7-C8-C9-OQ2
2	A	603	MYR	C5-C6-C7-C8
3	B	603	LPC	CE-CF-CG-CH
3	A	605	LPC	CK-CL-CM-CN
3	A	604	LPC	CG-CH-CI-CJ
3	A	604	LPC	CI-CJ-CK-CL
3	A	605	LPC	OQ2-CA-CB-CC
3	A	604	LPC	OQ2-CA-CB-CC
3	B	604	LPC	OQ2-CA-CB-CC
3	A	605	LPC	C3-C2-N1-C0B
3	A	605	LPC	CG-CH-CI-CJ
2	A	602	MYR	O2-C1-C2-C3
2	B	602	MYR	C7-C8-C9-C10
3	A	605	LPC	C3-C2-N1-C0A
3	A	606	LPC	OQ2-CA-CB-CC
3	A	604	LPC	OQ1-CA-CB-CC
3	A	605	LPC	OQ1-CA-CB-CC
3	A	606	LPC	CB-CC-CD-CE
2	B	606	MYR	O2-C1-C2-C3
2	A	601	MYR	O2-C1-C2-C3
2	A	602	MYR	O1-C1-C2-C3
2	A	603	MYR	O2-C1-C2-C3
2	A	601	MYR	O1-C1-C2-C3
3	A	606	LPC	OQ1-CA-CB-CC

There are no ring outliers.

12 monomers are involved in 205 short contacts:

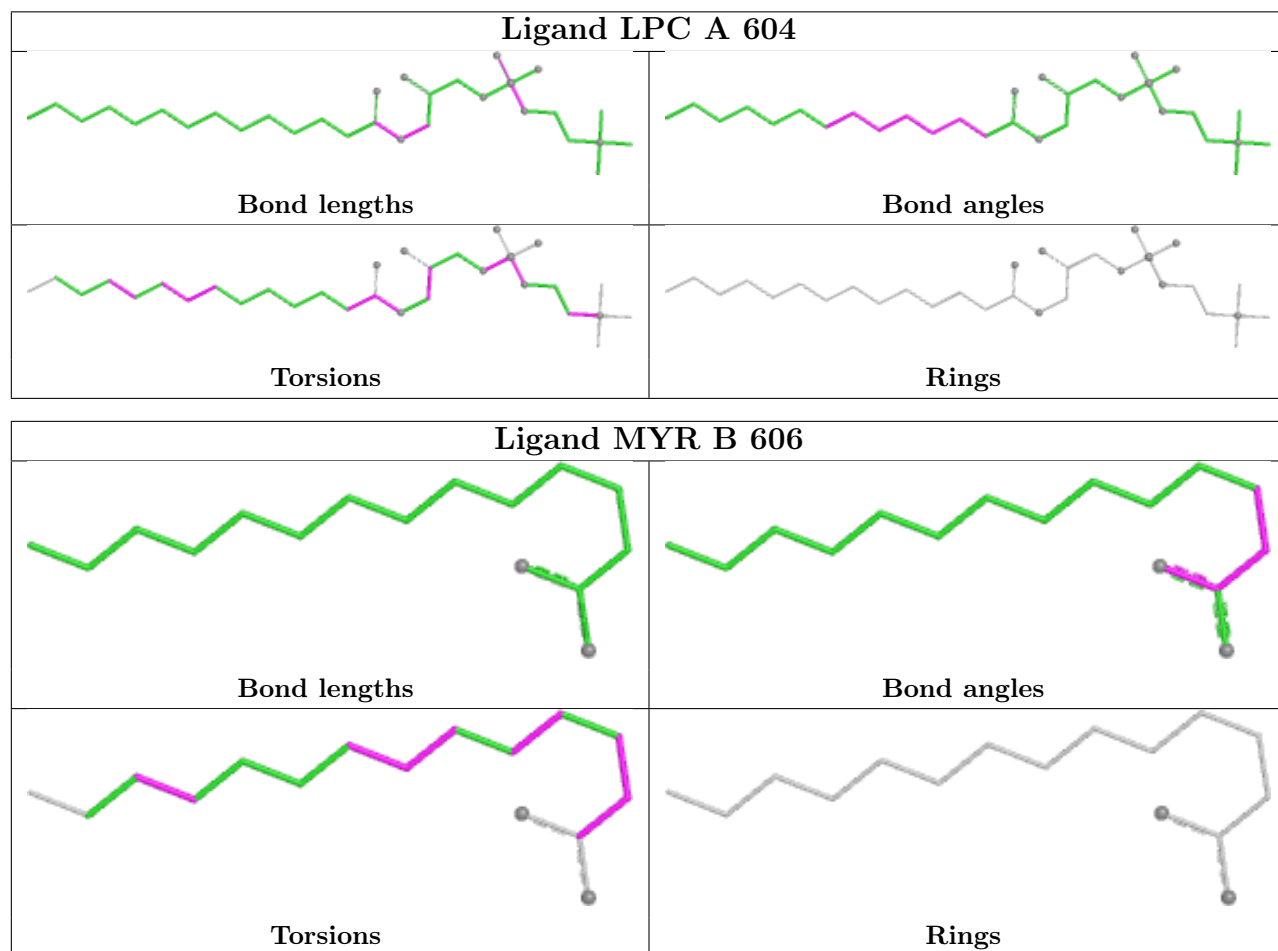
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	LPC	25	0
2	B	606	MYR	3	0
3	A	605	LPC	44	0
2	B	601	MYR	15	0
2	A	601	MYR	1	0
2	A	603	MYR	1	0
2	A	602	MYR	4	0
3	A	606	LPC	21	0
3	B	603	LPC	42	0

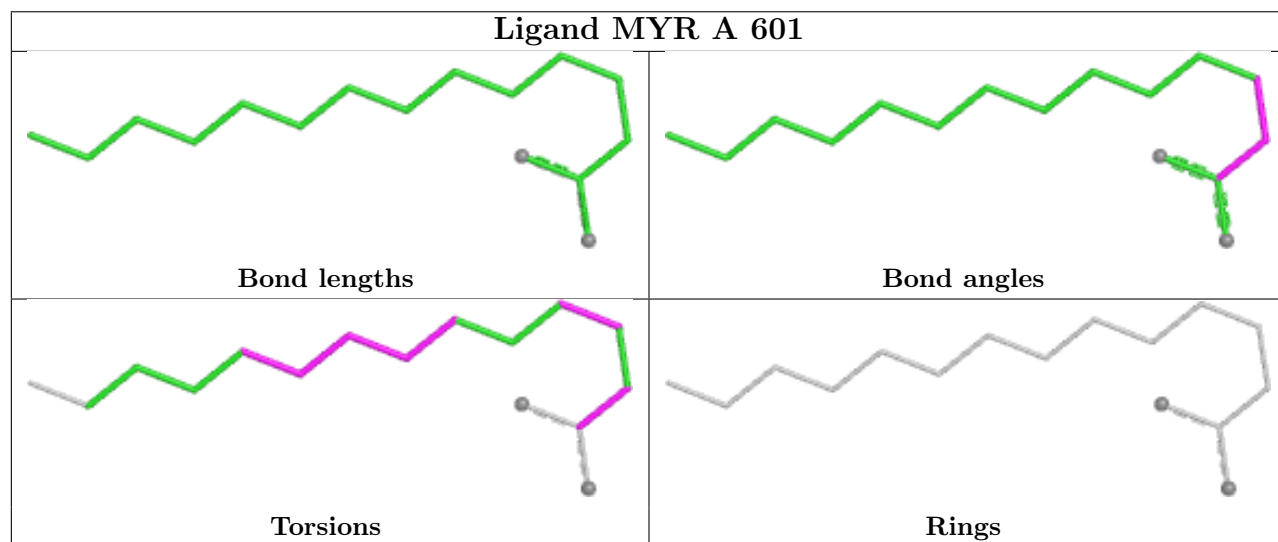
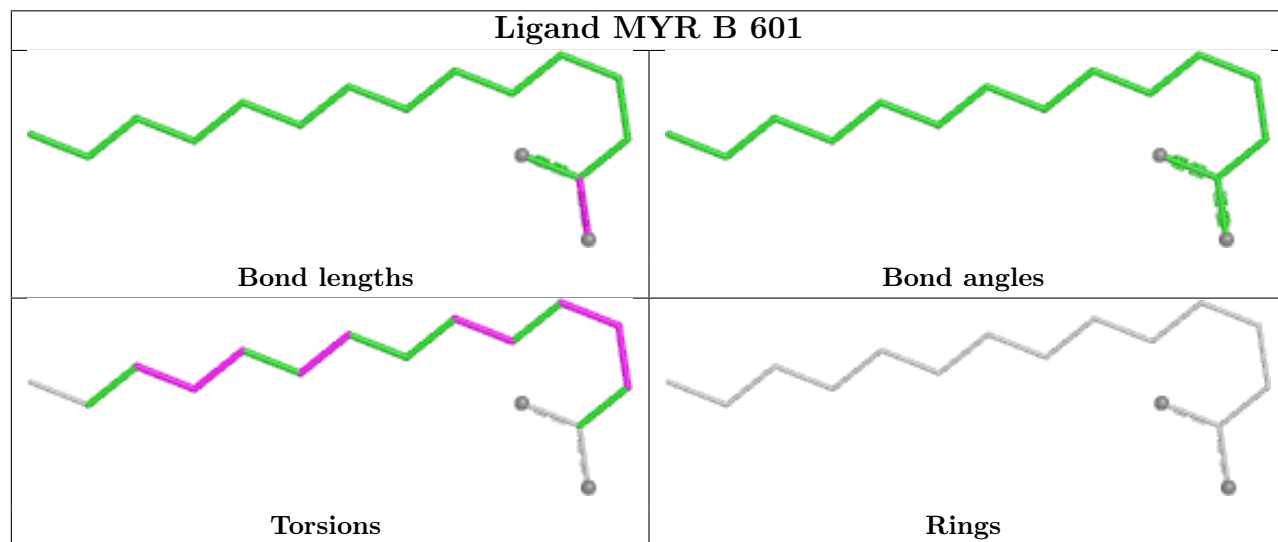
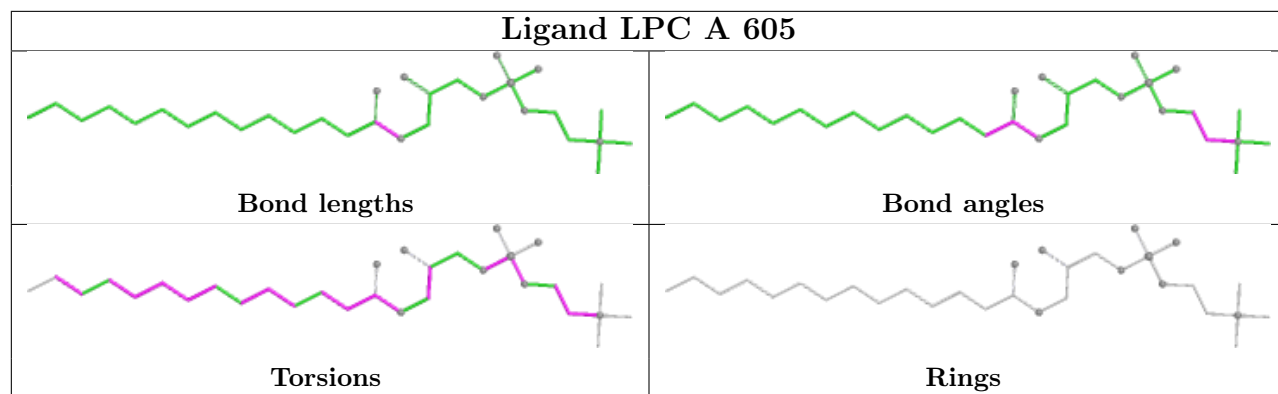
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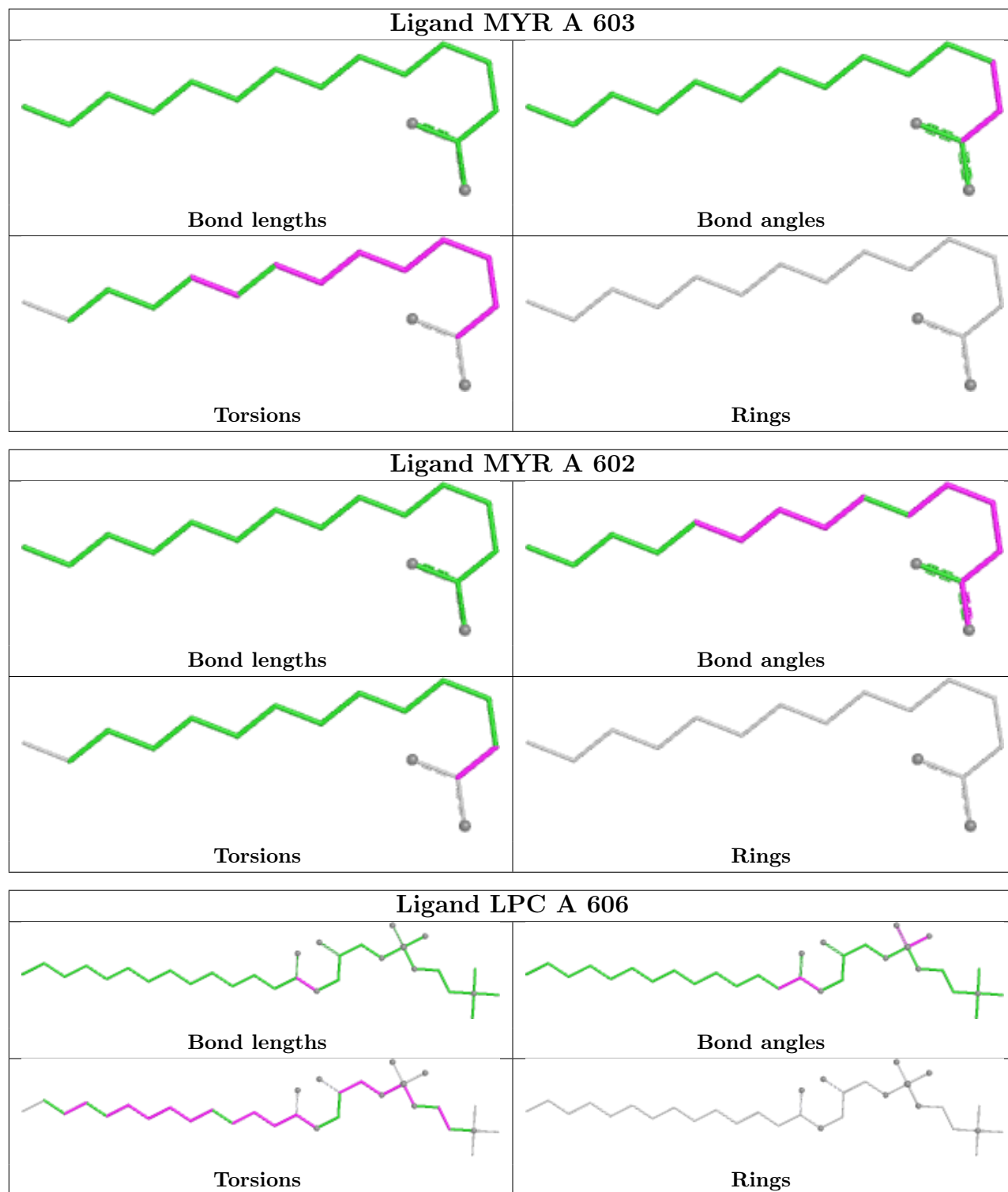
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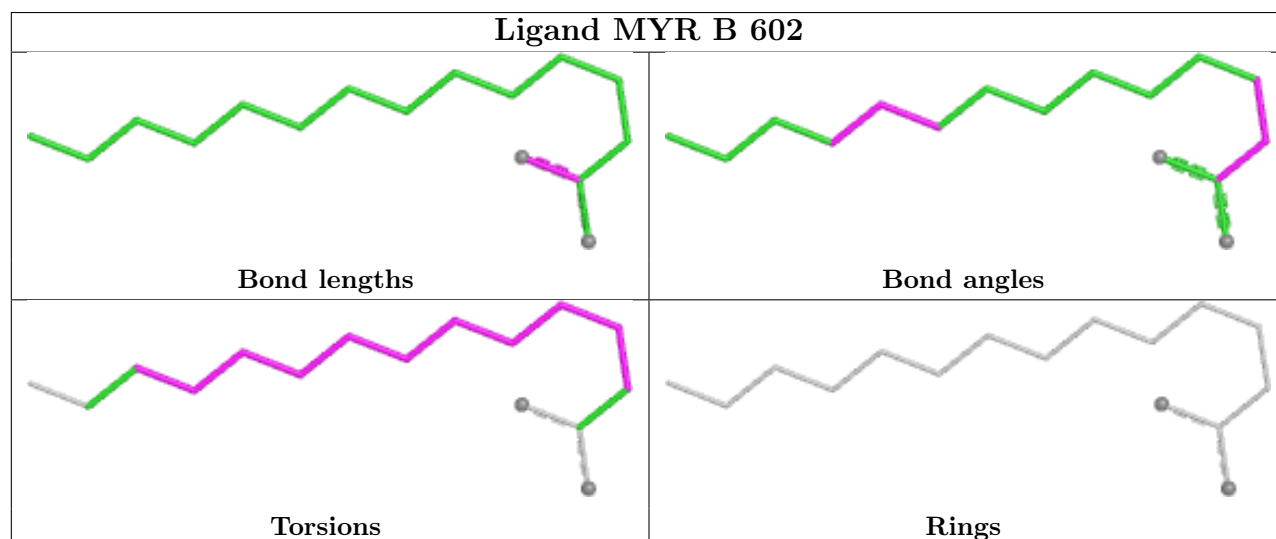
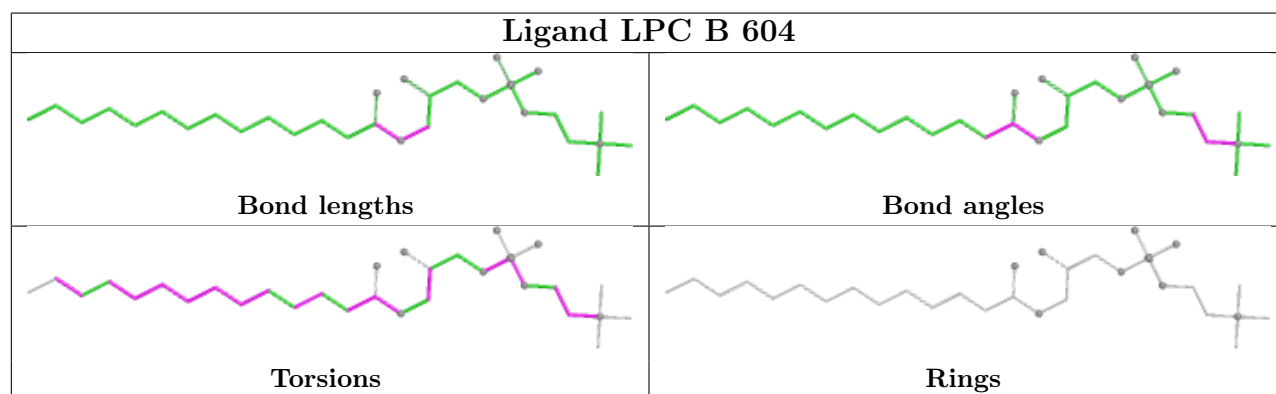
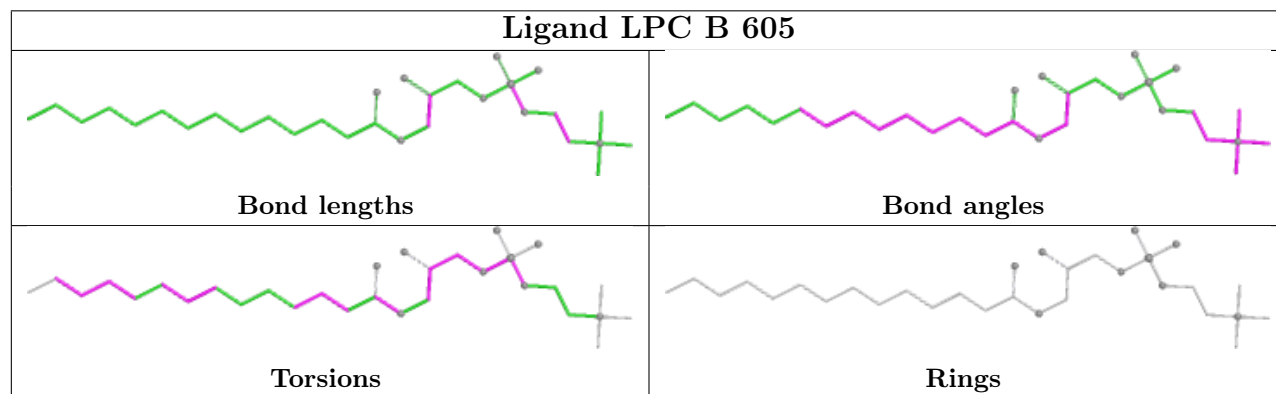
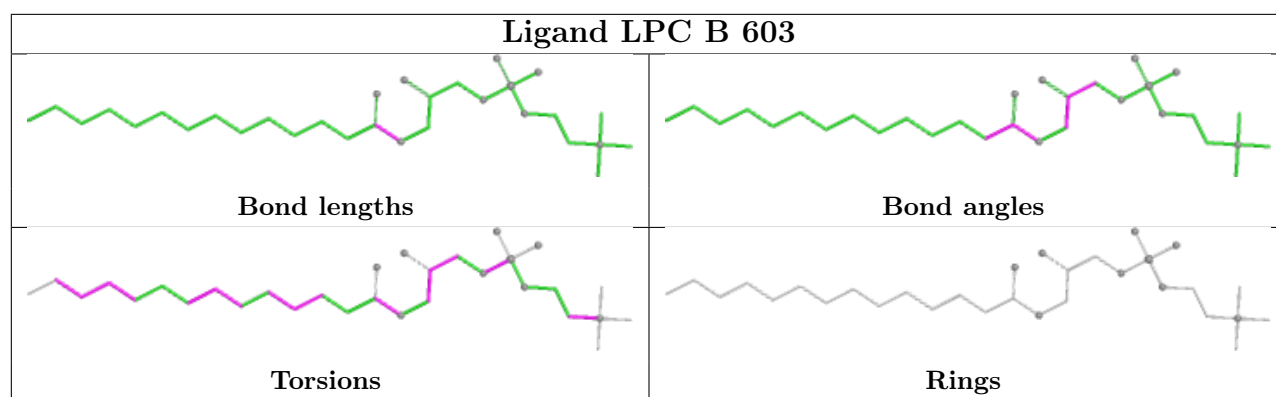
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	LPC	19	0
3	B	604	LPC	19	0
2	B	602	MYR	11	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	579/580 (99%)	0.22	9 (1%) 70 47	25, 50, 83, 154	0
1	B	579/580 (99%)	0.16	13 (2%) 62 38	21, 49, 83, 124	0
All	All	1158/1160 (99%)	0.19	22 (1%) 66 42	21, 50, 83, 154	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	CYS	4.4
1	B	95	GLU	4.3
1	B	170	GLN	3.8
1	B	568	PHE	3.7
1	B	561	ALA	3.0
1	A	433	VAL	3.0
1	B	396	GLU	2.9
1	B	563	ASP	2.8
1	A	561	ALA	2.7
1	A	365	ASP	2.7
1	A	575	LEU	2.6
1	B	525	LYS	2.3
1	B	437	CYS	2.3
1	B	569	ALA	2.2
1	B	439	LYS	2.2
1	A	390	GLN	2.2
1	B	442	GLU	2.2
1	A	301	ASP	2.2
1	B	143	ALA	2.1
1	B	448	CYS	2.1
1	A	549	ASP	2.1
1	A	426	VAL	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

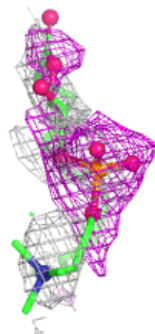
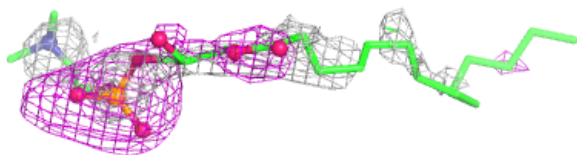
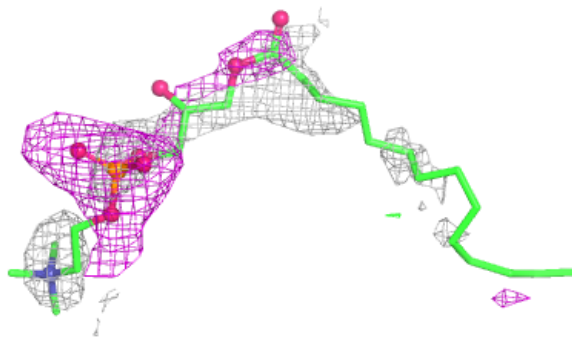
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LPC	A	606	31/31	0.51	0.22	49,58,66,70	0
3	LPC	B	603	31/31	0.59	0.22	44,53,65,66	0
3	LPC	B	605	31/31	0.63	0.20	48,56,63,65	0
3	LPC	A	604	31/31	0.66	0.20	43,49,57,59	0
3	LPC	A	605	31/31	0.67	0.19	43,48,55,63	0
3	LPC	B	604	31/31	0.68	0.20	42,49,58,60	0
2	MYR	B	601	16/16	0.77	0.22	54,63,72,78	0
2	MYR	A	601	16/16	0.78	0.18	40,48,67,68	0
2	MYR	B	602	16/16	0.78	0.21	40,48,60,61	0
2	MYR	A	603	16/16	0.83	0.15	39,42,61,63	0
2	MYR	B	606	16/16	0.83	0.17	38,43,50,52	0
2	MYR	A	602	16/16	0.84	0.18	47,50,56,56	0

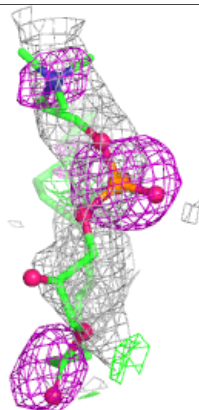
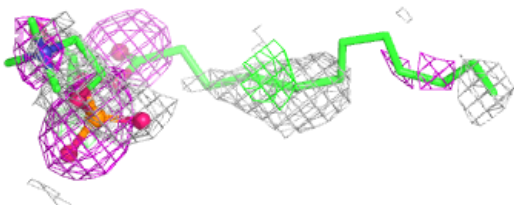
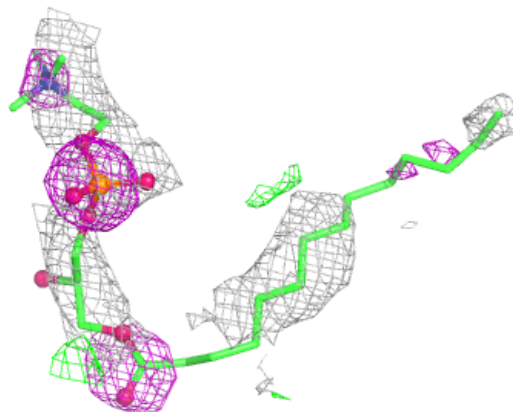
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LPC A 606:

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

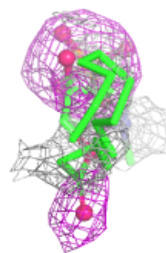
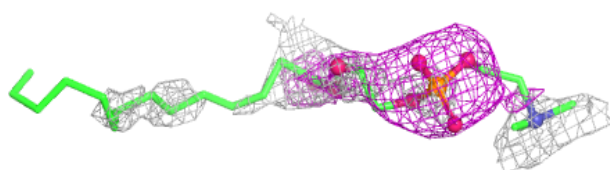
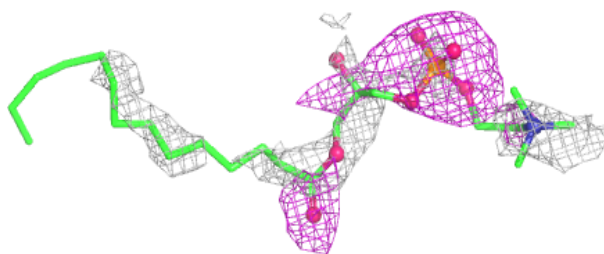
**Electron density around LPC B 603:**

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



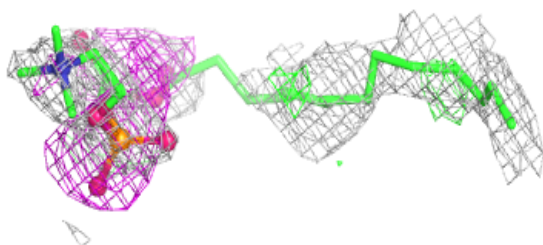
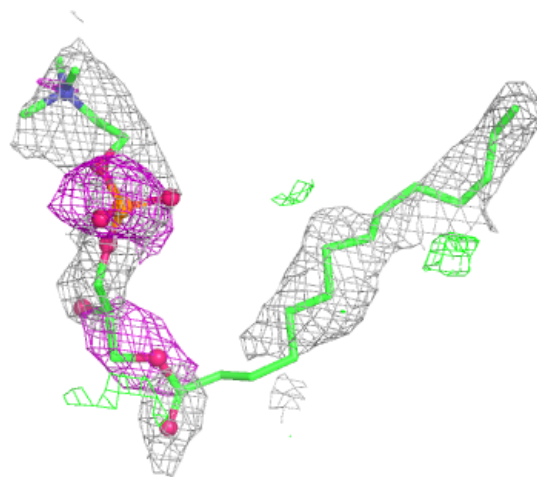
Electron density around LPC B 605:

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



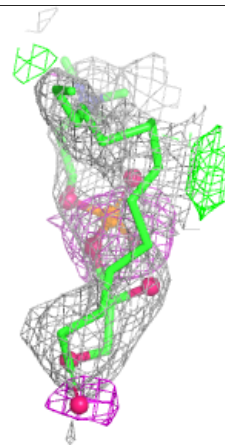
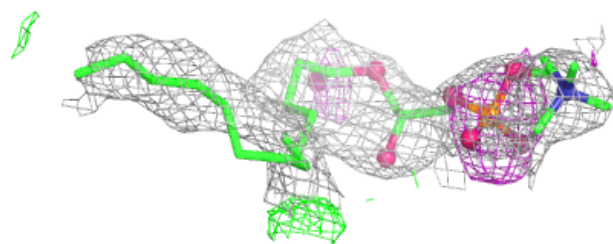
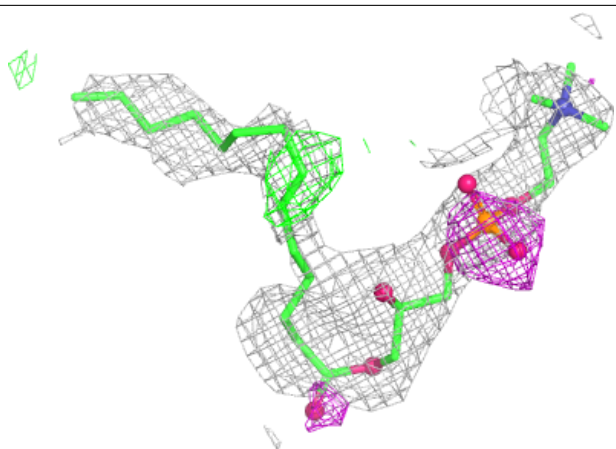
Electron density around LPC A 604:

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



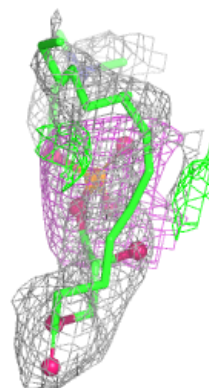
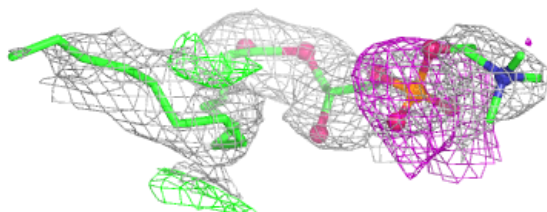
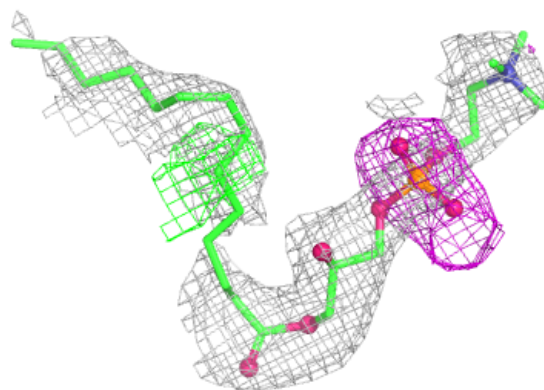
Electron density around LPC A 605:

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



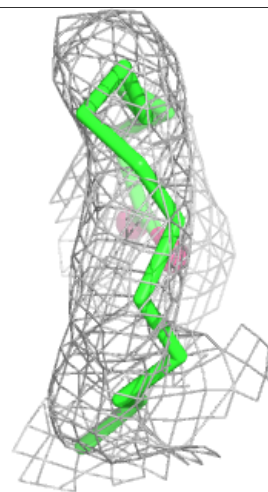
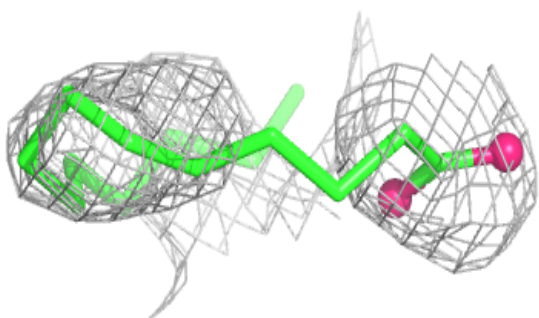
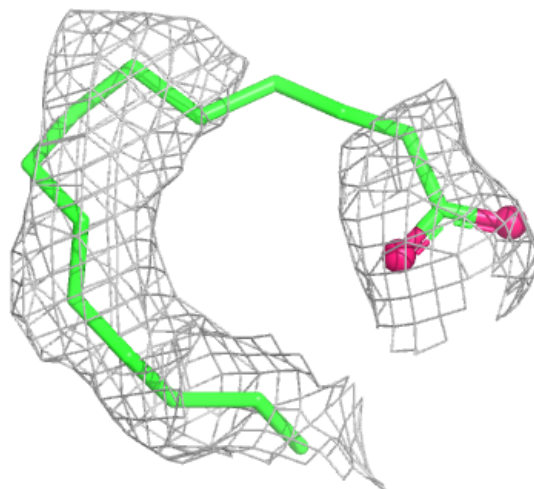
Electron density around LPC B 604:

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



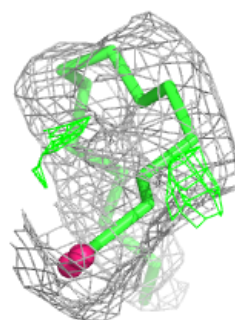
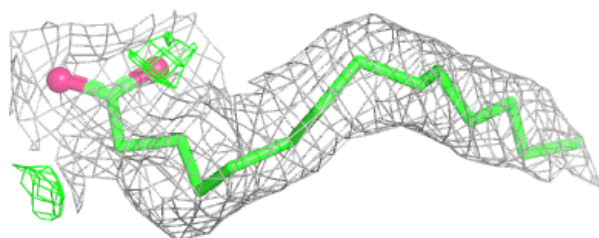
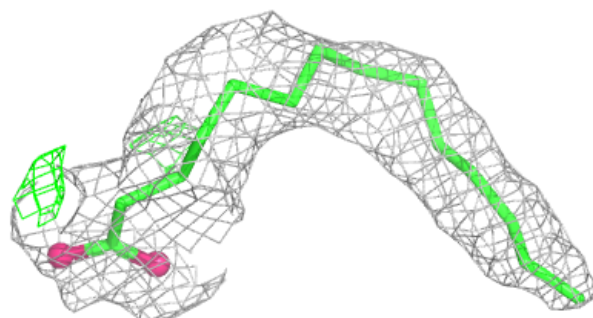
Electron density around MYR B 601:

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

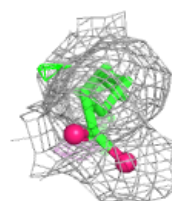
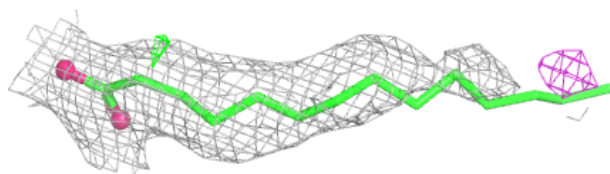
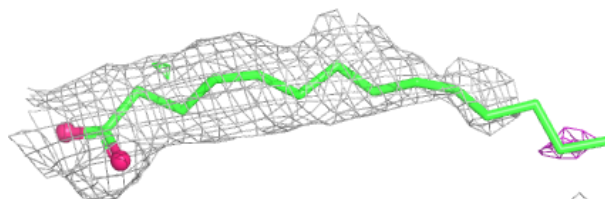


Electron density around MYR A 601:

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

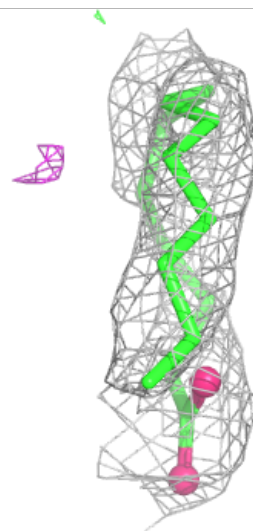
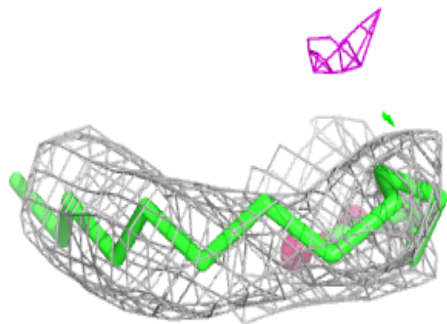
**Electron density around MYR B 602:**

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



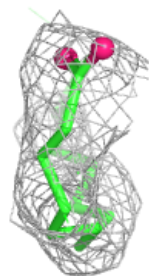
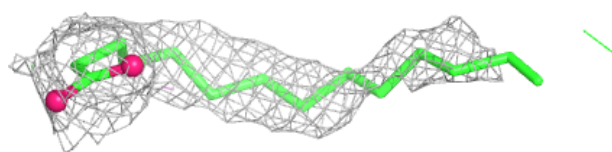
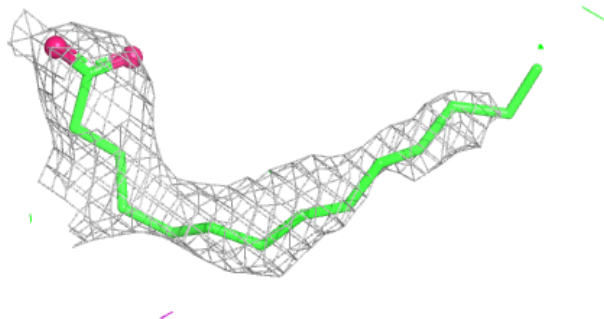
Electron density around MYR A 603:

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

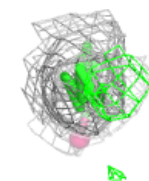
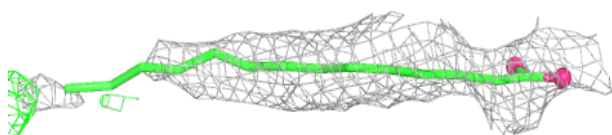
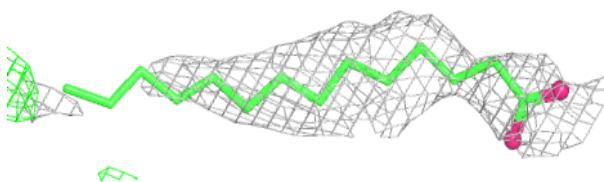


Electron density around MYR B 606:

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

**Electron density around MYR A 602:**

$2mF_o-DF_c$ (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.