



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 07:55 AM EST

PDB ID : 7LHE
EMDB ID : EMD-23337
Title : Structure of full-length IP3R1 channel reconstituted into lipid nanodisc in the apo-state
Authors : Baker, M.R.; Fan, G.; Baker, M.L.; Serysheva, I.I.
Deposited on : 2021-01-22
Resolution : 3.30 Å(reported)
Based on initial model : 6MU2

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

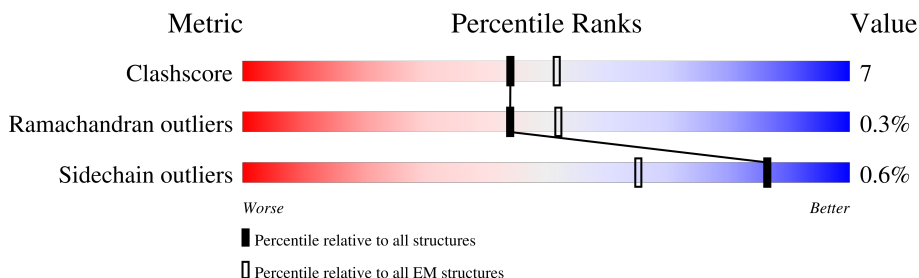
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2734	
1	B	2734	
1	C	2734	
1	D	2734	

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	PLX	A	2801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLX	A	2802	X	-	-	-
2	PLX	A	2803	X	-	-	-
2	PLX	A	2804	X	-	-	-
2	PLX	A	2806	X	-	-	-
2	PLX	A	2807	X	-	-	-
2	PLX	A	2808	X	-	-	-
2	PLX	B	2801	X	-	-	-
2	PLX	B	2802	X	-	-	-
2	PLX	B	2803	X	-	-	-
2	PLX	B	2804	X	-	-	-
2	PLX	B	2805	X	-	-	-
2	PLX	B	2806	X	-	-	-
2	PLX	B	2807	X	-	-	-
2	PLX	B	2808	X	-	-	-
2	PLX	C	2801	X	-	-	-
2	PLX	C	2802	X	-	-	-
2	PLX	C	2803	X	-	-	-
2	PLX	C	2804	X	-	-	-
2	PLX	C	2805	X	-	-	-
2	PLX	C	2807	X	-	-	-
2	PLX	C	2808	X	-	-	-
2	PLX	D	2801	X	-	-	-
2	PLX	D	2802	X	-	-	-
2	PLX	D	2803	X	-	-	-
2	PLX	D	2804	X	-	-	-
2	PLX	D	2806	X	-	-	-
2	PLX	D	2807	X	-	-	-

2 Entry composition ⓘ

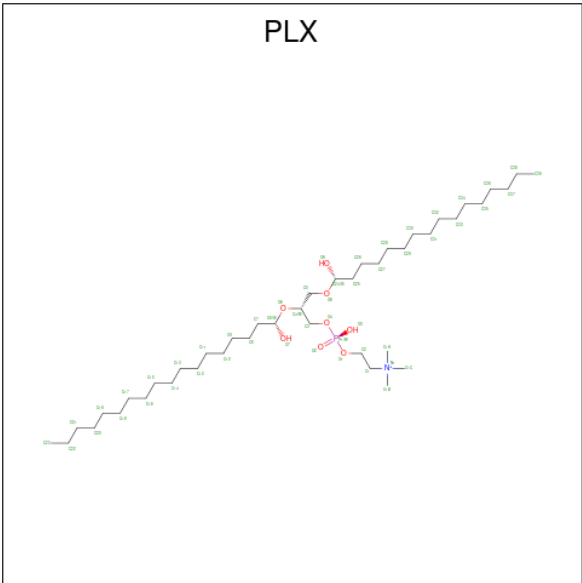
There are 3 unique types of molecules in this entry. The entry contains 73691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2298	Total 18148	11558	3171	3309	110	0	0
1	D	2298	Total 18148	11558	3171	3309	110	0	0
1	C	2298	Total 18148	11558	3171	3309	110	0	0
1	B	2298	Total 18148	11558	3171	3309	110	0	0

- Molecule 2 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOXOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total 274	204	7	56	7	0

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	A	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	A	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	A	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	A	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	D	1	Total	C	N	O	P	0
			234	174	6	48	6	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	C	1	Total	C	N	O	P	0
			274	204	7	56	7	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	

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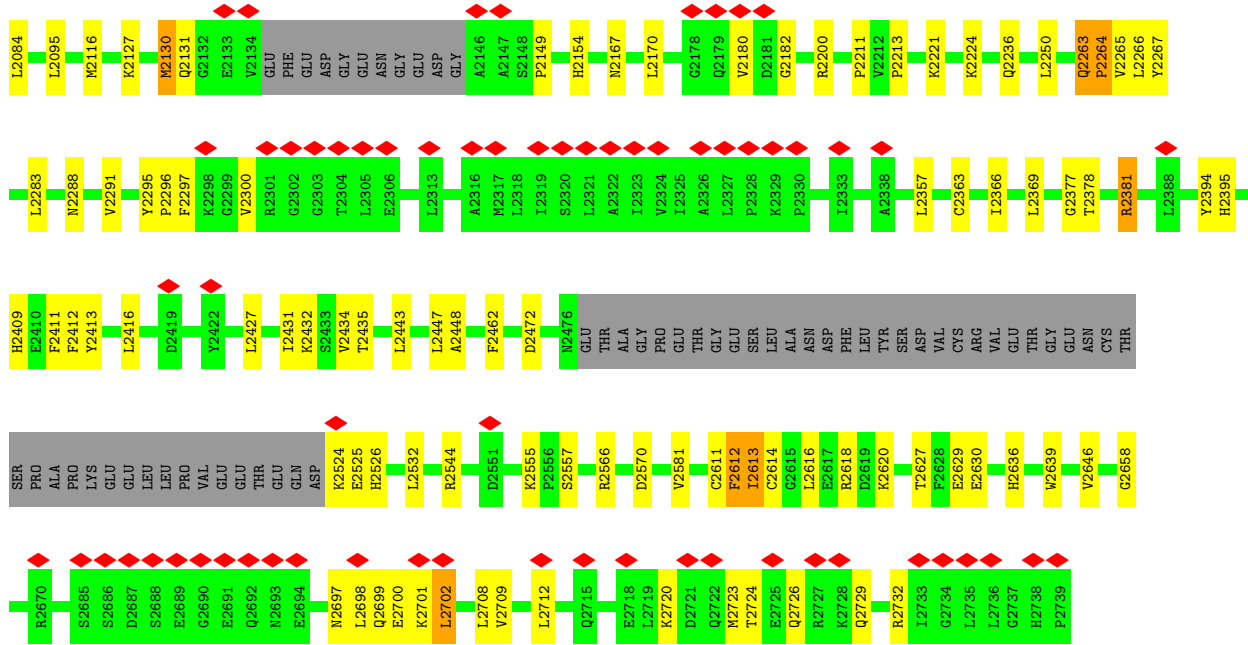
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	
2	B	1	Total	C	N	O	P	0
			313	233	8	64	8	

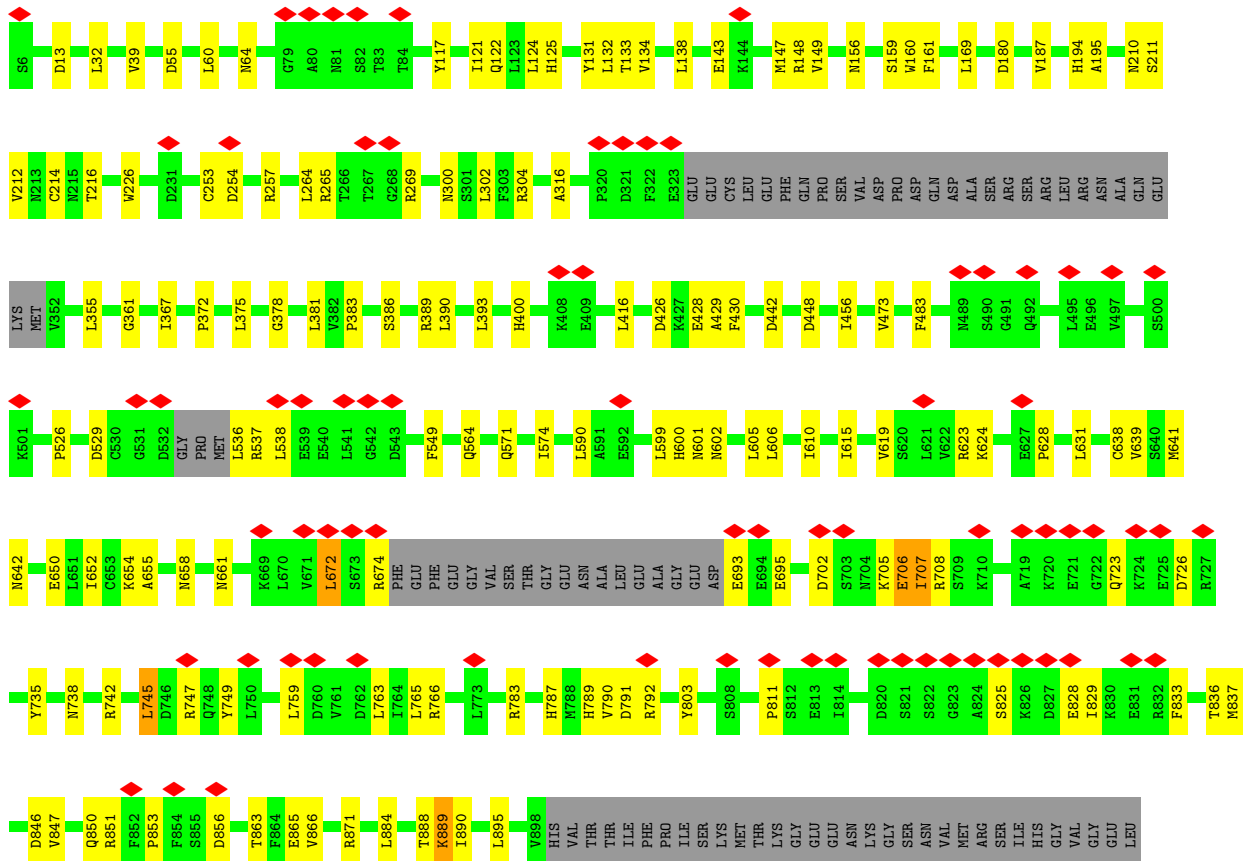
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

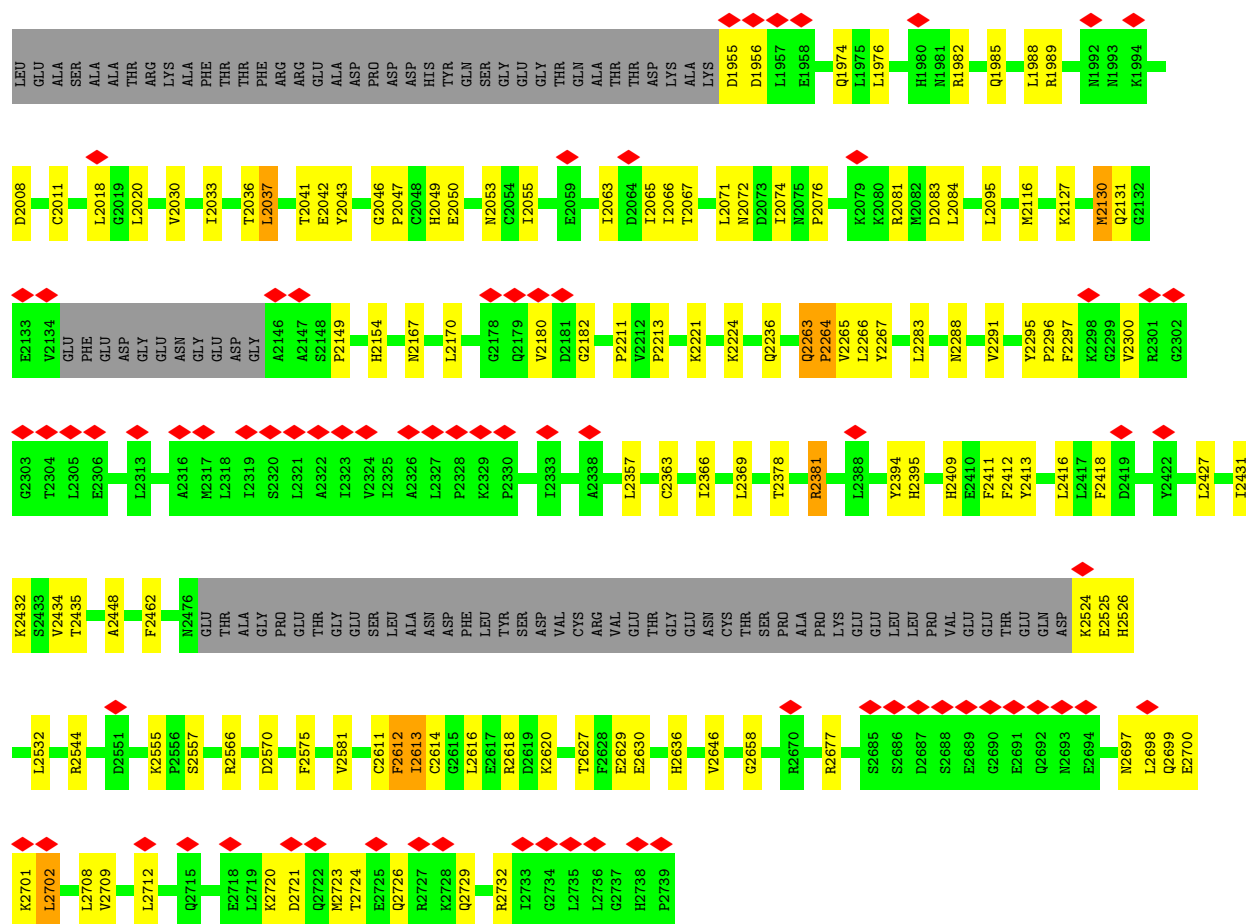




• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

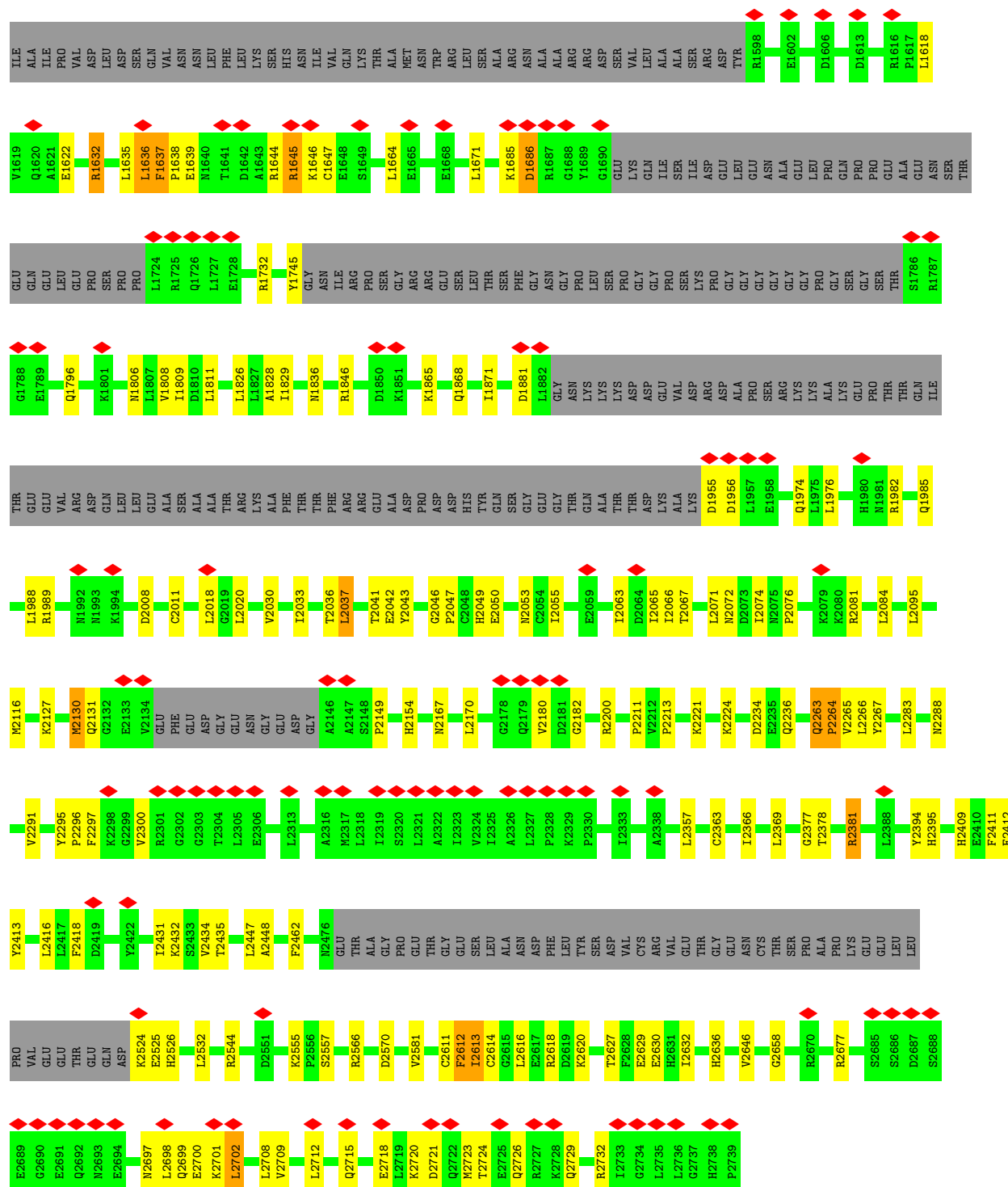












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	573723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	46943	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.754	Depositor
Minimum map value	-0.700	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.263	Depositor
Map size (\AA)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/18460	0.64	19/24875 (0.1%)
1	B	0.28	0/18460	0.64	19/24875 (0.1%)
1	C	0.28	0/18460	0.64	19/24875 (0.1%)
1	D	0.28	0/18460	0.64	19/24875 (0.1%)
All	All	0.28	0/73840	0.64	76/99500 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	A	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	C	1403	LEU	CA-CB-CG	9.26	136.59	115.30
1	D	1403	LEU	CA-CB-CG	9.24	136.56	115.30
1	A	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	D	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	C	381	LEU	CA-CB-CG	8.48	134.80	115.30
1	B	381	LEU	CA-CB-CG	8.48	134.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	672	LEU	CA-CB-CG	7.64	132.86	115.30
1	A	672	LEU	CA-CB-CG	7.63	132.84	115.30
1	B	672	LEU	CA-CB-CG	7.63	132.84	115.30
1	D	672	LEU	CA-CB-CG	7.62	132.84	115.30
1	A	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	D	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	C	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	1686	ASP	CB-CG-OD1	7.47	125.03	118.30
1	A	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	C	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	B	2702	LEU	CA-CB-CG	7.44	132.42	115.30
1	D	2702	LEU	CA-CB-CG	7.44	132.41	115.30
1	D	590	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	590	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	590	LEU	CA-CB-CG	6.82	130.98	115.30
1	C	590	LEU	CA-CB-CG	6.82	130.98	115.30
1	C	994	LEU	CA-CB-CG	6.53	130.32	115.30
1	D	994	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	994	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	994	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	D	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	C	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	745	LEU	CA-CB-CG	6.43	130.09	115.30
1	B	1636	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	1636	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	1636	LEU	CA-CB-CG	6.16	129.46	115.30
1	C	1636	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	D	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	D	2708	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	1365	MET	CA-CB-CG	5.97	123.45	113.30
1	B	2708	LEU	CA-CB-CG	5.97	129.03	115.30
1	C	1365	MET	CA-CB-CG	5.96	123.43	113.30
1	A	2708	LEU	CA-CB-CG	5.95	128.99	115.30
1	C	2708	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	599	LEU	CA-CB-CG	5.72	128.45	115.30
1	D	599	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	599	LEU	CA-CB-CG	5.70	128.42	115.30
1	C	599	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	1102	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	1102	LEU	CA-CB-CG	5.59	128.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1102	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	1102	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	2020	LEU	CA-CB-CG	5.56	128.09	115.30
1	D	2020	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	2723	MET	CA-CB-CG	5.52	122.69	113.30
1	A	2723	MET	CA-CB-CG	5.52	122.69	113.30
1	B	2723	MET	CA-CB-CG	5.49	122.63	113.30
1	C	2723	MET	CA-CB-CG	5.49	122.62	113.30
1	C	132	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	132	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	132	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	132	LEU	CA-CB-CG	5.41	127.73	115.30
1	C	2130	MET	CA-CB-CG	5.22	122.17	113.30
1	A	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	D	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	B	2130	MET	CA-CB-CG	5.20	122.14	113.30
1	C	1401	LEU	CA-CB-CG	5.19	127.25	115.30
1	B	1401	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	1401	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	1401	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	D	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	C	2037	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	2037	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1637	PHE	Peptide
1	A	2263	GLN	Peptide
1	A	2295	TYR	Peptide
1	A	2296	PRO	Peptide
1	A	2532	LEU	Peptide
1	A	706	GLU	Peptide
1	A	707	ILE	Peptide
1	B	1637	PHE	Peptide
1	B	2263	GLN	Peptide
1	B	2295	TYR	Peptide
1	B	2296	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	2532	LEU	Peptide
1	B	706	GLU	Peptide
1	B	707	ILE	Peptide
1	C	1637	PHE	Peptide
1	C	2263	GLN	Peptide
1	C	2295	TYR	Peptide
1	C	2296	PRO	Peptide
1	C	2532	LEU	Peptide
1	C	706	GLU	Peptide
1	C	707	ILE	Peptide
1	D	1637	PHE	Peptide
1	D	2263	GLN	Peptide
1	D	2295	TYR	Peptide
1	D	2296	PRO	Peptide
1	D	2532	LEU	Peptide
1	D	706	GLU	Peptide
1	D	707	ILE	Peptide

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	18148	0	17980	255	0
1	B	18148	0	17980	256	0
1	C	18148	0	17980	252	0
1	D	18148	0	17980	245	0
2	A	274	0	370	29	0
2	B	313	0	422	33	0
2	C	274	0	369	30	0
2	D	234	0	315	29	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	73691	0	73396	1013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1013) 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:2409:HIS:CG	2:C:2804:PLX:H51	1.37	1.58
1:D:2409:HIS:CG	2:D:2803:PLX:H51	1.40	1.54
1:A:2409:HIS:CG	2:A:2803:PLX:H51	1.46	1.49
1:C:2409:HIS:CD2	2:C:2804:PLX:H51	1.49	1.46
1:B:2409:HIS:CG	2:B:2807:PLX:H51	1.49	1.43
1:D:2409:HIS:CD2	2:D:2803:PLX:H51	1.56	1.40
1:B:2409:HIS:CE1	2:B:2807:PLX:H51	1.60	1.36
1:B:2409:HIS:CD2	2:B:2807:PLX:H51	1.61	1.36
1:B:2462:PHE:CD2	2:B:2802:PLX:O9	1.79	1.35
1:A:2409:HIS:CD2	2:A:2803:PLX:H51	1.62	1.35
1:B:2409:HIS:CD2	2:B:2807:PLX:H32	1.63	1.32
1:A:2409:HIS:CD2	2:A:2803:PLX:H32	1.66	1.30
1:B:2409:HIS:ND1	2:B:2807:PLX:H51	1.48	1.28
1:A:2570:ASP:OD2	1:D:2544:ARG:NH2	1.69	1.26
1:D:2570:ASP:OD2	1:C:2544:ARG:NH2	1.68	1.25
1:B:2409:HIS:CG	2:B:2807:PLX:C5	2.17	1.24
1:C:2462:PHE:CD2	2:C:2807:PLX:O9	1.91	1.24
1:A:2462:PHE:CD2	2:A:2806:PLX:O9	1.91	1.24
1:A:2544:ARG:NH2	1:B:2570:ASP:OD2	1.68	1.23
1:C:2570:ASP:OD2	1:B:2544:ARG:NH2	1.68	1.23
1:D:2409:HIS:CD2	2:D:2803:PLX:H32	1.77	1.20
1:C:2409:HIS:CG	2:C:2804:PLX:C5	2.25	1.19
1:A:2409:HIS:CG	2:A:2803:PLX:C5	2.23	1.19
1:A:2409:HIS:ND1	2:A:2803:PLX:H51	1.57	1.17
1:A:2409:HIS:CE1	2:A:2803:PLX:H51	1.78	1.17
1:B:2462:PHE:CG	2:B:2802:PLX:O9	1.98	1.16
1:D:2409:HIS:CG	2:D:2803:PLX:C5	2.29	1.14
1:C:2409:HIS:CD2	2:C:2804:PLX:H32	1.84	1.11
1:B:2409:HIS:NE2	2:B:2807:PLX:H51	1.66	1.09
1:B:2409:HIS:CD2	2:B:2807:PLX:C3	2.39	1.05
1:B:2409:HIS:CD2	2:B:2807:PLX:C5	2.38	1.05
1:B:2409:HIS:CE1	2:B:2807:PLX:C5	2.42	1.03
1:A:2409:HIS:CD2	2:A:2803:PLX:C3	2.42	1.03
1:B:2409:HIS:ND1	2:B:2807:PLX:C5	2.21	1.01
1:A:2409:HIS:CD2	2:A:2803:PLX:C5	2.42	1.00
1:C:2409:HIS:CD2	2:C:2804:PLX:C5	2.40	0.99
1:D:2409:HIS:CD2	2:D:2803:PLX:C5	2.46	0.99
1:C:2462:PHE:CG	2:C:2807:PLX:O9	2.17	0.97
1:D:2409:HIS:ND1	2:D:2803:PLX:H51	1.79	0.97
1:A:2409:HIS:NE2	2:A:2803:PLX:H51	1.79	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2462:PHE:CG	2:A:2806:PLX:O9	2.17	0.96
1:C:2409:HIS:ND1	2:C:2804:PLX:H51	1.87	0.89
1:D:2409:HIS:CD2	2:D:2803:PLX:C3	2.55	0.89
1:A:2409:HIS:ND1	2:A:2803:PLX:C5	2.34	0.88
1:A:2409:HIS:CE1	2:A:2803:PLX:C5	2.56	0.88
1:B:2409:HIS:HD2	2:B:2807:PLX:H32	1.40	0.86
1:B:2409:HIS:CG	2:B:2807:PLX:H52	2.08	0.86
1:D:2409:HIS:CE1	2:D:2803:PLX:H51	2.10	0.86
1:C:2409:HIS:CD2	2:C:2804:PLX:C3	2.60	0.83
1:A:623:ARG:HH12	1:A:628:PRO:HA	1.44	0.83
1:A:2409:HIS:HD2	2:A:2803:PLX:H32	1.44	0.83
1:B:623:ARG:HH12	1:B:628:PRO:HA	1.44	0.83
1:D:623:ARG:HH12	1:D:628:PRO:HA	1.44	0.81
1:C:623:ARG:HH12	1:C:628:PRO:HA	1.44	0.81
1:D:2462:PHE:CD1	2:D:2806:PLX:O8	2.32	0.79
1:A:2409:HIS:NE2	2:A:2803:PLX:H32	1.98	0.79
1:D:2409:HIS:NE2	2:D:2803:PLX:H51	1.98	0.79
1:C:2409:HIS:CE1	2:C:2804:PLX:H51	2.19	0.77
1:B:2409:HIS:NE2	2:B:2807:PLX:H32	1.99	0.77
1:C:2409:HIS:NE2	2:C:2804:PLX:H51	2.00	0.76
1:A:2462:PHE:CE2	2:A:2806:PLX:O9	2.41	0.74
1:B:2462:PHE:CE2	2:B:2802:PLX:O9	2.41	0.73
1:C:2462:PHE:CE2	2:C:2807:PLX:O9	2.41	0.73
1:D:2462:PHE:CE1	2:D:2806:PLX:C24	2.52	0.71
1:D:2409:HIS:CE1	2:D:2803:PLX:C5	2.74	0.71
1:D:2409:HIS:HD2	2:D:2803:PLX:H32	1.49	0.71
1:D:212:VAL:HG23	1:D:214:CYS:H	1.57	0.70
1:D:1374:TYR:HA	1:D:1377:HIS:HB3	1.74	0.70
1:C:1374:TYR:HA	1:C:1377:HIS:HB3	1.74	0.70
1:C:2409:HIS:ND1	2:C:2804:PLX:C5	2.51	0.70
1:A:212:VAL:HG23	1:A:214:CYS:H	1.57	0.69
1:B:1315:ILE:HG23	1:B:1316:VAL:HG23	1.74	0.69
1:C:1315:ILE:HG23	1:C:1316:VAL:HG23	1.74	0.69
1:A:1315:ILE:HG23	1:A:1316:VAL:HG23	1.74	0.68
1:B:1374:TYR:HA	1:B:1377:HIS:HB3	1.74	0.68
1:A:1374:TYR:HA	1:A:1377:HIS:HB3	1.74	0.68
1:C:2614:CYS:SG	1:C:2636:HIS:CE1	2.87	0.68
1:D:2614:CYS:SG	1:D:2636:HIS:CE1	2.87	0.68
1:B:212:VAL:HG23	1:B:214:CYS:H	1.57	0.68
1:C:212:VAL:HG23	1:C:214:CYS:H	1.57	0.68
1:D:1315:ILE:HG23	1:D:1316:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2409:HIS:CE1	2:C:2804:PLX:C5	2.76	0.68
1:B:2614:CYS:SG	1:B:2636:HIS:CE1	2.87	0.68
1:D:1636:LEU:HA	1:D:1639:GLU:HB3	1.76	0.67
1:A:1636:LEU:HA	1:A:1639:GLU:HB3	1.76	0.67
1:A:2614:CYS:SG	1:A:2636:HIS:CE1	2.87	0.67
1:C:2409:HIS:HD2	2:C:2804:PLX:H32	1.54	0.67
1:D:2409:HIS:ND1	2:D:2803:PLX:C5	2.49	0.67
1:B:2411:PHE:O	1:B:2413:TYR:N	2.26	0.67
1:B:1636:LEU:HA	1:B:1639:GLU:HB3	1.76	0.67
1:A:2409:HIS:CG	2:A:2803:PLX:H52	2.25	0.67
1:C:1636:LEU:HA	1:C:1639:GLU:HB3	1.75	0.67
1:C:2411:PHE:O	1:C:2413:TYR:N	2.26	0.66
1:B:1796:GLN:OE1	1:B:1836:ASN:ND2	2.29	0.66
1:A:1796:GLN:OE1	1:A:1836:ASN:ND2	2.29	0.66
1:D:2462:PHE:CZ	2:D:2806:PLX:C24	2.71	0.66
1:D:1796:GLN:OE1	1:D:1836:ASN:ND2	2.29	0.65
1:C:133:THR:HG22	1:C:159:SER:HB3	1.78	0.65
1:C:1796:GLN:OE1	1:C:1836:ASN:ND2	2.29	0.65
1:B:133:THR:HG22	1:B:159:SER:HB3	1.78	0.65
1:A:1408:ARG:HH12	1:A:1423:TYR:HB3	1.62	0.65
1:D:1408:ARG:HH12	1:D:1423:TYR:HB3	1.62	0.65
1:C:1408:ARG:HH12	1:C:1423:TYR:HB3	1.62	0.65
1:B:1408:ARG:HH12	1:B:1423:TYR:HB3	1.62	0.65
1:D:133:THR:HG22	1:D:159:SER:HB3	1.78	0.64
1:A:133:THR:HG22	1:A:159:SER:HB3	1.78	0.64
1:A:2411:PHE:O	1:A:2413:TYR:N	2.26	0.64
1:C:2074:ILE:HG21	1:C:2081:ARG:HH22	1.62	0.64
1:B:2074:ILE:HG21	1:B:2081:ARG:HH22	1.62	0.64
1:D:2411:PHE:O	1:D:2413:TYR:N	2.26	0.64
1:A:1187:CYS:SG	1:A:1206:ARG:NH2	2.71	0.64
1:A:2264:PRO:HA	1:A:2267:TYR:HB3	1.80	0.64
1:B:134:VAL:HG22	1:B:149:VAL:HG12	1.80	0.64
1:A:2074:ILE:HG21	1:A:2081:ARG:HH22	1.62	0.64
1:D:1187:CYS:SG	1:D:1206:ARG:NH2	2.71	0.64
1:D:2409:HIS:NE2	2:D:2803:PLX:H32	2.13	0.64
1:C:1187:CYS:SG	1:C:1206:ARG:NH2	2.71	0.64
1:B:654:LYS:O	1:B:658:ASN:ND2	2.31	0.64
1:D:2074:ILE:HG21	1:D:2081:ARG:HH22	1.62	0.63
1:C:134:VAL:HG22	1:C:149:VAL:HG12	1.80	0.63
1:B:2264:PRO:HA	1:B:2267:TYR:HB3	1.80	0.63
1:A:654:LYS:O	1:A:658:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2264:PRO:HA	1:C:2267:TYR:HB3	1.80	0.63
1:B:1187:CYS:SG	1:B:1206:ARG:NH2	2.71	0.63
1:D:2264:PRO:HA	1:D:2267:TYR:HB3	1.80	0.63
1:A:134:VAL:HG22	1:A:149:VAL:HG12	1.80	0.63
1:D:2555:LYS:H	1:D:2566:ARG:HH22	1.47	0.62
1:D:134:VAL:HG22	1:D:149:VAL:HG12	1.80	0.62
1:C:847:VAL:HG13	1:C:851:ARG:HE	1.65	0.61
1:A:847:VAL:HG13	1:A:851:ARG:HE	1.65	0.61
1:D:2462:PHE:CE1	2:D:2806:PLX:O8	2.52	0.61
1:B:847:VAL:HG13	1:B:851:ARG:HE	1.65	0.61
1:C:2076:PRO:O	1:C:2081:ARG:NH1	2.34	0.61
1:B:2555:LYS:H	1:B:2566:ARG:HH22	1.47	0.61
1:B:2076:PRO:O	1:B:2081:ARG:NH1	2.34	0.61
1:A:1312:LEU:HA	1:A:1315:ILE:HG22	1.82	0.61
1:D:1312:LEU:HA	1:D:1315:ILE:HG22	1.82	0.60
1:B:1312:LEU:HA	1:B:1315:ILE:HG22	1.82	0.60
1:A:2221:LYS:HD3	1:A:2224:LYS:HD2	1.83	0.60
1:A:2555:LYS:H	1:A:2566:ARG:HH22	1.47	0.60
1:D:2076:PRO:O	1:D:2081:ARG:NH1	2.34	0.60
1:C:654:LYS:O	1:C:658:ASN:ND2	2.31	0.60
1:D:650:GLU:O	1:D:654:LYS:NZ	2.35	0.60
1:D:706:GLU:HG3	1:D:707:ILE:H	1.67	0.60
1:A:2076:PRO:O	1:A:2081:ARG:NH1	2.34	0.60
1:A:2618:ARG:NH2	1:A:2629:GLU:OE2	2.35	0.60
1:D:2616:LEU:HD12	1:D:2620:LYS:HG3	1.83	0.60
1:C:2555:LYS:H	1:C:2566:ARG:HH22	1.47	0.60
1:D:2011:CYS:HB3	1:D:2065:ILE:HD11	1.84	0.60
1:C:2221:LYS:HD3	1:C:2224:LYS:HD2	1.83	0.60
1:B:706:GLU:HG3	1:B:707:ILE:H	1.67	0.60
1:D:654:LYS:O	1:D:658:ASN:ND2	2.31	0.60
1:D:847:VAL:HG13	1:D:851:ARG:HE	1.65	0.60
1:D:1644:ARG:NH1	1:D:1647:CYS:SG	2.75	0.60
1:D:2221:LYS:HD3	1:D:2224:LYS:HD2	1.83	0.60
1:C:1312:LEU:HA	1:C:1315:ILE:HG22	1.82	0.60
1:B:650:GLU:O	1:B:654:LYS:NZ	2.35	0.60
1:A:1644:ARG:NH1	1:A:1647:CYS:SG	2.75	0.60
1:B:2616:LEU:HD12	1:B:2620:LYS:HG3	1.83	0.60
1:B:2618:ARG:NH2	1:B:2629:GLU:OE2	2.35	0.60
1:C:1644:ARG:NH1	1:C:1647:CYS:SG	2.75	0.59
1:B:602:ASN:HB3	1:B:605:LEU:HD12	1.84	0.59
1:B:1974:GLN:HG3	1:B:2042:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:GLU:O	1:C:654:LYS:NZ	2.35	0.59
1:C:706:GLU:HG3	1:C:707:ILE:H	1.67	0.59
1:B:828:GLU:HG3	1:B:829:ILE:HG23	1.84	0.59
1:A:2011:CYS:HB3	1:A:2065:ILE:HD11	1.84	0.59
1:D:1974:GLN:HG3	1:D:2042:GLU:HG3	1.84	0.59
1:C:2616:LEU:HD12	1:C:2620:LYS:HG3	1.83	0.59
1:A:765:LEU:HD11	1:A:836:THR:HG22	1.85	0.59
1:B:2221:LYS:HD3	1:B:2224:LYS:HD2	1.83	0.59
1:A:2616:LEU:HD12	1:A:2620:LYS:HG3	1.83	0.59
1:D:2618:ARG:NH2	1:D:2629:GLU:OE2	2.35	0.59
1:C:2618:ARG:NH2	1:C:2629:GLU:OE2	2.35	0.59
1:B:989:ARG:HD2	1:B:1041:PHE:HE1	1.67	0.59
1:B:1644:ARG:NH1	1:B:1647:CYS:SG	2.75	0.59
1:D:989:ARG:HD2	1:D:1041:PHE:HE1	1.67	0.59
1:B:996:ILE:HA	1:B:999:ARG:HG2	1.85	0.59
1:A:706:GLU:HG3	1:A:707:ILE:H	1.67	0.59
1:A:828:GLU:HG3	1:A:829:ILE:HG23	1.84	0.59
1:D:169:LEU:HD21	1:C:429:ALA:HB3	1.85	0.59
1:C:1974:GLN:HG3	1:C:2042:GLU:HG3	1.84	0.59
1:A:996:ILE:HA	1:A:999:ARG:HG2	1.85	0.59
1:B:2409:HIS:CD2	2:B:2807:PLX:C4	2.86	0.59
1:A:650:GLU:O	1:A:654:LYS:NZ	2.35	0.58
1:D:996:ILE:HA	1:D:999:ARG:HG2	1.85	0.58
1:C:996:ILE:HA	1:C:999:ARG:HG2	1.85	0.58
1:C:2524:LYS:HE2	1:C:2526:HIS:HB2	1.85	0.58
1:B:2524:LYS:HE2	1:B:2526:HIS:HB2	1.85	0.58
1:A:989:ARG:HD2	1:A:1041:PHE:HE1	1.67	0.58
1:D:765:LEU:HD11	1:D:836:THR:HG22	1.85	0.58
1:C:2011:CYS:HB3	1:C:2065:ILE:HD11	1.84	0.58
1:B:765:LEU:HD11	1:B:836:THR:HG22	1.85	0.58
1:D:602:ASN:HB3	1:D:605:LEU:HD12	1.84	0.58
1:D:759:LEU:HD13	1:D:763:LEU:HG	1.86	0.58
1:C:602:ASN:HB3	1:C:605:LEU:HD12	1.84	0.58
1:A:1974:GLN:HG3	1:A:2042:GLU:HG3	1.84	0.58
1:A:1982:ARG:HA	1:A:1985:GLN:HB3	1.86	0.58
1:C:765:LEU:HD11	1:C:836:THR:HG22	1.85	0.58
1:A:429:ALA:HB3	1:B:169:LEU:HD21	1.85	0.58
1:A:759:LEU:HD13	1:A:763:LEU:HG	1.86	0.58
1:C:828:GLU:HG3	1:C:829:ILE:HG23	1.84	0.58
1:C:1982:ARG:HA	1:C:1985:GLN:HB3	1.86	0.58
1:A:602:ASN:HB3	1:A:605:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2524:LYS:HE2	1:A:2526:HIS:HB2	1.85	0.58
1:D:2524:LYS:HE2	1:D:2526:HIS:HB2	1.85	0.58
1:C:169:LEU:HD21	1:B:429:ALA:HB3	1.85	0.58
1:B:790:VAL:O	1:B:792:ARG:NH1	2.37	0.58
1:B:2011:CYS:HB3	1:B:2065:ILE:HD11	1.84	0.58
1:D:1982:ARG:HA	1:D:1985:GLN:HB3	1.86	0.57
1:C:606:LEU:HD13	1:C:610:ILE:HD12	1.86	0.57
1:C:989:ARG:HD2	1:C:1041:PHE:HE1	1.67	0.57
1:D:606:LEU:HD13	1:D:610:ILE:HD12	1.86	0.57
1:A:790:VAL:O	1:A:792:ARG:NH1	2.37	0.57
1:C:790:VAL:O	1:C:792:ARG:NH1	2.37	0.57
1:B:846:ASP:OD2	1:B:850:GLN:NE2	2.37	0.57
1:A:143:GLU:OE1	1:A:210:ASN:ND2	2.38	0.57
1:D:828:GLU:HG3	1:D:829:ILE:HG23	1.84	0.57
1:D:846:ASP:OD2	1:D:850:GLN:NE2	2.37	0.57
1:C:1985:GLN:NE2	1:C:2043:TYR:O	2.38	0.57
1:A:1632:ARG:NH2	1:A:1635:LEU:O	2.38	0.57
1:C:846:ASP:OD2	1:C:850:GLN:NE2	2.37	0.57
1:C:2409:HIS:NE2	2:C:2804:PLX:H32	2.18	0.57
1:A:169:LEU:HD21	1:D:429:ALA:HB3	1.85	0.57
1:D:1985:GLN:NE2	1:D:2043:TYR:O	2.38	0.57
1:D:1632:ARG:NH2	1:D:1635:LEU:O	2.38	0.57
1:C:1808:VAL:HG11	1:C:1828:ALA:HB2	1.87	0.57
1:C:655:ALA:O	1:C:661:ASN:ND2	2.38	0.56
1:C:1632:ARG:NH2	1:C:1635:LEU:O	2.38	0.56
1:B:1982:ARG:HA	1:B:1985:GLN:HB3	1.86	0.56
1:A:537:ARG:HH12	1:A:549:PHE:HE2	1.54	0.56
1:A:846:ASP:OD2	1:A:850:GLN:NE2	2.37	0.56
1:D:790:VAL:O	1:D:792:ARG:NH1	2.37	0.56
1:D:1808:VAL:HG11	1:D:1828:ALA:HB2	1.87	0.56
1:C:143:GLU:OE1	1:C:210:ASN:ND2	2.38	0.56
1:C:537:ARG:HH12	1:C:549:PHE:HE2	1.54	0.56
1:C:759:LEU:HD13	1:C:763:LEU:HG	1.86	0.56
1:B:759:LEU:HD13	1:B:763:LEU:HG	1.86	0.56
1:B:1632:ARG:NH2	1:B:1635:LEU:O	2.38	0.56
1:A:606:LEU:HD13	1:A:610:ILE:HD12	1.86	0.56
1:D:537:ARG:HH12	1:D:549:PHE:HE2	1.54	0.56
1:C:571:GLN:HB3	1:C:605:LEU:HD11	1.88	0.56
1:B:143:GLU:OE1	1:B:210:ASN:ND2	2.38	0.56
1:B:606:LEU:HD13	1:B:610:ILE:HD12	1.86	0.56
1:B:1808:VAL:HG11	1:B:1828:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:GLN:HB3	1:D:605:LEU:HD11	1.88	0.56
1:B:537:ARG:HH12	1:B:549:PHE:HE2	1.54	0.56
1:A:571:GLN:HB3	1:A:605:LEU:HD11	1.88	0.56
1:D:143:GLU:OE1	1:D:210:ASN:ND2	2.38	0.55
1:D:655:ALA:O	1:D:661:ASN:ND2	2.38	0.55
1:C:13:ASP:OD1	1:C:226:TRP:N	2.40	0.55
1:B:1985:GLN:NE2	1:B:2043:TYR:O	2.38	0.55
1:A:888:THR:HG21	1:A:981:ILE:HD13	1.88	0.55
1:A:1985:GLN:NE2	1:A:2043:TYR:O	2.38	0.55
1:D:2418:PHE:HE2	2:D:2804:PLX:H301	1.72	0.55
2:D:2801:PLX:H251	2:D:2801:PLX:H72	1.89	0.55
1:C:888:THR:HG21	1:C:981:ILE:HD13	1.88	0.55
1:A:1808:VAL:HG11	1:A:1828:ALA:HB2	1.87	0.55
1:C:389:ARG:NH2	1:C:426:ASP:OD1	2.40	0.55
1:D:888:THR:HG21	1:D:981:ILE:HD13	1.88	0.55
1:B:264:LEU:HD12	1:B:416:LEU:HD21	1.89	0.55
1:A:304:ARG:NH1	1:A:361:GLY:O	2.40	0.55
1:A:389:ARG:NH2	1:A:426:ASP:OD1	2.40	0.55
1:C:304:ARG:NH1	1:C:361:GLY:O	2.40	0.55
1:B:389:ARG:NH2	1:B:426:ASP:OD1	2.40	0.55
1:B:655:ALA:O	1:B:661:ASN:ND2	2.38	0.55
1:A:2049:HIS:O	1:A:2053:ASN:ND2	2.40	0.55
1:D:389:ARG:NH2	1:D:426:ASP:OD1	2.40	0.55
1:C:2049:HIS:O	1:C:2053:ASN:ND2	2.40	0.55
1:B:2180:VAL:HG12	1:B:2182:GLY:H	1.72	0.55
1:D:2049:HIS:O	1:D:2053:ASN:ND2	2.40	0.55
1:C:264:LEU:HD12	1:C:416:LEU:HD21	1.89	0.55
1:C:2180:VAL:HG12	1:C:2182:GLY:H	1.72	0.55
1:B:571:GLN:HB3	1:B:605:LEU:HD11	1.88	0.54
2:C:2802:PLX:H72	2:C:2802:PLX:H251	1.89	0.54
1:B:304:ARG:NH1	1:B:361:GLY:O	2.40	0.54
1:B:2049:HIS:O	1:B:2053:ASN:ND2	2.40	0.54
1:D:2448:ALA:HB2	1:D:2581:VAL:HG11	1.89	0.54
1:A:655:ALA:O	1:A:661:ASN:ND2	2.38	0.54
1:A:2180:VAL:HG12	1:A:2182:GLY:H	1.72	0.54
1:D:264:LEU:HD12	1:D:416:LEU:HD21	1.89	0.54
1:D:304:ARG:NH1	1:D:361:GLY:O	2.40	0.54
1:B:888:THR:HG21	1:B:981:ILE:HD13	1.88	0.54
1:B:2418:PHE:HE2	2:B:2808:PLX:H301	1.72	0.54
1:A:13:ASP:OD1	1:A:226:TRP:N	2.40	0.54
2:B:2805:PLX:H72	2:B:2805:PLX:H251	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:CYS:SG	1:C:254:ASP:N	2.81	0.54
1:D:13:ASP:OD1	1:D:226:TRP:N	2.40	0.54
1:C:2283:LEU:HD11	1:C:2357:LEU:HD22	1.90	0.54
1:A:2409:HIS:CD2	2:A:2803:PLX:C4	2.90	0.54
1:D:253:CYS:SG	1:D:254:ASP:N	2.81	0.54
1:C:2448:ALA:HB2	1:C:2581:VAL:HG11	1.89	0.54
1:A:2448:ALA:HB2	1:A:2581:VAL:HG11	1.89	0.54
1:B:2283:LEU:HD11	1:B:2357:LEU:HD22	1.90	0.53
1:A:302:LEU:HB3	1:A:367:ILE:HD11	1.91	0.53
1:B:13:ASP:OD1	1:B:226:TRP:N	2.40	0.53
1:A:1073:PRO:HB2	1:A:1075:LEU:H	1.72	0.53
1:A:1306:VAL:HG21	1:A:1370:PRO:HD2	1.90	0.53
1:D:2180:VAL:HG12	1:D:2182:GLY:H	1.72	0.53
1:B:1306:VAL:HG21	1:B:1370:PRO:HD2	1.90	0.53
1:B:1989:ARG:HH21	1:B:2050:GLU:HG3	1.74	0.53
1:A:1989:ARG:HH21	1:A:2050:GLU:HG3	1.74	0.53
1:D:1073:PRO:HB2	1:D:1075:LEU:H	1.72	0.53
1:C:1989:ARG:HH21	1:C:2050:GLU:HG3	1.74	0.53
1:C:2409:HIS:CE1	2:C:2804:PLX:O8	2.61	0.53
1:A:264:LEU:HD12	1:A:416:LEU:HD21	1.89	0.53
1:A:982:LEU:HD23	1:A:985:ARG:HD3	1.91	0.53
1:C:674:ARG:NH1	1:C:693:GLU:O	2.42	0.53
1:B:1073:PRO:HB2	1:B:1075:LEU:H	1.72	0.53
1:D:2283:LEU:HD11	1:D:2357:LEU:HD22	1.90	0.53
1:B:302:LEU:HB3	1:B:367:ILE:HD11	1.91	0.53
1:A:702:ASP:OD2	1:A:708:ARG:NH2	2.42	0.53
1:A:2378:THR:HA	1:A:2381:ARG:HE	1.73	0.53
1:C:1073:PRO:HB2	1:C:1075:LEU:H	1.72	0.53
1:B:702:ASP:OD2	1:B:708:ARG:NH2	2.42	0.53
1:B:982:LEU:HD23	1:B:985:ARG:HD3	1.91	0.53
1:A:253:CYS:SG	1:A:254:ASP:N	2.81	0.53
1:A:2283:LEU:HD11	1:A:2357:LEU:HD22	1.90	0.53
1:D:302:LEU:HB3	1:D:367:ILE:HD11	1.91	0.53
1:D:2074:ILE:HG22	1:D:2076:PRO:HD2	1.91	0.53
1:C:1242:GLN:HE21	1:C:1275:HIS:HB3	1.73	0.53
1:B:1002:ASP:HA	1:B:1005:ASN:HB2	1.91	0.53
1:B:2074:ILE:HG22	1:B:2076:PRO:HD2	1.91	0.53
1:A:1002:ASP:HA	1:A:1005:ASN:HB2	1.91	0.53
1:A:1242:GLN:HE21	1:A:1275:HIS:HB3	1.73	0.53
1:A:1316:VAL:HG11	1:A:1330:VAL:HB	1.91	0.53
1:D:1316:VAL:HG11	1:D:1330:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1989:ARG:HH21	1:D:2050:GLU:HG3	1.74	0.53
1:C:982:LEU:HD23	1:C:985:ARG:HD3	1.91	0.53
1:C:2071:LEU:HD11	1:C:2116:MET:HG3	1.91	0.53
1:B:674:ARG:NH1	1:B:693:GLU:O	2.42	0.53
1:A:390:LEU:HD22	1:A:430:PHE:HZ	1.74	0.53
1:D:702:ASP:OD2	1:D:708:ARG:NH2	2.42	0.53
1:D:982:LEU:HD23	1:D:985:ARG:HD3	1.91	0.53
1:C:1306:VAL:HG21	1:C:1370:PRO:HD2	1.90	0.53
1:C:2074:ILE:HG22	1:C:2076:PRO:HD2	1.91	0.53
1:C:2378:THR:HA	1:C:2381:ARG:HE	1.73	0.53
1:B:253:CYS:SG	1:B:254:ASP:N	2.81	0.53
1:B:2448:ALA:HB2	1:B:2581:VAL:HG11	1.89	0.53
1:A:2071:LEU:HD11	1:A:2116:MET:HG3	1.91	0.52
1:D:811:PRO:HG3	1:D:998:LYS:HE2	1.92	0.52
1:D:1242:GLN:HE21	1:D:1275:HIS:HB3	1.73	0.52
1:D:1306:VAL:HG21	1:D:1370:PRO:HD2	1.90	0.52
1:D:2008:ASP:HA	1:D:2065:ILE:HD13	1.91	0.52
1:C:702:ASP:OD2	1:C:708:ARG:NH2	2.42	0.52
1:C:2008:ASP:HA	1:C:2065:ILE:HD13	1.91	0.52
1:B:811:PRO:HG3	1:B:998:LYS:HE2	1.92	0.52
1:B:2071:LEU:HD11	1:B:2116:MET:HG3	1.91	0.52
1:D:674:ARG:NH1	1:D:693:GLU:O	2.42	0.52
1:B:2008:ASP:HA	1:B:2065:ILE:HD13	1.91	0.52
1:D:2071:LEU:HD11	1:D:2116:MET:HG3	1.91	0.52
1:D:1002:ASP:HA	1:D:1005:ASN:HB2	1.91	0.52
1:D:1318:ALA:HA	1:D:1322:PHE:HB2	1.92	0.52
1:C:1316:VAL:HG11	1:C:1330:VAL:HB	1.91	0.52
1:A:811:PRO:HG3	1:A:998:LYS:HE2	1.92	0.52
1:A:1252:GLN:NE2	1:A:1276:ILE:O	2.43	0.52
1:A:2018:LEU:O	1:A:2072:ASN:ND2	2.43	0.52
1:C:302:LEU:HB3	1:C:367:ILE:HD11	1.91	0.52
1:C:2066:ILE:HG12	1:C:2095:LEU:HD22	1.91	0.52
1:B:390:LEU:HD22	1:B:430:PHE:HZ	1.74	0.52
1:B:1064:LEU:HD21	1:B:1082:LEU:HD23	1.92	0.52
1:D:2018:LEU:O	1:D:2072:ASN:ND2	2.43	0.52
1:D:2263:GLN:HB3	1:D:2266:LEU:HB3	1.92	0.52
1:D:2378:THR:HA	1:D:2381:ARG:HE	1.73	0.52
1:C:390:LEU:HD22	1:C:430:PHE:HZ	1.74	0.52
1:C:811:PRO:HG3	1:C:998:LYS:HE2	1.92	0.52
1:B:2378:THR:HA	1:B:2381:ARG:HE	1.73	0.52
1:A:674:ARG:NH1	1:A:693:GLU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2074:ILE:HG22	1:A:2076:PRO:HD2	1.91	0.52
1:D:1809:ILE:HG21	1:D:1846:ARG:HG2	1.92	0.52
1:D:2066:ILE:HG12	1:D:2095:LEU:HD22	1.91	0.52
1:C:400:HIS:HB2	1:C:428:GLU:HG3	1.92	0.52
1:C:2263:GLN:HB3	1:C:2266:LEU:HB3	1.92	0.52
1:A:2066:ILE:HG12	1:A:2095:LEU:HD22	1.91	0.52
1:C:1064:LEU:HD21	1:C:1082:LEU:HD23	1.92	0.52
1:C:1809:ILE:HG21	1:C:1846:ARG:HG2	1.92	0.52
1:B:1242:GLN:HE21	1:B:1275:HIS:HB3	1.73	0.52
1:B:2066:ILE:HG12	1:B:2095:LEU:HD22	1.91	0.52
1:D:390:LEU:HD22	1:D:430:PHE:HZ	1.74	0.51
1:B:1316:VAL:HG11	1:B:1330:VAL:HB	1.91	0.51
1:A:1809:ILE:HG21	1:A:1846:ARG:HG2	1.92	0.51
1:A:2008:ASP:HA	1:A:2065:ILE:HD13	1.91	0.51
1:C:1252:GLN:NE2	1:C:1276:ILE:O	2.43	0.51
1:B:2018:LEU:O	1:B:2072:ASN:ND2	2.43	0.51
1:C:1318:ALA:HA	1:C:1322:PHE:HB2	1.92	0.51
1:B:2263:GLN:HB3	1:B:2266:LEU:HB3	1.92	0.51
1:B:2409:HIS:NE2	2:B:2807:PLX:C5	2.51	0.51
1:A:1064:LEU:HD21	1:A:1082:LEU:HD23	1.92	0.51
1:D:1252:GLN:NE2	1:D:1276:ILE:O	2.43	0.51
1:B:1252:GLN:NE2	1:B:1276:ILE:O	2.43	0.51
1:B:1809:ILE:HG21	1:B:1846:ARG:HG2	1.92	0.51
1:C:1002:ASP:HA	1:C:1005:ASN:HB2	1.91	0.51
1:C:2018:LEU:O	1:C:2072:ASN:ND2	2.43	0.51
1:B:400:HIS:HB2	1:B:428:GLU:HG3	1.92	0.51
1:A:1318:ALA:HA	1:A:1322:PHE:HB2	1.92	0.51
1:B:1125:ILE:HG22	1:B:1172:ASN:HB2	1.93	0.51
1:A:2263:GLN:HB3	1:A:2266:LEU:HB3	1.92	0.51
1:D:400:HIS:HB2	1:D:428:GLU:HG3	1.92	0.51
1:A:400:HIS:HB2	1:A:428:GLU:HG3	1.92	0.50
1:A:1064:LEU:HB3	1:A:1083:LEU:HD12	1.94	0.50
1:D:1064:LEU:HD21	1:D:1082:LEU:HD23	1.92	0.50
1:D:1064:LEU:HB3	1:D:1083:LEU:HD12	1.94	0.50
1:D:1125:ILE:HG22	1:D:1172:ASN:HB2	1.93	0.50
1:B:871:ARG:HD3	1:B:973:LYS:HE2	1.94	0.50
1:B:1064:LEU:HB3	1:B:1083:LEU:HD12	1.94	0.50
1:B:1318:ALA:HA	1:B:1322:PHE:HB2	1.92	0.50
1:C:1064:LEU:HB3	1:C:1083:LEU:HD12	1.94	0.50
1:A:871:ARG:HD3	1:A:973:LYS:HE2	1.94	0.50
1:C:871:ARG:HD3	1:C:973:LYS:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:871:ARG:HD3	1:D:973:LYS:HE2	1.94	0.49
1:D:2067:THR:OG1	1:D:2116:MET:SD	2.63	0.49
1:C:1125:ILE:HG22	1:C:1172:ASN:HB2	1.93	0.49
1:A:615:ILE:O	1:A:619:VAL:N	2.44	0.49
1:A:1125:ILE:HG22	1:A:1172:ASN:HB2	1.93	0.49
1:C:738:ASN:OD1	1:C:783:ARG:NH1	2.45	0.49
1:C:2613:ILE:H	1:C:2613:ILE:HD12	1.78	0.49
1:C:2213:PRO:HG2	1:C:2646:VAL:HG23	1.94	0.49
1:B:2067:THR:OG1	1:B:2116:MET:SD	2.63	0.49
1:A:2544:ARG:NH2	1:B:2570:ASP:CG	2.60	0.49
1:D:2213:PRO:HG2	1:D:2646:VAL:HG23	1.94	0.49
1:D:2627:THR:OG1	1:D:2630:GLU:OE1	2.31	0.49
1:D:738:ASN:OD1	1:D:783:ARG:NH1	2.45	0.49
1:D:783:ARG:NH2	1:D:865:GLU:OE2	2.46	0.49
1:D:863:THR:HA	1:D:866:VAL:HG12	1.95	0.49
1:D:2575:PHE:HD2	2:D:2807:PLX:C36	2.26	0.49
1:C:863:THR:HA	1:C:866:VAL:HG12	1.95	0.49
1:C:2131:GLN:HG2	1:C:2149:PRO:HG2	1.94	0.49
1:B:1191:SER:OG	1:B:1195:ARG:NH2	2.46	0.49
1:A:1191:SER:OG	1:A:1195:ARG:NH2	2.46	0.49
1:C:2067:THR:OG1	1:C:2116:MET:SD	2.63	0.49
1:B:194:HIS:HA	1:B:216:THR:HG21	1.94	0.49
1:A:738:ASN:OD1	1:A:783:ARG:NH1	2.45	0.49
2:A:2801:PLX:H72	2:A:2801:PLX:H251	1.94	0.49
1:D:2613:ILE:HD12	1:D:2613:ILE:H	1.78	0.49
1:C:971:LYS:HA	1:C:974:ILE:HG12	1.95	0.49
1:A:863:THR:HA	1:A:866:VAL:HG12	1.95	0.48
1:A:971:LYS:HA	1:A:974:ILE:HG12	1.95	0.48
1:D:2131:GLN:HG2	1:D:2149:PRO:HG2	1.94	0.48
1:A:194:HIS:HA	1:A:216:THR:HG21	1.94	0.48
1:A:783:ARG:NH2	1:A:865:GLU:OE2	2.46	0.48
1:D:194:HIS:HA	1:D:216:THR:HG21	1.94	0.48
1:B:2613:ILE:HD12	1:B:2613:ILE:H	1.78	0.48
1:A:1881:ASP:OD1	1:A:1881:ASP:N	2.46	0.48
1:A:2432:LYS:HA	1:A:2435:THR:HG22	1.96	0.48
1:D:1191:SER:OG	1:D:1195:ARG:NH2	2.46	0.48
1:C:194:HIS:HA	1:C:216:THR:HG21	1.94	0.48
1:B:600:HIS:CG	1:B:601:ASN:H	2.31	0.48
1:B:863:THR:HA	1:B:866:VAL:HG12	1.95	0.48
1:A:600:HIS:CG	1:A:601:ASN:H	2.31	0.48
1:A:2213:PRO:HG2	1:A:2646:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2613:ILE:HD12	1:A:2613:ILE:H	1.78	0.48
1:D:971:LYS:HA	1:D:974:ILE:HG12	1.95	0.48
1:D:2726:GLN:OE1	1:D:2729:GLN:NE2	2.47	0.48
1:C:600:HIS:CG	1:C:601:ASN:H	2.31	0.48
1:C:783:ARG:NH2	1:C:865:GLU:OE2	2.46	0.48
1:C:1191:SER:OG	1:C:1195:ARG:NH2	2.46	0.48
1:B:2131:GLN:HG2	1:B:2149:PRO:HG2	1.94	0.48
1:B:2213:PRO:HG2	1:B:2646:VAL:HG23	1.94	0.48
1:B:2726:GLN:OE1	1:B:2729:GLN:NE2	2.46	0.48
1:A:2726:GLN:OE1	1:A:2729:GLN:NE2	2.46	0.48
1:B:971:LYS:HA	1:B:974:ILE:HG12	1.95	0.48
1:B:2627:THR:OG1	1:B:2630:GLU:OE1	2.31	0.48
1:B:738:ASN:OD1	1:B:783:ARG:NH1	2.45	0.48
1:A:2131:GLN:HG2	1:A:2149:PRO:HG2	1.94	0.48
1:D:600:HIS:CG	1:D:601:ASN:H	2.31	0.48
1:B:783:ARG:NH2	1:B:865:GLU:OE2	2.46	0.48
1:B:856:ASP:OD1	1:B:856:ASP:N	2.47	0.48
1:D:2432:LYS:HA	1:D:2435:THR:HG22	1.96	0.48
1:C:138:LEU:HD23	1:C:148:ARG:HH22	1.79	0.48
1:D:2413:TYR:HA	1:D:2416:LEU:HG	1.96	0.47
1:C:2726:GLN:OE1	1:C:2729:GLN:NE2	2.46	0.47
1:B:702:ASP:OD1	1:B:702:ASP:N	2.47	0.47
1:A:138:LEU:HD23	1:A:148:ARG:HH22	1.79	0.47
1:D:456:ILE:HD13	1:D:473:VAL:HB	1.96	0.47
1:C:2409:HIS:CD2	2:C:2804:PLX:C4	2.97	0.47
1:B:1976:LEU:HD23	1:B:1988:LEU:HD11	1.96	0.47
1:A:702:ASP:OD1	1:A:702:ASP:N	2.47	0.47
1:C:2627:THR:OG1	1:C:2630:GLU:OE1	2.31	0.47
1:B:789:HIS:CD2	1:B:790:VAL:HG13	2.49	0.47
1:A:856:ASP:N	1:A:856:ASP:OD1	2.47	0.47
1:D:2724:THR:HG21	1:C:2720:LYS:NZ	2.29	0.47
1:C:789:HIS:CD2	1:C:790:VAL:HG13	2.49	0.47
1:C:2698:LEU:HA	1:C:2701:LYS:HE2	1.97	0.47
1:B:2432:LYS:HA	1:B:2435:THR:HG22	1.95	0.47
1:A:456:ILE:HD13	1:A:473:VAL:HB	1.96	0.47
1:A:2557:SER:O	1:A:2557:SER:OG	2.31	0.47
1:C:2413:TYR:HA	1:C:2416:LEU:HG	1.96	0.47
1:A:2627:THR:OG1	1:A:2630:GLU:OE1	2.31	0.47
1:A:2724:THR:HG21	1:D:2720:LYS:NZ	2.30	0.47
1:D:2698:LEU:HA	1:D:2701:LYS:HE2	1.97	0.47
1:C:64:ASN:HD22	1:C:122:GLN:HE21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2697:ASN:O	1:B:2700:GLU:HG3	2.15	0.47
1:A:160:TRP:HE3	1:A:187:VAL:HG11	1.80	0.47
1:A:789:HIS:CD2	1:A:790:VAL:HG13	2.49	0.47
1:A:2697:ASN:O	1:A:2700:GLU:HG3	2.15	0.47
1:D:138:LEU:HD23	1:D:148:ARG:HH22	1.79	0.47
1:D:641:MET:HG3	1:D:642:ASN:H	1.80	0.47
1:D:789:HIS:CD2	1:D:790:VAL:HG13	2.49	0.47
1:C:1976:LEU:HD23	1:C:1988:LEU:HD11	1.96	0.47
1:C:2432:LYS:HA	1:C:2435:THR:HG22	1.96	0.47
1:B:1982:ARG:NH1	1:B:2047:PRO:O	2.48	0.47
1:D:160:TRP:HE3	1:D:187:VAL:HG11	1.80	0.47
1:D:1881:ASP:OD1	1:D:1881:ASP:N	2.46	0.47
1:C:856:ASP:OD1	1:C:856:ASP:N	2.47	0.47
1:B:456:ILE:HD13	1:B:473:VAL:HB	1.96	0.47
1:C:2724:THR:HG21	1:B:2720:LYS:NZ	2.29	0.47
1:B:2698:LEU:HA	1:B:2701:LYS:HE2	1.97	0.47
2:A:2803:PLX:H1A2	2:A:2803:PLX:H21	1.75	0.47
1:C:1982:ARG:NH1	1:C:2047:PRO:O	2.48	0.47
1:C:641:MET:HG3	1:C:642:ASN:H	1.80	0.46
1:A:147:MET:HB3	1:A:211:SER:HB3	1.98	0.46
1:D:64:ASN:HD22	1:D:122:GLN:HE21	1.63	0.46
1:D:117:TYR:OH	1:D:180:ASP:OD2	2.34	0.46
1:D:147:MET:HB3	1:D:211:SER:HB3	1.98	0.46
1:C:2697:ASN:O	1:C:2700:GLU:HG3	2.15	0.46
1:B:2413:TYR:HA	1:B:2416:LEU:HG	1.96	0.46
1:A:2413:TYR:HA	1:A:2416:LEU:HG	1.96	0.46
1:C:117:TYR:OH	1:C:180:ASP:OD2	2.34	0.46
1:C:2409:HIS:ND1	2:C:2804:PLX:O8	2.47	0.46
1:B:160:TRP:HE3	1:B:187:VAL:HG11	1.80	0.46
1:A:1301:THR:HB	1:B:138:LEU:HG	1.97	0.46
1:A:1976:LEU:HD23	1:A:1988:LEU:HD11	1.96	0.46
1:D:2409:HIS:CD2	2:D:2803:PLX:C4	2.97	0.46
1:C:160:TRP:HE3	1:C:187:VAL:HG11	1.80	0.46
1:C:1373:MET:O	1:C:1377:HIS:N	2.48	0.46
1:B:138:LEU:HD23	1:B:148:ARG:HH22	1.79	0.46
1:A:2698:LEU:HA	1:A:2701:LYS:HE2	1.97	0.46
1:B:147:MET:HB3	1:B:211:SER:HB3	1.98	0.46
1:C:316:ALA:HB2	1:C:355:LEU:HD23	1.98	0.46
1:C:456:ILE:HD13	1:C:473:VAL:HB	1.96	0.46
1:C:702:ASP:OD1	1:C:702:ASP:N	2.47	0.46
1:A:747:ARG:NH1	1:A:749:TYR:OH	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2618:ARG:HH21	1:B:2236:GLN:HG3	1.81	0.46
1:A:2720:LYS:NZ	1:B:2724:THR:HG21	2.30	0.46
1:C:1117:GLN:NE2	1:C:1118:ASP:OD1	2.49	0.46
1:C:2409:HIS:NE2	2:C:2804:PLX:C5	2.70	0.46
1:C:2570:ASP:CG	1:B:2544:ARG:NH2	2.61	0.46
2:C:2802:PLX:H252	2:C:2803:PLX:H72	1.97	0.46
1:A:1073:PRO:HG2	1:A:1076:VAL:H	1.81	0.46
1:D:1685:LYS:HG2	1:D:1686:ASP:H	1.81	0.46
1:D:2570:ASP:CG	1:C:2544:ARG:NH2	2.61	0.46
1:B:117:TYR:OH	1:B:180:ASP:OD2	2.34	0.46
1:B:745:LEU:HA	1:B:787:HIS:HB3	1.98	0.46
1:A:117:TYR:OH	1:A:180:ASP:OD2	2.34	0.46
1:D:889:LYS:HD2	1:D:890:ILE:HG23	1.98	0.46
1:D:1976:LEU:HD23	1:D:1988:LEU:HD11	1.96	0.46
1:D:2697:ASN:O	1:D:2700:GLU:HG3	2.15	0.46
2:D:2801:PLX:H252	2:D:2802:PLX:H72	1.96	0.46
1:C:138:LEU:HG	1:B:1301:THR:HB	1.98	0.46
1:C:147:MET:HB3	1:C:211:SER:HB3	1.98	0.46
1:C:745:LEU:HA	1:C:787:HIS:HB3	1.98	0.46
2:B:2805:PLX:H252	2:B:2806:PLX:H72	1.98	0.46
1:A:742:ARG:HA	1:A:745:LEU:HD23	1.98	0.46
1:A:1685:LYS:HG2	1:A:1686:ASP:H	1.81	0.46
1:D:1982:ARG:NH1	1:D:2047:PRO:O	2.48	0.46
1:C:1956:ASP:OD1	1:C:1956:ASP:N	2.49	0.46
1:B:747:ARG:NH1	1:B:749:TYR:OH	2.49	0.46
1:B:1117:GLN:NE2	1:B:1118:ASP:OD1	2.49	0.46
1:A:1125:ILE:HD12	1:A:1176:VAL:HG22	1.98	0.45
1:A:1373:MET:O	1:A:1377:HIS:N	2.48	0.45
1:A:2236:GLN:HG3	1:D:2618:ARG:HH21	1.81	0.45
1:D:316:ALA:HB2	1:D:355:LEU:HD23	1.98	0.45
1:C:1685:LYS:HG2	1:C:1686:ASP:H	1.81	0.45
1:C:2226:ARG:O	1:C:2230:THR:OG1	2.32	0.45
1:B:64:ASN:HD22	1:B:122:GLN:HE21	1.63	0.45
1:B:1125:ILE:HD12	1:B:1176:VAL:HG22	1.98	0.45
1:A:316:ALA:HB2	1:A:355:LEU:HD23	1.98	0.45
1:A:641:MET:HG3	1:A:642:ASN:H	1.80	0.45
1:A:889:LYS:HD2	1:A:890:ILE:HG23	1.98	0.45
1:D:39:VAL:HG21	1:D:195:ALA:HB1	1.98	0.45
1:D:856:ASP:OD1	1:D:856:ASP:N	2.47	0.45
1:C:889:LYS:HD2	1:C:890:ILE:HG23	1.98	0.45
1:B:889:LYS:HD2	1:B:890:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1073:PRO:HG2	1:B:1076:VAL:H	1.81	0.45
1:A:64:ASN:HD22	1:A:122:GLN:HE21	1.63	0.45
1:D:564:GLN:NE2	1:D:574:ILE:HD12	2.32	0.45
1:D:1956:ASP:N	1:D:1956:ASP:OD1	2.49	0.45
1:D:1117:GLN:NE2	1:D:1118:ASP:OD1	2.49	0.45
1:D:1327:GLN:HA	1:D:1330:VAL:HG12	1.99	0.45
1:C:1327:GLN:HA	1:C:1330:VAL:HG12	1.99	0.45
1:B:742:ARG:HA	1:B:745:LEU:HD23	1.98	0.45
1:B:1034:GLU:OE2	1:B:1732:ARG:NH1	2.50	0.45
1:B:1806:ASN:HA	1:B:1809:ILE:HG22	1.99	0.45
1:A:442:ASP:HB2	1:A:483:PHE:HE1	1.82	0.45
1:D:442:ASP:HB2	1:D:483:PHE:HE1	1.82	0.45
1:D:742:ARG:HA	1:D:745:LEU:HD23	1.98	0.45
1:D:1393:THR:HB	1:D:1396:LYS:HB3	1.99	0.45
1:B:641:MET:HG3	1:B:642:ASN:H	1.80	0.45
1:A:564:GLN:NE2	1:A:574:ILE:HD12	2.32	0.45
1:C:1393:THR:HB	1:C:1396:LYS:HB3	1.99	0.45
1:A:1393:THR:HB	1:A:1396:LYS:HB3	1.99	0.45
1:A:1982:ARG:NH1	1:A:2047:PRO:O	2.48	0.45
1:D:138:LEU:HG	1:C:1301:THR:HB	1.98	0.45
1:C:39:VAL:HG21	1:C:195:ALA:HB1	1.98	0.45
1:C:442:ASP:HB2	1:C:483:PHE:HE1	1.82	0.45
1:C:742:ARG:HA	1:C:745:LEU:HD23	1.98	0.45
1:C:1034:GLU:OE2	1:C:1732:ARG:NH1	2.50	0.45
1:C:1125:ILE:HD12	1:C:1176:VAL:HG22	1.98	0.45
1:C:2236:GLN:HG3	1:B:2618:ARG:HH21	1.81	0.45
2:C:2804:PLX:H21	2:C:2804:PLX:H1A2	1.77	0.45
1:B:2557:SER:O	1:B:2557:SER:OG	2.31	0.45
2:B:2802:PLX:H252	2:B:2802:PLX:H51	1.72	0.45
1:A:1034:GLU:OE2	1:A:1732:ARG:NH1	2.50	0.45
1:D:1080:LEU:HD22	1:D:1671:LEU:HD21	1.99	0.45
1:D:1806:ASN:HA	1:D:1809:ILE:HG22	1.99	0.45
1:D:2409:HIS:CE1	2:D:2803:PLX:O8	2.70	0.45
1:B:442:ASP:HB2	1:B:483:PHE:HE1	1.82	0.45
1:B:564:GLN:NE2	1:B:574:ILE:HD12	2.32	0.45
1:B:1881:ASP:OD1	1:B:1881:ASP:N	2.46	0.45
1:D:1034:GLU:OE2	1:D:1732:ARG:NH1	2.50	0.45
1:D:1073:PRO:HG2	1:D:1076:VAL:H	1.81	0.45
1:D:2288:ASN:HA	1:D:2291:VAL:HG12	1.99	0.45
1:B:372:PRO:HG2	1:B:375:LEU:HD23	1.99	0.45
1:B:628:PRO:HB2	1:B:735:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:GLN:HA	1:B:1330:VAL:HG12	1.99	0.45
1:A:745:LEU:HA	1:A:787:HIS:HB3	1.98	0.45
1:A:1327:GLN:HA	1:A:1330:VAL:HG12	1.99	0.45
1:D:747:ARG:NH1	1:D:749:TYR:OH	2.49	0.45
1:D:1125:ILE:HD12	1:D:1176:VAL:HG22	1.98	0.45
1:C:564:GLN:NE2	1:C:574:ILE:HD12	2.32	0.45
1:B:39:VAL:HG21	1:B:195:ALA:HB1	1.98	0.45
1:B:2288:ASN:HA	1:B:2291:VAL:HG12	1.99	0.45
1:A:1117:GLN:NE2	1:A:1118:ASP:OD1	2.49	0.44
1:D:372:PRO:HG2	1:D:375:LEU:HD23	1.99	0.44
1:C:1664:LEU:HD12	1:C:1811:LEU:HD12	2.00	0.44
1:B:1080:LEU:HD22	1:B:1671:LEU:HD21	1.99	0.44
1:B:1685:LYS:HG2	1:B:1686:ASP:H	1.81	0.44
1:A:138:LEU:HG	1:D:1301:THR:HB	1.98	0.44
1:D:745:LEU:HA	1:D:787:HIS:HB3	1.98	0.44
1:D:1955:ASP:OD1	1:D:1955:ASP:N	2.51	0.44
1:D:2236:GLN:HG3	1:C:2618:ARG:HH21	1.81	0.44
1:C:1881:ASP:N	1:C:1881:ASP:OD1	2.46	0.44
1:B:600:HIS:CD2	1:B:601:ASN:H	2.35	0.44
1:A:372:PRO:HG2	1:A:375:LEU:HD23	1.99	0.44
1:A:1080:LEU:HD22	1:A:1671:LEU:HD21	1.99	0.44
1:A:2409:HIS:NE2	2:A:2803:PLX:C5	2.61	0.44
1:D:600:HIS:CD2	1:D:601:ASN:H	2.35	0.44
1:D:2033:ILE:HA	1:D:2036:THR:HG22	2.00	0.44
2:D:2803:PLX:H1A2	2:D:2803:PLX:H21	1.77	0.44
1:C:372:PRO:HG2	1:C:375:LEU:HD23	1.99	0.44
1:C:2288:ASN:HA	1:C:2291:VAL:HG12	1.99	0.44
1:B:316:ALA:HB2	1:B:355:LEU:HD23	1.98	0.44
1:B:1664:LEU:HD12	1:B:1811:LEU:HD12	2.00	0.44
1:A:1806:ASN:HA	1:A:1809:ILE:HG22	1.99	0.44
1:D:1214:VAL:HG21	1:D:1240:PHE:HE2	1.83	0.44
1:C:526:PRO:HA	1:C:529:ASP:HB3	1.99	0.44
1:C:1806:ASN:HA	1:C:1809:ILE:HG22	1.99	0.44
2:C:2807:PLX:H1C2	2:C:2807:PLX:H21	1.79	0.44
1:B:1280:ASN:HD22	1:B:1283:LEU:HB2	1.83	0.44
1:B:1373:MET:O	1:B:1377:HIS:N	2.48	0.44
1:B:2167:ASN:HD22	1:B:2170:LEU:HB2	1.83	0.44
1:A:2288:ASN:HA	1:A:2291:VAL:HG12	1.99	0.44
1:D:1664:LEU:HD12	1:D:1811:LEU:HD12	2.00	0.44
1:D:1865:LYS:HD2	1:D:1868:GLN:HE21	1.83	0.44
1:B:1393:THR:HB	1:B:1396:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:PRO:HA	1:A:529:ASP:HB3	1.99	0.44
1:A:600:HIS:CD2	1:A:601:ASN:H	2.35	0.44
1:A:628:PRO:HB2	1:A:735:TYR:HD2	1.82	0.44
1:D:194:HIS:CD2	1:D:212:VAL:HG22	2.53	0.44
1:C:600:HIS:CD2	1:C:601:ASN:H	2.35	0.44
1:C:1214:VAL:HG21	1:C:1240:PHE:HE2	1.83	0.44
1:C:1280:ASN:HD22	1:C:1283:LEU:HB2	1.83	0.44
1:C:2127:LYS:HA	1:C:2130:MET:SD	2.58	0.44
1:B:2033:ILE:HA	1:B:2036:THR:HG22	2.00	0.44
1:B:2127:LYS:HA	1:B:2130:MET:SD	2.58	0.44
1:A:2127:LYS:HA	1:A:2130:MET:SD	2.58	0.44
1:A:2729:GLN:HA	1:A:2732:ARG:HG3	2.00	0.44
1:D:628:PRO:HB2	1:D:735:TYR:HD2	1.82	0.44
1:C:1080:LEU:HD22	1:C:1671:LEU:HD21	1.99	0.44
1:C:2033:ILE:HA	1:C:2036:THR:HG22	2.00	0.44
1:A:39:VAL:HG21	1:A:195:ALA:HB1	1.98	0.44
1:A:2033:ILE:HA	1:A:2036:THR:HG22	2.00	0.44
1:A:2363:CYS:HA	1:A:2366:ILE:HG22	2.00	0.44
1:D:1373:MET:O	1:D:1377:HIS:N	2.48	0.44
1:C:194:HIS:CD2	1:C:212:VAL:HG22	2.53	0.44
1:C:615:ILE:O	1:C:619:VAL:N	2.44	0.44
1:B:1088:SER:O	1:B:1088:SER:OG	2.36	0.44
1:A:791:ASP:N	1:A:791:ASP:OD1	2.51	0.44
1:D:2127:LYS:HA	1:D:2130:MET:SD	2.58	0.44
1:C:791:ASP:N	1:C:791:ASP:OD1	2.51	0.44
1:C:2154:HIS:CD2	1:C:2211:PRO:HB3	2.53	0.44
1:B:2154:HIS:CD2	1:B:2211:PRO:HB3	2.53	0.44
1:A:194:HIS:CD2	1:A:212:VAL:HG22	2.53	0.43
1:A:1956:ASP:N	1:A:1956:ASP:OD1	2.49	0.43
1:D:884:LEU:HD12	1:D:981:ILE:HG22	2.00	0.43
1:C:133:THR:HG21	1:C:156:ASN:HB3	2.00	0.43
1:C:2037:LEU:O	1:C:2041:THR:HG23	2.18	0.43
2:C:2803:PLX:H1B2	2:C:2803:PLX:H21	1.73	0.43
2:C:2807:PLX:H252	2:C:2807:PLX:H51	1.87	0.43
1:B:1955:ASP:N	1:B:1955:ASP:OD1	2.51	0.43
1:B:2394:TYR:HB2	2:B:2808:PLX:H81	2.00	0.43
1:A:1408:ARG:O	1:A:1412:HIS:ND1	2.51	0.43
1:A:1865:LYS:HD2	1:A:1868:GLN:HE21	1.83	0.43
1:A:2067:THR:OG1	1:A:2116:MET:SD	2.63	0.43
2:A:2802:PLX:H262	2:A:2802:PLX:H291	1.67	0.43
1:D:300:ASN:ND2	1:D:378:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:526:PRO:HA	1:D:529:ASP:HB3	1.99	0.43
1:D:2394:TYR:HB2	2:D:2804:PLX:H81	2.01	0.43
1:C:1300:GLU:OE2	1:C:1337:SER:OG	2.30	0.43
1:A:1214:VAL:HG21	1:A:1240:PHE:HE2	1.83	0.43
1:D:791:ASP:OD1	1:D:791:ASP:N	2.51	0.43
1:B:2055:ILE:HG22	1:B:2063:ILE:HD11	2.01	0.43
1:A:1664:LEU:HD12	1:A:1811:LEU:HD12	2.00	0.43
1:D:1280:ASN:HD22	1:D:1283:LEU:HB2	1.83	0.43
1:D:1391:VAL:HG22	1:D:1434:THR:HG21	2.01	0.43
1:D:2363:CYS:HA	1:D:2366:ILE:HG22	2.00	0.43
1:D:2729:GLN:HA	1:D:2732:ARG:HG3	2.00	0.43
1:C:2055:ILE:HG22	1:C:2063:ILE:HD11	2.01	0.43
1:C:2083:ASP:OD1	1:C:2083:ASP:N	2.51	0.43
2:C:2807:PLX:H322	2:C:2807:PLX:H351	1.86	0.43
1:B:1865:LYS:HD2	1:B:1868:GLN:HE21	1.83	0.43
1:B:1956:ASP:OD1	1:B:1956:ASP:N	2.49	0.43
1:A:2167:ASN:HD22	1:A:2170:LEU:HB2	1.83	0.43
1:D:2154:HIS:CD2	1:D:2211:PRO:HB3	2.53	0.43
1:D:2167:ASN:HD22	1:D:2170:LEU:HB2	1.83	0.43
1:C:1073:PRO:HG2	1:C:1076:VAL:H	1.81	0.43
1:C:2729:GLN:HA	1:C:2732:ARG:HG3	2.00	0.43
1:B:194:HIS:CD2	1:B:212:VAL:HG22	2.53	0.43
1:B:969:ASP:O	1:B:973:LYS:HG2	2.19	0.43
1:A:300:ASN:ND2	1:A:378:GLY:O	2.51	0.43
1:D:2037:LEU:O	1:D:2041:THR:HG23	2.18	0.43
1:D:2677:ARG:HD3	1:D:2677:ARG:HA	1.87	0.43
1:C:672:LEU:HA	1:C:695:GLU:HG3	2.01	0.43
1:C:969:ASP:O	1:C:973:LYS:HG2	2.19	0.43
1:C:1865:LYS:HD2	1:C:1868:GLN:HE21	1.83	0.43
1:C:1955:ASP:OD1	1:C:1955:ASP:N	2.51	0.43
2:C:2807:PLX:H111	2:C:2808:PLX:H141	2.01	0.43
1:B:884:LEU:HD12	1:B:981:ILE:HG22	2.00	0.43
1:B:1408:ARG:O	1:B:1412:HIS:ND1	2.51	0.43
1:A:884:LEU:HD12	1:A:981:ILE:HG22	2.00	0.43
1:A:1955:ASP:OD1	1:A:1955:ASP:N	2.51	0.43
1:A:2154:HIS:CD2	1:A:2211:PRO:HB3	2.53	0.43
1:D:969:ASP:O	1:D:973:LYS:HG2	2.19	0.43
1:D:2055:ILE:HG22	1:D:2063:ILE:HD11	2.01	0.43
1:D:2083:ASP:N	1:D:2083:ASP:OD1	2.51	0.43
1:C:628:PRO:HB2	1:C:735:TYR:HD2	1.82	0.43
2:B:2802:PLX:H322	2:B:2802:PLX:H351	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2807:PLX:H292	2:B:2807:PLX:H321	1.84	0.43
1:A:133:THR:HG21	1:A:156:ASN:HB3	2.00	0.43
1:A:1203:ARG:HA	1:A:1206:ARG:HH11	1.84	0.43
1:A:1280:ASN:HD22	1:A:1283:LEU:HB2	1.83	0.43
1:D:803:TYR:HE2	1:D:1099:GLN:HG3	1.84	0.43
1:C:825:SER:HB2	1:C:829:ILE:HD11	2.01	0.43
1:C:1293:GLN:HA	1:C:1296:VAL:HG23	2.01	0.43
1:C:1391:VAL:HG22	1:C:1434:THR:HG21	2.01	0.43
1:B:526:PRO:HA	1:B:529:ASP:HB3	1.99	0.43
1:B:791:ASP:OD1	1:B:791:ASP:N	2.51	0.43
1:B:833:PHE:O	1:B:837:MET:HG2	2.19	0.43
1:B:1214:VAL:HG21	1:B:1240:PHE:HE2	1.83	0.43
1:B:1285:SER:O	1:B:1325:LYS:NZ	2.43	0.43
1:B:1391:VAL:HG22	1:B:1434:THR:HG21	2.01	0.43
1:B:2037:LEU:O	1:B:2041:THR:HG23	2.18	0.43
1:B:2263:GLN:O	1:B:2265:VAL:N	2.52	0.43
1:A:638:CYS:SG	1:A:639:VAL:HG23	2.59	0.43
1:A:1293:GLN:HA	1:A:1296:VAL:HG23	2.01	0.43
1:D:1408:ARG:O	1:D:1412:HIS:ND1	2.51	0.43
1:C:747:ARG:NH1	1:C:749:TYR:OH	2.49	0.43
1:C:747:ARG:NH2	1:C:792:ARG:HB2	2.34	0.43
1:C:803:TYR:HE2	1:C:1099:GLN:HG3	1.84	0.43
1:C:2394:TYR:HB2	2:C:2805:PLX:H81	2.01	0.43
2:C:2803:PLX:H291	2:C:2803:PLX:H262	1.65	0.43
1:B:672:LEU:HA	1:B:695:GLU:HG3	2.01	0.43
1:B:1203:ARG:HA	1:B:1206:ARG:HH11	1.84	0.43
1:B:2363:CYS:HA	1:B:2366:ILE:HG22	2.00	0.43
2:B:2806:PLX:H1B2	2:B:2806:PLX:H21	1.74	0.43
2:A:2806:PLX:H111	2:A:2807:PLX:H141	2.01	0.43
1:D:825:SER:HB2	1:D:829:ILE:HD11	2.01	0.43
1:D:833:PHE:O	1:D:837:MET:HG2	2.19	0.43
1:D:2263:GLN:O	1:D:2265:VAL:N	2.52	0.43
1:D:2409:HIS:NE2	2:D:2803:PLX:C5	2.72	0.43
1:C:2297:PHE:HA	1:C:2300:VAL:HG13	2.01	0.43
1:B:638:CYS:SG	1:B:639:VAL:HG23	2.59	0.43
1:B:1618:LEU:O	1:B:1622:GLU:HB2	2.19	0.43
1:A:969:ASP:O	1:A:973:LYS:HG2	2.19	0.42
1:A:2055:ILE:HG22	1:A:2063:ILE:HD11	2.01	0.42
1:A:2083:ASP:OD1	1:A:2083:ASP:N	2.51	0.42
1:A:2394:TYR:HB2	2:A:2804:PLX:H81	2.00	0.42
1:D:124:LEU:HD12	1:D:131:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:ASN:ND2	1:C:378:GLY:O	2.51	0.42
1:C:2167:ASN:HD22	1:C:2170:LEU:HB2	1.83	0.42
1:B:803:TYR:HE2	1:B:1099:GLN:HG3	1.84	0.42
1:A:124:LEU:HD12	1:A:131:TYR:CZ	2.54	0.42
1:A:803:TYR:HE2	1:A:1099:GLN:HG3	1.84	0.42
1:A:2127:LYS:NZ	1:A:2149:PRO:O	2.51	0.42
1:A:2525:GLU:O	1:A:2526:HIS:ND1	2.53	0.42
1:D:638:CYS:SG	1:D:639:VAL:HG23	2.59	0.42
1:D:2699:GLN:HA	1:D:2702:LEU:HD23	2.01	0.42
1:C:1408:ARG:O	1:C:1412:HIS:ND1	2.51	0.42
1:C:1618:LEU:O	1:C:1622:GLU:HB2	2.19	0.42
1:C:2250:LEU:HD23	1:C:2250:LEU:HA	1.85	0.42
1:A:2030:VAL:HG11	1:A:2084:LEU:HG	2.01	0.42
1:A:2699:GLN:HA	1:A:2702:LEU:HD23	2.01	0.42
1:D:133:THR:HG21	1:D:156:ASN:HB3	2.00	0.42
1:C:884:LEU:HD12	1:C:981:ILE:HG22	2.00	0.42
1:B:1104:VAL:HG22	1:B:1105:THR:H	1.84	0.42
1:A:833:PHE:O	1:A:837:MET:HG2	2.19	0.42
1:D:747:ARG:NH2	1:D:792:ARG:HB2	2.34	0.42
1:B:133:THR:HG21	1:B:156:ASN:HB3	2.00	0.42
1:B:1632:ARG:HG3	1:B:1745:TYR:HE1	1.85	0.42
1:A:2037:LEU:O	1:A:2041:THR:HG23	2.18	0.42
1:D:672:LEU:HA	1:D:695:GLU:HG3	2.01	0.42
1:C:1104:VAL:HG22	1:C:1105:THR:H	1.84	0.42
1:C:2263:GLN:O	1:C:2265:VAL:N	2.52	0.42
1:B:300:ASN:ND2	1:B:378:GLY:O	2.51	0.42
1:B:895:LEU:HD21	1:B:974:ILE:HD11	2.02	0.42
1:B:2297:PHE:HA	1:B:2300:VAL:HG13	2.01	0.42
1:B:2525:GLU:O	1:B:2526:HIS:ND1	2.53	0.42
1:A:895:LEU:HD21	1:A:974:ILE:HD11	2.02	0.42
1:A:2046:GLY:HA2	1:A:2658:GLY:HA3	2.02	0.42
1:A:2263:GLN:O	1:A:2265:VAL:N	2.52	0.42
2:A:2806:PLX:H1C2	2:A:2806:PLX:H21	1.79	0.42
1:D:1618:LEU:O	1:D:1622:GLU:HB2	2.19	0.42
1:D:2046:GLY:HA2	1:D:2658:GLY:HA3	2.02	0.42
1:D:2721:ASP:O	1:D:2724:THR:OG1	2.31	0.42
1:C:638:CYS:SG	1:C:639:VAL:HG23	2.59	0.42
1:C:833:PHE:O	1:C:837:MET:HG2	2.19	0.42
1:C:2525:GLU:O	1:C:2526:HIS:ND1	2.53	0.42
1:B:55:ASP:O	1:B:125:HIS:NE2	2.53	0.42
1:B:124:LEU:HD12	1:B:131:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:747:ARG:NH2	1:B:792:ARG:HB2	2.34	0.42
1:B:2729:GLN:HA	1:B:2732:ARG:HG3	2.00	0.42
1:A:825:SER:HB2	1:A:829:ILE:HD11	2.01	0.42
1:A:2250:LEU:HD23	1:A:2250:LEU:HA	1.85	0.42
1:D:723:GLN:HB2	1:D:726:ASP:HB2	2.02	0.42
1:D:2297:PHE:HA	1:D:2300:VAL:HG13	2.01	0.42
1:C:60:LEU:HD12	1:C:121:ILE:HG12	2.02	0.42
1:C:2363:CYS:HA	1:C:2366:ILE:HG22	2.00	0.42
1:A:723:GLN:HB2	1:A:726:ASP:HB2	2.02	0.42
1:A:1391:VAL:HG22	1:A:1434:THR:HG21	2.01	0.42
1:D:615:ILE:O	1:D:619:VAL:N	2.44	0.42
1:D:624:LYS:HD2	1:D:624:LYS:HA	1.89	0.42
1:D:1203:ARG:HA	1:D:1206:ARG:HH11	1.84	0.42
1:D:2431:ILE:HA	1:D:2434:VAL:HG12	2.01	0.42
1:C:55:ASP:O	1:C:125:HIS:NE2	2.53	0.42
1:C:124:LEU:HD12	1:C:131:TYR:CZ	2.54	0.42
1:C:2699:GLN:HA	1:C:2702:LEU:HD23	2.01	0.42
1:B:536:LEU:HB3	1:B:538:LEU:HD23	2.02	0.42
1:B:1244:PHE:O	1:B:1251:ASN:ND2	2.53	0.42
1:B:1293:GLN:HA	1:B:1296:VAL:HG23	2.00	0.42
1:B:2409:HIS:CB	2:B:2807:PLX:H52	2.49	0.42
1:A:1244:PHE:O	1:A:1251:ASN:ND2	2.53	0.42
2:A:2803:PLX:H321	2:A:2803:PLX:H292	1.86	0.42
1:D:55:ASP:O	1:D:125:HIS:NE2	2.53	0.42
1:D:60:LEU:HD12	1:D:121:ILE:HG12	2.02	0.42
1:C:723:GLN:HB2	1:C:726:ASP:HB2	2.02	0.42
1:B:2699:GLN:HA	1:B:2702:LEU:HD23	2.01	0.42
1:A:1104:VAL:HG22	1:A:1105:THR:H	1.84	0.42
1:D:1104:VAL:HG22	1:D:1105:THR:H	1.84	0.42
1:D:1293:GLN:HA	1:D:1296:VAL:HG23	2.01	0.42
1:C:1203:ARG:HA	1:C:1206:ARG:HH11	1.84	0.42
1:C:2431:ILE:HA	1:C:2434:VAL:HG12	2.01	0.42
1:B:265:ARG:O	1:B:269:ARG:NH2	2.53	0.42
1:B:623:ARG:NH1	1:B:631:LEU:HB2	2.35	0.42
1:B:825:SER:HB2	1:B:829:ILE:HD11	2.01	0.42
2:B:2807:PLX:H1A2	2:B:2807:PLX:H21	1.76	0.42
1:A:672:LEU:HA	1:A:695:GLU:HG3	2.01	0.41
2:A:2802:PLX:H21	2:A:2802:PLX:H1B2	1.74	0.41
1:D:2525:GLU:O	1:D:2526:HIS:ND1	2.53	0.41
1:C:1271:VAL:HA	1:C:1274:GLN:HB3	2.02	0.41
1:B:2127:LYS:NZ	1:B:2149:PRO:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ARG:NH1	1:A:631:LEU:HB2	2.35	0.41
1:A:747:ARG:NH2	1:A:792:ARG:HB2	2.34	0.41
1:C:895:LEU:HD21	1:C:974:ILE:HD11	2.02	0.41
1:C:1632:ARG:HG3	1:C:1745:TYR:HE1	1.85	0.41
1:C:2200:ARG:HD3	1:C:2200:ARG:HA	1.89	0.41
1:C:2721:ASP:O	1:C:2724:THR:OG1	2.31	0.41
1:B:2030:VAL:HG11	1:B:2084:LEU:HG	2.01	0.41
1:B:2632:ILE:HD13	1:B:2632:ILE:HA	1.94	0.41
1:B:2721:ASP:O	1:B:2724:THR:OG1	2.31	0.41
2:B:2806:PLX:H291	2:B:2806:PLX:H262	1.66	0.41
1:A:1618:LEU:O	1:A:1622:GLU:HB2	2.19	0.41
1:A:1644:ARG:HA	1:A:1647:CYS:HB3	2.03	0.41
1:A:2297:PHE:HA	1:A:2300:VAL:HG13	2.01	0.41
1:D:1271:VAL:HA	1:D:1274:GLN:HB3	2.02	0.41
1:D:2614:CYS:SG	1:D:2616:LEU:HD23	2.61	0.41
1:C:623:ARG:NH1	1:C:631:LEU:HB2	2.35	0.41
1:C:1403:LEU:HG	1:C:1406:ILE:HB	2.03	0.41
1:B:723:GLN:HB2	1:B:726:ASP:HB2	2.02	0.41
1:B:1203:ARG:HH21	1:B:1247:GLY:H	1.68	0.41
1:B:1203:ARG:NH1	1:B:1248:ASN:OD1	2.54	0.41
1:A:1025:PRO:HB2	1:A:1026:GLY:H	1.64	0.41
1:A:1203:ARG:HH21	1:A:1247:GLY:H	1.68	0.41
1:A:2443:LEU:HD23	1:A:2443:LEU:HA	1.88	0.41
1:C:2369:LEU:HD21	1:C:2395:HIS:HB3	2.03	0.41
2:B:2802:PLX:H131	2:B:2802:PLX:H162	1.95	0.41
1:A:55:ASP:O	1:A:125:HIS:NE2	2.53	0.41
1:A:404:ILE:HA	1:A:405:PRO:HD3	1.95	0.41
1:A:1403:LEU:HG	1:A:1406:ILE:HB	2.03	0.41
1:A:2369:LEU:HD21	1:A:2395:HIS:HB3	2.03	0.41
1:D:265:ARG:O	1:D:269:ARG:NH2	2.53	0.41
1:D:623:ARG:NH1	1:D:631:LEU:HB2	2.35	0.41
1:D:1403:LEU:HG	1:D:1406:ILE:HB	2.03	0.41
1:D:2544:ARG:H	1:D:2544:ARG:HG2	1.72	0.41
1:C:2614:CYS:SG	1:C:2616:LEU:HD23	2.61	0.41
1:B:2409:HIS:CE1	2:B:2807:PLX:O8	2.71	0.41
2:B:2802:PLX:H111	2:B:2803:PLX:H141	2.02	0.41
1:A:1088:SER:O	1:A:1088:SER:OG	2.36	0.41
1:A:1271:VAL:HA	1:A:1274:GLN:HB3	2.02	0.41
1:A:2200:ARG:HD3	1:A:2200:ARG:HA	1.89	0.41
1:D:536:LEU:HB3	1:D:538:LEU:HD23	2.02	0.41
1:D:895:LEU:HD21	1:D:974:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1203:ARG:NH1	1:D:1248:ASN:OD1	2.54	0.41
1:D:2030:VAL:HG11	1:D:2084:LEU:HG	2.01	0.41
1:C:265:ARG:O	1:C:269:ARG:NH2	2.53	0.41
1:C:1244:PHE:O	1:C:1251:ASN:ND2	2.53	0.41
1:B:871:ARG:NH2	1:B:976:GLU:OE2	2.51	0.41
1:B:1271:VAL:HA	1:B:1274:GLN:HB3	2.03	0.41
1:A:122:GLN:OE1	1:A:159:SER:OG	2.30	0.41
1:A:300:ASN:HB2	1:B:2732:ARG:NH2	2.36	0.41
1:A:1203:ARG:NH1	1:A:1248:ASN:OD1	2.54	0.41
1:A:2377:GLY:O	1:A:2381:ARG:NE	2.54	0.41
1:D:1644:ARG:HA	1:D:1647:CYS:HB3	2.03	0.41
1:D:2611:CYS:SG	1:D:2612:PHE:N	2.94	0.41
2:D:2806:PLX:H1C2	2:D:2806:PLX:H21	1.82	0.41
1:C:785:MET:O	1:C:789:HIS:ND1	2.53	0.41
1:C:2709:VAL:O	1:C:2712:LEU:HG	2.21	0.41
1:A:265:ARG:O	1:A:269:ARG:NH2	2.53	0.41
1:A:383:PRO:HG2	1:A:386:SER:HB3	2.03	0.41
1:D:1203:ARG:HH21	1:D:1247:GLY:H	1.68	0.41
1:D:1632:ARG:HG3	1:D:1745:TYR:HE1	1.85	0.41
1:D:1674:LYS:HD2	1:D:1674:LYS:HA	1.90	0.41
1:D:2369:LEU:HD21	1:D:2395:HIS:HB3	2.03	0.41
1:C:2557:SER:O	1:C:2557:SER:OG	2.31	0.41
1:B:60:LEU:HD12	1:B:121:ILE:HG12	2.02	0.41
1:B:383:PRO:HG2	1:B:386:SER:HB3	2.03	0.41
1:B:1403:LEU:HG	1:B:1406:ILE:HB	2.03	0.41
1:B:1644:ARG:HA	1:B:1647:CYS:HB3	2.03	0.41
1:A:45:ASP:N	1:A:45:ASP:OD1	2.53	0.41
1:A:871:ARG:NH2	1:A:976:GLU:OE2	2.51	0.41
1:A:1632:ARG:HG3	1:A:1745:TYR:HE1	1.85	0.41
1:D:1244:PHE:O	1:D:1251:ASN:ND2	2.53	0.41
1:D:2575:PHE:CD2	2:D:2807:PLX:C36	3.03	0.41
2:D:2803:PLX:H292	2:D:2803:PLX:H321	1.79	0.41
1:C:536:LEU:HB3	1:C:538:LEU:HD23	2.02	0.41
1:C:585:ILE:HD11	1:C:595:ILE:HG21	2.03	0.41
1:C:2030:VAL:HG11	1:C:2084:LEU:HG	2.01	0.41
1:C:2611:CYS:SG	1:C:2612:PHE:N	2.94	0.41
1:C:2732:ARG:NH2	1:B:300:ASN:HB2	2.36	0.41
1:B:625:ASN:O	1:B:626:ARG:NE	2.51	0.41
1:B:1645:ARG:NH1	1:B:1646:LYS:HB2	2.36	0.41
1:B:1826:LEU:HD23	1:B:1829:ILE:HD12	2.03	0.41
1:B:2046:GLY:HA2	1:B:2658:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2377:GLY:O	1:B:2381:ARG:NE	2.54	0.41
1:A:60:LEU:HD12	1:A:121:ILE:HG12	2.02	0.41
1:A:2431:ILE:HA	1:A:2434:VAL:HG12	2.01	0.41
1:D:2557:SER:O	1:D:2557:SER:OG	2.31	0.41
1:C:383:PRO:HG2	1:C:386:SER:HB3	2.03	0.41
1:C:1645:ARG:NH1	1:C:1646:LYS:HB2	2.36	0.41
1:C:2046:GLY:HA2	1:C:2658:GLY:HA3	2.02	0.41
1:C:2377:GLY:O	1:C:2381:ARG:NE	2.54	0.41
1:B:32:LEU:HD23	1:B:445:PHE:HB2	2.03	0.41
1:B:2431:ILE:HA	1:B:2434:VAL:HG12	2.02	0.41
1:B:2611:CYS:SG	1:B:2612:PHE:N	2.94	0.41
1:B:2709:VAL:O	1:B:2712:LEU:HG	2.21	0.41
2:A:2804:PLX:H141	2:A:2804:PLX:H111	1.95	0.40
2:A:2806:PLX:H252	2:A:2806:PLX:H51	1.85	0.40
1:D:32:LEU:N	1:D:448:ASP:OD2	2.54	0.40
1:D:871:ARG:NH2	1:D:976:GLU:OE2	2.51	0.40
1:D:1179:ILE:HD12	1:D:1179:ILE:HA	1.92	0.40
1:D:1450:LEU:O	1:D:1454:PHE:HB2	2.22	0.40
1:C:32:LEU:N	1:C:448:ASP:OD2	2.55	0.40
1:C:250:PHE:HB2	1:C:262:VAL:HG22	2.03	0.40
1:A:121:ILE:HG22	1:A:161:PHE:HB2	2.03	0.40
1:A:496:GLU:HB3	1:A:499:PHE:HE2	1.86	0.40
1:A:501:LYS:HA	1:A:502:PRO:HD3	1.87	0.40
1:A:638:CYS:HB2	1:A:652:ILE:HD13	2.04	0.40
1:A:1450:LEU:O	1:A:1454:PHE:HB2	2.22	0.40
1:A:1645:ARG:NH1	1:A:1646:LYS:HB2	2.36	0.40
1:A:1826:LEU:HD23	1:A:1829:ILE:HD12	2.03	0.40
1:A:2614:CYS:SG	1:A:2616:LEU:HD23	2.61	0.40
1:D:121:ILE:HG22	1:D:161:PHE:HB2	2.03	0.40
1:D:638:CYS:HB2	1:D:652:ILE:HD13	2.04	0.40
1:C:1644:ARG:HA	1:C:1647:CYS:HB3	2.03	0.40
1:C:1826:LEU:HD23	1:C:1826:LEU:HA	1.86	0.40
1:B:121:ILE:HG22	1:B:161:PHE:HB2	2.03	0.40
1:B:607:GLU:HB3	1:B:647:VAL:HG11	2.03	0.40
1:B:615:ILE:O	1:B:619:VAL:N	2.44	0.40
1:B:2234:ASP:N	1:B:2234:ASP:OD1	2.55	0.40
1:A:1620:GLN:O	1:A:1624:SER:OG	2.30	0.40
1:A:2427:LEU:HD11	1:B:2447:LEU:HD22	2.03	0.40
1:A:2472:ASP:OD1	1:A:2472:ASP:N	2.55	0.40
1:D:1645:ARG:NH1	1:D:1646:LYS:HB2	2.36	0.40
1:C:121:ILE:HG22	1:C:161:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:ASN:O	1:C:626:ARG:NE	2.51	0.40
1:C:1203:ARG:HH21	1:C:1247:GLY:H	1.68	0.40
1:C:1826:LEU:HD23	1:C:1829:ILE:HD12	2.03	0.40
1:B:2369:LEU:HD21	1:B:2395:HIS:HB3	2.03	0.40
1:B:2677:ARG:HD3	1:B:2677:ARG:HA	1.87	0.40
1:A:32:LEU:N	1:A:448:ASP:OD2	2.55	0.40
1:A:2224:LYS:HG3	1:A:2639:TRP:CZ2	2.57	0.40
1:A:2611:CYS:SG	1:A:2612:PHE:N	2.94	0.40
1:A:2709:VAL:O	1:A:2712:LEU:HG	2.21	0.40
1:D:2732:ARG:NH2	1:C:300:ASN:HB2	2.36	0.40
1:C:178:ILE:HD13	1:C:178:ILE:HA	1.88	0.40
1:C:1637:PHE:HD1	1:C:1638:PRO:HD3	1.87	0.40
1:B:1404:ASP:O	1:B:1408:ARG:HG2	2.21	0.40
1:B:1416:ILE:HD13	1:B:1416:ILE:HA	1.93	0.40
1:B:1637:PHE:HD1	1:B:1638:PRO:HD3	1.87	0.40
1:B:1871:ILE:H	1:B:1871:ILE:HG12	1.69	0.40
1:B:2715:GLN:HA	1:B:2718:GLU:HG3	2.04	0.40
1:A:536:LEU:HB3	1:A:538:LEU:HD23	2.02	0.40
1:A:826:LYS:HD2	1:A:826:LYS:HA	1.90	0.40
1:A:1871:ILE:H	1:A:1871:ILE:HG12	1.69	0.40
1:A:2447:LEU:HD22	1:D:2427:LEU:HD11	2.03	0.40
1:D:383:PRO:HG2	1:D:386:SER:HB3	2.03	0.40
1:D:2709:VAL:O	1:D:2712:LEU:HG	2.21	0.40
1:C:314:LEU:HD12	1:C:314:LEU:HA	1.94	0.40
1:C:624:LYS:HD2	1:C:624:LYS:HA	1.89	0.40
1:C:669:LYS:HA	1:C:669:LYS:HD2	1.93	0.40
1:C:1228:THR:OG1	1:C:1229:LYS:N	2.53	0.40
1:B:496:GLU:HB3	1:B:499:PHE:HE2	1.87	0.40
1:B:624:LYS:HA	1:B:624:LYS:HD2	1.89	0.40
1:B:2200:ARG:HD3	1:B:2200:ARG:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	B	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	C	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
1	D	2270/2734 (83%)	2018 (89%)	246 (11%)	6 (0%)	41	71
All	All	9080/10936 (83%)	8072 (89%)	984 (11%)	24 (0%)	44	71

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2412	PHE
1	D	2412	PHE
1	C	2412	PHE
1	B	2412	PHE
1	A	2612	PHE
1	D	2612	PHE
1	C	2612	PHE
1	B	2612	PHE
1	A	393	LEU
1	A	2264	PRO
1	D	393	LEU
1	D	2264	PRO
1	C	393	LEU
1	C	2264	PRO
1	B	393	LEU
1	B	2264	PRO
1	A	853	PRO
1	D	853	PRO
1	C	853	PRO
1	B	853	PRO
1	A	2613	ILE
1	D	2613	ILE
1	C	2613	ILE
1	B	2613	ILE

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 PDB entries followed by that with respect to all EM entries.

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	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	B	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	C	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
1	D	1972/2444 (81%)	1961 (99%)	11 (1%)	86	91
All	All	7888/9776 (81%)	7844 (99%)	44 (1%)	86	91

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	705	LYS
1	A	766	ARG
1	A	889	LYS
1	A	1206	ARG
1	A	1229	LYS
1	A	1304	ARG
1	A	1348	ARG
1	A	1632	ARG
1	A	1645	ARG
1	A	2381	ARG
1	D	257	ARG
1	D	705	LYS
1	D	766	ARG
1	D	889	LYS
1	D	1206	ARG
1	D	1229	LYS
1	D	1304	ARG
1	D	1348	ARG
1	D	1632	ARG
1	D	1645	ARG
1	D	2381	ARG
1	C	257	ARG
1	C	705	LYS
1	C	766	ARG
1	C	889	LYS
1	C	1206	ARG
1	C	1229	LYS
1	C	1304	ARG
1	C	1348	ARG

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Mol	Chain	Res	Type
1	C	1632	ARG
1	C	1645	ARG
1	C	2381	ARG
1	B	257	ARG
1	B	705	LYS
1	B	766	ARG
1	B	889	LYS
1	B	1206	ARG
1	B	1229	LYS
1	B	1304	ARG
1	B	1348	ARG
1	B	1632	ARG
1	B	1645	ARG
1	B	2381	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	122	GLN
1	A	1242	GLN
1	A	1252	GLN
1	A	1836	ASN
1	A	2053	ASN
1	A	2108	ASN
1	A	2729	GLN
1	D	103	ASN
1	D	122	GLN
1	D	1242	GLN
1	D	1252	GLN
1	D	1836	ASN
1	D	2053	ASN
1	D	2108	ASN
1	D	2729	GLN
1	C	103	ASN
1	C	122	GLN
1	C	1242	GLN
1	C	1252	GLN
1	C	1836	ASN
1	C	2053	ASN
1	C	2108	ASN
1	C	2729	GLN

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Mol	Chain	Res	Type
1	B	64	ASN
1	B	1242	GLN
1	B	1252	GLN
1	B	1836	ASN
1	B	2053	ASN
1	B	2108	ASN
1	B	2729	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 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
2	PLX	D	2802	-	35,35,51	2.02	4 (11%)	39,43,59	1.62	6 (15%)
2	PLX	B	2808	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	A	2804	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	C	2805	-	38,38,51	1.95	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	A	2801	-	33,33,51	2.07	4 (12%)	37,41,59	1.72	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLX	C	2802	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	A	2807	-	42,42,51	1.86	4 (9%)	46,50,59	1.54	5 (10%)
2	PLX	C	2804	-	35,35,51	2.02	5 (14%)	39,43,59	1.69	5 (12%)
2	PLX	B	2807	-	35,35,51	2.02	5 (14%)	39,43,59	1.71	5 (12%)
2	PLX	B	2803	-	41,41,51	1.88	4 (9%)	45,49,59	1.56	5 (11%)
2	PLX	B	2802	-	45,45,51	1.79	4 (8%)	49,53,59	1.51	5 (10%)
2	PLX	C	2807	-	45,45,51	1.79	4 (8%)	49,53,59	1.57	5 (10%)
2	PLX	B	2801	-	39,39,51	1.92	4 (10%)	43,47,59	1.61	5 (11%)
2	PLX	D	2803	-	35,35,51	2.01	4 (11%)	39,43,59	1.70	5 (12%)
2	PLX	C	2808	-	42,42,51	1.86	4 (9%)	46,50,59	1.55	5 (10%)
2	PLX	C	2803	-	35,35,51	2.02	4 (11%)	39,43,59	1.63	6 (15%)
2	PLX	C	2801	-	39,39,51	1.92	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	D	2804	-	38,38,51	1.96	4 (10%)	42,46,59	1.62	5 (11%)
2	PLX	B	2806	-	35,35,51	2.02	4 (11%)	39,43,59	1.62	6 (15%)
2	PLX	A	2806	-	45,45,51	1.79	4 (8%)	49,53,59	1.56	5 (10%)
2	PLX	A	2803	-	35,35,51	2.02	4 (11%)	39,43,59	1.71	6 (15%)
2	PLX	D	2807	-	42,42,51	1.86	4 (9%)	46,50,59	1.54	5 (10%)
2	PLX	B	2805	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	D	2801	-	33,33,51	2.07	4 (12%)	37,41,59	1.73	5 (13%)
2	PLX	D	2806	-	45,45,51	1.69	6 (13%)	49,53,59	1.66	6 (12%)
2	PLX	A	2808	-	39,39,51	1.92	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	B	2804	-	39,39,51	1.91	4 (10%)	43,47,59	1.60	5 (11%)
2	PLX	A	2802	-	35,35,51	2.02	4 (11%)	39,43,59	1.63	6 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	D	2802	-	3/3/5/5	19/39/39/55	-
2	PLX	B	2808	-	3/3/5/5	24/42/42/55	-
2	PLX	A	2804	-	3/3/5/5	26/42/42/55	-
2	PLX	C	2805	-	3/3/5/5	23/42/42/55	-
2	PLX	A	2801	-	3/3/5/5	17/37/37/55	-
2	PLX	C	2802	-	3/3/5/5	18/37/37/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	A	2807	-	3/3/5/5	25/46/46/55	-
2	PLX	C	2804	-	3/3/5/5	18/39/39/55	-
2	PLX	B	2807	-	3/3/5/5	16/39/39/55	-
2	PLX	B	2803	-	3/3/5/5	24/45/45/55	-
2	PLX	B	2802	-	3/3/5/5	26/49/49/55	-
2	PLX	C	2807	-	3/3/5/5	25/49/49/55	-
2	PLX	B	2801	-	3/3/5/5	23/43/43/55	-
2	PLX	D	2803	-	3/3/5/5	21/39/39/55	-
2	PLX	C	2808	-	3/3/5/5	25/46/46/55	-
2	PLX	C	2803	-	3/3/5/5	19/39/39/55	-
2	PLX	C	2801	-	3/3/5/5	21/43/43/55	-
2	PLX	D	2804	-	3/3/5/5	24/42/42/55	-
2	PLX	B	2806	-	3/3/5/5	19/39/39/55	-
2	PLX	A	2806	-	3/3/5/5	25/49/49/55	-
2	PLX	A	2803	-	3/3/5/5	17/39/39/55	-
2	PLX	D	2807	-	3/3/5/5	26/46/46/55	-
2	PLX	B	2805	-	3/3/5/5	18/37/37/55	-
2	PLX	D	2801	-	3/3/5/5	18/37/37/55	-
2	PLX	D	2806	-	3/3/5/5	25/49/49/55	-
2	PLX	A	2808	-	3/3/5/5	20/43/43/55	-
2	PLX	B	2804	-	3/3/5/5	22/43/43/55	-
2	PLX	A	2802	-	3/3/5/5	19/39/39/55	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2801	PLX	O7-C6	-7.25	1.18	1.39
2	C	2804	PLX	O7-C6	-7.24	1.18	1.39
2	C	2803	PLX	O7-C6	-7.24	1.18	1.39
2	B	2808	PLX	O7-C6	-7.23	1.18	1.39
2	C	2808	PLX	O7-C6	-7.23	1.18	1.39
2	B	2806	PLX	O7-C6	-7.22	1.18	1.39
2	A	2803	PLX	O7-C6	-7.22	1.18	1.39
2	C	2801	PLX	O7-C6	-7.22	1.18	1.39
2	A	2802	PLX	O7-C6	-7.22	1.18	1.39
2	A	2807	PLX	O7-C6	-7.22	1.18	1.39
2	B	2807	PLX	O7-C6	-7.22	1.18	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2808	PLX	O7-C6	-7.22	1.19	1.39
2	D	2804	PLX	O7-C6	-7.22	1.19	1.39
2	D	2802	PLX	O7-C6	-7.21	1.19	1.39
2	B	2805	PLX	O7-C6	-7.21	1.19	1.39
2	A	2804	PLX	O7-C6	-7.21	1.19	1.39
2	D	2807	PLX	O7-C6	-7.21	1.19	1.39
2	B	2804	PLX	O7-C6	-7.21	1.19	1.39
2	C	2802	PLX	O7-C6	-7.21	1.19	1.39
2	D	2803	PLX	O7-C6	-7.21	1.19	1.39
2	D	2801	PLX	O7-C6	-7.20	1.19	1.39
2	C	2805	PLX	O7-C6	-7.20	1.19	1.39
2	B	2803	PLX	O7-C6	-7.20	1.19	1.39
2	A	2801	PLX	O7-C6	-7.20	1.19	1.39
2	A	2806	PLX	O9-C24	-7.19	1.19	1.39
2	B	2802	PLX	O7-C6	-7.18	1.19	1.39
2	A	2806	PLX	O7-C6	-7.16	1.19	1.39
2	C	2807	PLX	O7-C6	-7.15	1.19	1.39
2	D	2804	PLX	O9-C24	-7.15	1.19	1.39
2	A	2804	PLX	O9-C24	-7.15	1.19	1.39
2	B	2808	PLX	O9-C24	-7.15	1.19	1.39
2	A	2802	PLX	O9-C24	-7.14	1.19	1.39
2	D	2802	PLX	O9-C24	-7.14	1.19	1.39
2	C	2807	PLX	O9-C24	-7.14	1.19	1.39
2	D	2806	PLX	O7-C6	-7.14	1.19	1.39
2	A	2807	PLX	O9-C24	-7.13	1.19	1.39
2	C	2805	PLX	O9-C24	-7.13	1.19	1.39
2	B	2803	PLX	O9-C24	-7.13	1.19	1.39
2	C	2808	PLX	O9-C24	-7.13	1.19	1.39
2	B	2802	PLX	O9-C24	-7.12	1.19	1.39
2	B	2806	PLX	O9-C24	-7.12	1.19	1.39
2	A	2803	PLX	O9-C24	-7.12	1.19	1.39
2	C	2803	PLX	O9-C24	-7.11	1.19	1.39
2	B	2807	PLX	O9-C24	-7.11	1.19	1.39
2	D	2801	PLX	O9-C24	-7.11	1.19	1.39
2	C	2804	PLX	O9-C24	-7.11	1.19	1.39
2	A	2801	PLX	O9-C24	-7.10	1.19	1.39
2	B	2805	PLX	O9-C24	-7.10	1.19	1.39
2	C	2802	PLX	O9-C24	-7.10	1.19	1.39
2	C	2801	PLX	O9-C24	-7.10	1.19	1.39
2	D	2807	PLX	O9-C24	-7.10	1.19	1.39
2	B	2801	PLX	O9-C24	-7.09	1.19	1.39
2	B	2804	PLX	O9-C24	-7.08	1.19	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2808	PLX	O9-C24	-7.08	1.19	1.39
2	D	2803	PLX	O9-C24	-7.08	1.19	1.39
2	D	2806	PLX	O9-C24	-5.27	1.24	1.39
2	A	2803	PLX	O6-C4	-3.41	1.40	1.44
2	B	2803	PLX	O6-C4	-3.35	1.40	1.44
2	A	2807	PLX	O6-C4	-3.33	1.40	1.44
2	B	2807	PLX	O6-C4	-3.33	1.40	1.44
2	C	2808	PLX	O6-C4	-3.31	1.40	1.44
2	D	2807	PLX	O6-C4	-3.31	1.40	1.44
2	C	2804	PLX	O6-C4	-3.22	1.40	1.44
2	A	2808	PLX	O6-C4	-3.20	1.40	1.44
2	A	2804	PLX	O6-C4	-3.20	1.40	1.44
2	B	2801	PLX	O6-C4	-3.19	1.40	1.44
2	D	2803	PLX	O6-C4	-3.19	1.40	1.44
2	C	2805	PLX	O6-C4	-3.17	1.40	1.44
2	B	2808	PLX	O6-C4	-3.17	1.40	1.44
2	D	2804	PLX	O6-C4	-3.16	1.40	1.44
2	B	2804	PLX	O6-C4	-3.15	1.40	1.44
2	C	2803	PLX	O6-C4	-3.14	1.40	1.44
2	C	2801	PLX	O6-C4	-3.13	1.40	1.44
2	D	2802	PLX	O6-C4	-3.11	1.40	1.44
2	A	2801	PLX	O6-C4	-3.07	1.40	1.44
2	B	2806	PLX	O6-C4	-3.07	1.40	1.44
2	D	2801	PLX	O6-C4	-3.06	1.40	1.44
2	A	2802	PLX	O6-C4	-3.06	1.40	1.44
2	B	2805	PLX	O6-C4	-3.05	1.40	1.44
2	C	2802	PLX	O6-C4	-3.02	1.40	1.44
2	A	2806	PLX	O6-C4	-2.97	1.40	1.44
2	C	2807	PLX	O6-C4	-2.93	1.40	1.44
2	B	2802	PLX	O6-C4	-2.87	1.40	1.44
2	D	2806	PLX	C25-C24	2.72	1.56	1.50
2	D	2806	PLX	C7-C6	2.49	1.56	1.50
2	D	2806	PLX	O6-C4	-2.24	1.41	1.44
2	C	2807	PLX	C7-C6	2.21	1.55	1.50
2	A	2806	PLX	C7-C6	2.20	1.55	1.50
2	A	2808	PLX	C7-C6	2.19	1.55	1.50
2	B	2802	PLX	C7-C6	2.19	1.55	1.50
2	A	2804	PLX	C7-C6	2.18	1.55	1.50
2	C	2805	PLX	C7-C6	2.17	1.55	1.50
2	D	2804	PLX	C7-C6	2.17	1.55	1.50
2	B	2804	PLX	C7-C6	2.16	1.55	1.50
2	C	2801	PLX	C7-C6	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2808	PLX	C7-C6	2.14	1.55	1.50
2	B	2801	PLX	C7-C6	2.14	1.55	1.50
2	A	2807	PLX	C7-C6	2.13	1.55	1.50
2	D	2801	PLX	C7-C6	2.13	1.55	1.50
2	B	2803	PLX	C7-C6	2.13	1.55	1.50
2	D	2807	PLX	C7-C6	2.12	1.55	1.50
2	D	2806	PLX	O8-C24	2.12	1.43	1.40
2	C	2802	PLX	C7-C6	2.11	1.55	1.50
2	C	2808	PLX	C7-C6	2.11	1.55	1.50
2	D	2803	PLX	C7-C6	2.10	1.55	1.50
2	C	2803	PLX	C7-C6	2.10	1.55	1.50
2	A	2801	PLX	C7-C6	2.09	1.55	1.50
2	C	2804	PLX	C7-C6	2.09	1.55	1.50
2	B	2805	PLX	C7-C6	2.08	1.55	1.50
2	A	2802	PLX	C7-C6	2.06	1.55	1.50
2	D	2802	PLX	C7-C6	2.06	1.55	1.50
2	A	2803	PLX	C7-C6	2.06	1.55	1.50
2	B	2806	PLX	C7-C6	2.05	1.55	1.50
2	B	2807	PLX	P1-O4	2.02	1.67	1.59
2	B	2807	PLX	C7-C6	2.01	1.55	1.50
2	C	2804	PLX	P1-O4	2.00	1.67	1.59

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2806	PLX	O9-C24-C25	7.26	122.58	109.12
2	C	2807	PLX	O9-C24-C25	6.48	121.13	109.12
2	A	2806	PLX	O9-C24-C25	6.45	121.08	109.12
2	D	2803	PLX	O9-C24-C25	6.02	120.28	109.12
2	C	2804	PLX	O9-C24-C25	5.98	120.20	109.12
2	A	2804	PLX	O7-C6-C7	5.95	120.14	109.12
2	D	2804	PLX	O7-C6-C7	5.94	120.13	109.12
2	B	2801	PLX	O9-C24-C25	5.93	120.11	109.12
2	B	2804	PLX	O9-C24-C25	5.93	120.11	109.12
2	A	2808	PLX	O9-C24-C25	5.92	120.10	109.12
2	C	2805	PLX	O7-C6-C7	5.92	120.09	109.12
2	B	2808	PLX	O7-C6-C7	5.92	120.08	109.12
2	B	2805	PLX	O9-C24-C25	5.91	120.08	109.12
2	D	2801	PLX	O9-C24-C25	5.91	120.07	109.12
2	D	2803	PLX	O7-C6-C7	5.90	120.05	109.12
2	C	2801	PLX	O9-C24-C25	5.89	120.04	109.12
2	C	2804	PLX	O7-C6-C7	5.89	120.04	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2802	PLX	O9-C24-C25	5.88	120.02	109.12
2	A	2801	PLX	O9-C24-C25	5.88	120.01	109.12
2	C	2807	PLX	O7-C6-C7	5.88	120.01	109.12
2	A	2803	PLX	O7-C6-C7	5.87	119.99	109.12
2	B	2805	PLX	O7-C6-C7	5.85	119.97	109.12
2	B	2807	PLX	O7-C6-C7	5.85	119.96	109.12
2	B	2807	PLX	O9-C24-C25	5.84	119.95	109.12
2	C	2802	PLX	O7-C6-C7	5.83	119.92	109.12
2	D	2801	PLX	O7-C6-C7	5.82	119.91	109.12
2	A	2806	PLX	O7-C6-C7	5.81	119.89	109.12
2	A	2801	PLX	O7-C6-C7	5.81	119.88	109.12
2	B	2801	PLX	O7-C6-C7	5.80	119.87	109.12
2	C	2808	PLX	O7-C6-C7	5.79	119.86	109.12
2	A	2807	PLX	O7-C6-C7	5.78	119.83	109.12
2	B	2802	PLX	O9-C24-C25	5.77	119.81	109.12
2	B	2803	PLX	O7-C6-C7	5.77	119.81	109.12
2	B	2804	PLX	O7-C6-C7	5.77	119.80	109.12
2	C	2801	PLX	O7-C6-C7	5.76	119.78	109.12
2	B	2808	PLX	O9-C24-C25	5.75	119.78	109.12
2	A	2808	PLX	O7-C6-C7	5.75	119.78	109.12
2	D	2807	PLX	O7-C6-C7	5.75	119.77	109.12
2	D	2804	PLX	O9-C24-C25	5.74	119.75	109.12
2	C	2805	PLX	O9-C24-C25	5.72	119.71	109.12
2	A	2804	PLX	O9-C24-C25	5.71	119.70	109.12
2	A	2803	PLX	O9-C24-C25	5.69	119.66	109.12
2	C	2808	PLX	O9-C24-C25	5.67	119.63	109.12
2	A	2807	PLX	O9-C24-C25	5.65	119.59	109.12
2	B	2803	PLX	O9-C24-C25	5.64	119.58	109.12
2	D	2807	PLX	O9-C24-C25	5.64	119.56	109.12
2	B	2802	PLX	O7-C6-C7	5.62	119.54	109.12
2	A	2802	PLX	O9-C24-C25	5.51	119.34	109.12
2	C	2803	PLX	O9-C24-C25	5.50	119.32	109.12
2	C	2803	PLX	O7-C6-C7	5.50	119.30	109.12
2	B	2806	PLX	O7-C6-C7	5.50	119.30	109.12
2	B	2806	PLX	O9-C24-C25	5.48	119.28	109.12
2	D	2802	PLX	O9-C24-C25	5.48	119.28	109.12
2	D	2802	PLX	O7-C6-C7	5.48	119.28	109.12
2	A	2802	PLX	O7-C6-C7	5.48	119.27	109.12
2	D	2806	PLX	O7-C6-C7	5.03	118.44	109.12
2	D	2806	PLX	C1B-N1-C1C	3.99	119.24	108.97
2	D	2806	PLX	C26-C25-C24	3.96	122.54	113.38
2	C	2807	PLX	C1B-N1-C1C	3.96	119.14	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2802	PLX	C1B-N1-C1C	3.95	119.13	108.97
2	A	2806	PLX	C1B-N1-C1C	3.94	119.10	108.97
2	A	2807	PLX	C1B-N1-C1C	3.85	118.87	108.97
2	B	2803	PLX	C1B-N1-C1C	3.85	118.86	108.97
2	A	2803	PLX	C1B-N1-C1C	3.85	118.86	108.97
2	D	2807	PLX	C1B-N1-C1C	3.83	118.82	108.97
2	C	2808	PLX	C1B-N1-C1C	3.82	118.79	108.97
2	B	2807	PLX	C1B-N1-C1C	3.80	118.75	108.97
2	A	2801	PLX	C1B-N1-C1C	3.80	118.74	108.97
2	C	2802	PLX	C1B-N1-C1C	3.80	118.73	108.97
2	D	2801	PLX	C1B-N1-C1C	3.79	118.72	108.97
2	B	2805	PLX	C1B-N1-C1C	3.78	118.70	108.97
2	C	2804	PLX	C1B-N1-C1C	3.75	118.62	108.97
2	D	2803	PLX	C1B-N1-C1C	3.75	118.62	108.97
2	C	2805	PLX	C1B-N1-C1C	3.72	118.54	108.97
2	D	2804	PLX	C1B-N1-C1C	3.72	118.53	108.97
2	B	2808	PLX	C1B-N1-C1C	3.71	118.52	108.97
2	A	2808	PLX	C1B-N1-C1C	3.70	118.48	108.97
2	A	2804	PLX	C1B-N1-C1C	3.70	118.47	108.97
2	B	2801	PLX	C1B-N1-C1C	3.68	118.43	108.97
2	B	2804	PLX	C1B-N1-C1C	3.67	118.42	108.97
2	C	2801	PLX	C1B-N1-C1C	3.66	118.39	108.97
2	C	2803	PLX	C1B-N1-C1C	3.65	118.35	108.97
2	A	2802	PLX	C1B-N1-C1C	3.64	118.33	108.97
2	D	2802	PLX	C1B-N1-C1C	3.64	118.33	108.97
2	B	2806	PLX	C1B-N1-C1C	3.63	118.32	108.97
2	C	2803	PLX	O8-C24-C25	3.58	120.61	109.49
2	B	2806	PLX	O8-C24-C25	3.58	120.60	109.49
2	A	2802	PLX	O8-C24-C25	3.57	120.58	109.49
2	D	2802	PLX	O8-C24-C25	3.57	120.58	109.49
2	D	2804	PLX	O8-C24-C25	3.57	120.57	109.49
2	C	2805	PLX	O8-C24-C25	3.57	120.56	109.49
2	B	2808	PLX	O8-C24-C25	3.57	120.56	109.49
2	A	2804	PLX	O8-C24-C25	3.55	120.53	109.49
2	B	2803	PLX	O8-C24-C25	3.55	120.50	109.49
2	D	2807	PLX	O8-C24-C25	3.54	120.49	109.49
2	C	2808	PLX	O8-C24-C25	3.53	120.44	109.49
2	A	2807	PLX	O8-C24-C25	3.52	120.42	109.49
2	C	2802	PLX	O8-C24-C25	3.38	119.97	109.49
2	A	2801	PLX	O8-C24-C25	3.37	119.95	109.49
2	D	2801	PLX	O8-C24-C25	3.37	119.95	109.49
2	B	2805	PLX	O8-C24-C25	3.36	119.93	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2802	PLX	O8-C24-C25	3.33	119.82	109.49
2	C	2801	PLX	O8-C24-C25	3.31	119.76	109.49
2	B	2801	PLX	O8-C24-C25	3.30	119.73	109.49
2	B	2804	PLX	O8-C24-C25	3.30	119.73	109.49
2	A	2808	PLX	O8-C24-C25	3.30	119.73	109.49
2	A	2806	PLX	O8-C24-C25	3.25	119.59	109.49
2	C	2807	PLX	O8-C24-C25	3.25	119.58	109.49
2	C	2804	PLX	O8-C24-C25	3.11	119.15	109.49
2	D	2803	PLX	O8-C24-C25	3.10	119.10	109.49
2	B	2807	PLX	O8-C24-C25	3.05	118.97	109.49
2	A	2803	PLX	O8-C24-C25	3.04	118.92	109.49
2	B	2802	PLX	O6-C6-C7	2.32	120.44	110.05
2	B	2804	PLX	O6-C6-C7	2.28	120.28	110.05
2	A	2808	PLX	O6-C6-C7	2.28	120.28	110.05
2	B	2801	PLX	O6-C6-C7	2.28	120.28	110.05
2	C	2804	PLX	O6-C6-C7	2.28	120.26	110.05
2	C	2801	PLX	O6-C6-C7	2.28	120.26	110.05
2	A	2806	PLX	O6-C6-C7	2.27	120.23	110.05
2	C	2807	PLX	O6-C6-C7	2.26	120.21	110.05
2	D	2806	PLX	O6-C6-C7	2.25	120.13	110.05
2	D	2807	PLX	O6-C6-C7	2.24	120.10	110.05
2	B	2803	PLX	O6-C6-C7	2.24	120.08	110.05
2	A	2807	PLX	O6-C6-C7	2.24	120.08	110.05
2	C	2808	PLX	O6-C6-C7	2.23	120.04	110.05
2	A	2803	PLX	O6-C6-C7	2.22	120.01	110.05
2	A	2801	PLX	O6-C6-C7	2.22	119.99	110.05
2	A	2804	PLX	O6-C6-C7	2.22	119.99	110.05
2	B	2805	PLX	O6-C6-C7	2.22	119.99	110.05
2	C	2805	PLX	O6-C6-C7	2.21	119.98	110.05
2	B	2808	PLX	O6-C6-C7	2.21	119.98	110.05
2	D	2803	PLX	O6-C6-C7	2.21	119.96	110.05
2	C	2802	PLX	O6-C6-C7	2.21	119.96	110.05
2	D	2804	PLX	O6-C6-C7	2.21	119.95	110.05
2	D	2801	PLX	O6-C6-C7	2.20	119.94	110.05
2	D	2802	PLX	O6-C6-C7	2.20	119.90	110.05
2	B	2807	PLX	O6-C6-C7	2.20	119.90	110.05
2	C	2803	PLX	O6-C6-C7	2.19	119.86	110.05
2	A	2802	PLX	O6-C6-C7	2.18	119.85	110.05
2	B	2806	PLX	O6-C6-C7	2.18	119.85	110.05
2	A	2802	PLX	C5-O8-C24	2.10	117.86	113.80
2	C	2803	PLX	C5-O8-C24	2.09	117.82	113.80
2	D	2802	PLX	C5-O8-C24	2.07	117.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2806	PLX	O8-C5-C4	2.07	115.90	110.90
2	B	2806	PLX	C5-O8-C24	2.07	117.79	113.80
2	A	2803	PLX	O8-C5-C4	-2.06	105.94	110.90

All (84) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2801	PLX	C24
2	A	2801	PLX	C6
2	A	2801	PLX	C4
2	A	2802	PLX	C24
2	A	2802	PLX	C6
2	A	2802	PLX	C4
2	A	2803	PLX	C24
2	A	2803	PLX	C6
2	A	2803	PLX	C4
2	A	2804	PLX	C24
2	A	2804	PLX	C6
2	A	2804	PLX	C4
2	A	2806	PLX	C24
2	A	2806	PLX	C6
2	A	2806	PLX	C4
2	A	2807	PLX	C24
2	A	2807	PLX	C6
2	A	2807	PLX	C4
2	A	2808	PLX	C24
2	A	2808	PLX	C6
2	A	2808	PLX	C4
2	D	2801	PLX	C24
2	D	2801	PLX	C6
2	D	2801	PLX	C4
2	D	2802	PLX	C24
2	D	2802	PLX	C6
2	D	2802	PLX	C4
2	D	2803	PLX	C24
2	D	2803	PLX	C6
2	D	2803	PLX	C4
2	D	2804	PLX	C24
2	D	2804	PLX	C6
2	D	2804	PLX	C4
2	D	2806	PLX	C24
2	D	2806	PLX	C6

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Mol	Chain	Res	Type	Atom
2	D	2806	PLX	C4
2	D	2807	PLX	C24
2	D	2807	PLX	C6
2	D	2807	PLX	C4
2	C	2801	PLX	C24
2	C	2801	PLX	C6
2	C	2801	PLX	C4
2	C	2802	PLX	C24
2	C	2802	PLX	C6
2	C	2802	PLX	C4
2	C	2803	PLX	C24
2	C	2803	PLX	C6
2	C	2803	PLX	C4
2	C	2804	PLX	C24
2	C	2804	PLX	C6
2	C	2804	PLX	C4
2	C	2805	PLX	C24
2	C	2805	PLX	C6
2	C	2805	PLX	C4
2	C	2807	PLX	C24
2	C	2807	PLX	C6
2	C	2807	PLX	C4
2	C	2808	PLX	C24
2	C	2808	PLX	C6
2	C	2808	PLX	C4
2	B	2801	PLX	C24
2	B	2801	PLX	C6
2	B	2801	PLX	C4
2	B	2802	PLX	C24
2	B	2802	PLX	C6
2	B	2802	PLX	C4
2	B	2803	PLX	C24
2	B	2803	PLX	C6
2	B	2803	PLX	C4
2	B	2804	PLX	C24
2	B	2804	PLX	C6
2	B	2804	PLX	C4
2	B	2805	PLX	C24
2	B	2805	PLX	C6
2	B	2805	PLX	C4
2	B	2806	PLX	C24
2	B	2806	PLX	C6

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Mol	Chain	Res	Type	Atom
2	B	2806	PLX	C4
2	B	2807	PLX	C24
2	B	2807	PLX	C6
2	B	2807	PLX	C4
2	B	2808	PLX	C24
2	B	2808	PLX	C6
2	B	2808	PLX	C4

All (603) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2801	PLX	O7-C6-C7-C8
2	A	2801	PLX	C3-O4-P1-O2
2	A	2801	PLX	C3-O4-P1-O3
2	A	2801	PLX	O9-C24-C25-C26
2	A	2802	PLX	O7-C6-O6-C4
2	A	2802	PLX	C3-O4-P1-O2
2	A	2802	PLX	C3-O4-P1-O3
2	A	2803	PLX	O7-C6-C7-C8
2	A	2803	PLX	O7-C6-O6-C4
2	A	2803	PLX	C3-O4-P1-O2
2	A	2803	PLX	C3-O4-P1-O3
2	A	2803	PLX	O9-C24-C25-C26
2	A	2804	PLX	O7-C6-O6-C4
2	A	2804	PLX	C3-O4-P1-O1
2	A	2804	PLX	C3-O4-P1-O2
2	A	2804	PLX	C3-O4-P1-O3
2	A	2804	PLX	C2-O1-P1-O2
2	A	2804	PLX	C25-C24-O8-C5
2	A	2804	PLX	O9-C24-C25-C26
2	A	2806	PLX	O7-C6-O6-C4
2	A	2806	PLX	C3-O4-P1-O2
2	A	2807	PLX	O7-C6-O6-C4
2	A	2807	PLX	C3-O4-P1-O3
2	A	2807	PLX	C25-C24-O8-C5
2	A	2807	PLX	O9-C24-C25-C26
2	A	2808	PLX	O7-C6-O6-C4
2	A	2808	PLX	C3-O4-P1-O1
2	A	2808	PLX	C3-O4-P1-O2
2	A	2808	PLX	C3-O4-P1-O3
2	A	2808	PLX	N1-C1-C2-O1
2	A	2808	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	D	2801	PLX	O7-C6-C7-C8
2	D	2801	PLX	C3-O4-P1-O2
2	D	2801	PLX	C3-O4-P1-O3
2	D	2801	PLX	O9-C24-C25-C26
2	D	2802	PLX	O7-C6-O6-C4
2	D	2802	PLX	C3-O4-P1-O2
2	D	2802	PLX	C3-O4-P1-O3
2	D	2803	PLX	O7-C6-C7-C8
2	D	2803	PLX	O7-C6-O6-C4
2	D	2803	PLX	C3-O4-P1-O2
2	D	2803	PLX	C3-O4-P1-O3
2	D	2803	PLX	O9-C24-C25-C26
2	D	2804	PLX	O7-C6-O6-C4
2	D	2804	PLX	C3-O4-P1-O1
2	D	2804	PLX	C3-O4-P1-O2
2	D	2804	PLX	C3-O4-P1-O3
2	D	2804	PLX	C2-O1-P1-O2
2	D	2804	PLX	C25-C24-O8-C5
2	D	2804	PLX	O9-C24-C25-C26
2	D	2806	PLX	O7-C6-O6-C4
2	D	2806	PLX	N1-C1-C2-O1
2	D	2807	PLX	O7-C6-O6-C4
2	D	2807	PLX	C3-O4-P1-O3
2	D	2807	PLX	C25-C24-O8-C5
2	D	2807	PLX	O9-C24-C25-C26
2	C	2801	PLX	O7-C6-O6-C4
2	C	2801	PLX	C3-O4-P1-O2
2	C	2801	PLX	C3-O4-P1-O3
2	C	2801	PLX	N1-C1-C2-O1
2	C	2801	PLX	O8-C24-C25-C26
2	C	2802	PLX	O7-C6-C7-C8
2	C	2802	PLX	C3-O4-P1-O2
2	C	2802	PLX	C3-O4-P1-O3
2	C	2802	PLX	O9-C24-C25-C26
2	C	2803	PLX	O7-C6-O6-C4
2	C	2803	PLX	C3-O4-P1-O2
2	C	2803	PLX	C3-O4-P1-O3
2	C	2804	PLX	O7-C6-C7-C8
2	C	2804	PLX	O7-C6-O6-C4
2	C	2804	PLX	C3-O4-P1-O2
2	C	2804	PLX	C3-O4-P1-O3
2	C	2804	PLX	O9-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	C	2805	PLX	O7-C6-O6-C4
2	C	2805	PLX	C3-O4-P1-O1
2	C	2805	PLX	C3-O4-P1-O2
2	C	2805	PLX	C3-O4-P1-O3
2	C	2805	PLX	C2-O1-P1-O2
2	C	2805	PLX	C25-C24-O8-C5
2	C	2805	PLX	O9-C24-C25-C26
2	C	2807	PLX	O7-C6-O6-C4
2	C	2807	PLX	C3-O4-P1-O2
2	C	2808	PLX	O7-C6-O6-C4
2	C	2808	PLX	C3-O4-P1-O3
2	C	2808	PLX	C25-C24-O8-C5
2	C	2808	PLX	O9-C24-C25-C26
2	B	2801	PLX	O7-C6-O6-C4
2	B	2801	PLX	C3-O4-P1-O1
2	B	2801	PLX	C3-O4-P1-O2
2	B	2801	PLX	C3-O4-P1-O3
2	B	2801	PLX	N1-C1-C2-O1
2	B	2801	PLX	O8-C24-C25-C26
2	B	2802	PLX	O7-C6-O6-C4
2	B	2802	PLX	C3-O4-P1-O1
2	B	2802	PLX	C3-O4-P1-O2
2	B	2803	PLX	O7-C6-O6-C4
2	B	2803	PLX	C3-O4-P1-O1
2	B	2803	PLX	C3-O4-P1-O3
2	B	2803	PLX	C25-C24-O8-C5
2	B	2803	PLX	O9-C24-C25-C26
2	B	2804	PLX	O7-C6-O6-C4
2	B	2804	PLX	C3-O4-P1-O2
2	B	2804	PLX	C3-O4-P1-O3
2	B	2804	PLX	N1-C1-C2-O1
2	B	2804	PLX	O8-C24-C25-C26
2	B	2805	PLX	O7-C6-C7-C8
2	B	2805	PLX	C3-O4-P1-O2
2	B	2805	PLX	C3-O4-P1-O3
2	B	2805	PLX	O9-C24-C25-C26
2	B	2806	PLX	O7-C6-O6-C4
2	B	2806	PLX	C3-O4-P1-O2
2	B	2806	PLX	C3-O4-P1-O3
2	B	2807	PLX	O7-C6-C7-C8
2	B	2807	PLX	O7-C6-O6-C4
2	B	2807	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
2	B	2807	PLX	C3-O4-P1-O3
2	B	2807	PLX	O9-C24-C25-C26
2	B	2808	PLX	O7-C6-O6-C4
2	B	2808	PLX	C3-O4-P1-O1
2	B	2808	PLX	C3-O4-P1-O2
2	B	2808	PLX	C3-O4-P1-O3
2	B	2808	PLX	C2-O1-P1-O2
2	B	2808	PLX	C25-C24-O8-C5
2	B	2808	PLX	O9-C24-C25-C26
2	A	2802	PLX	C26-C27-C28-C29
2	D	2802	PLX	C26-C27-C28-C29
2	B	2806	PLX	C26-C27-C28-C29
2	A	2804	PLX	C11-C12-C13-C14
2	C	2803	PLX	C26-C27-C28-C29
2	D	2804	PLX	C11-C12-C13-C14
2	C	2805	PLX	C11-C12-C13-C14
2	B	2808	PLX	C11-C12-C13-C14
2	A	2807	PLX	O6-C4-C5-O8
2	C	2808	PLX	O6-C4-C5-O8
2	B	2803	PLX	O6-C4-C5-O8
2	A	2804	PLX	C2-C1-N1-C1A
2	D	2804	PLX	C2-C1-N1-C1A
2	C	2805	PLX	C2-C1-N1-C1A
2	B	2808	PLX	C2-C1-N1-C1A
2	B	2802	PLX	C30-C31-C32-C33
2	A	2801	PLX	C3-O4-P1-O1
2	A	2802	PLX	C3-O4-P1-O1
2	A	2803	PLX	C3-O4-P1-O1
2	A	2804	PLX	C2-O1-P1-O4
2	A	2807	PLX	C3-O4-P1-O1
2	D	2801	PLX	C3-O4-P1-O1
2	D	2802	PLX	C3-O4-P1-O1
2	D	2803	PLX	C3-O4-P1-O1
2	D	2804	PLX	C2-O1-P1-O4
2	D	2807	PLX	C3-O4-P1-O1
2	C	2801	PLX	C3-O4-P1-O1
2	C	2802	PLX	C3-O4-P1-O1
2	C	2803	PLX	C3-O4-P1-O1
2	C	2804	PLX	C3-O4-P1-O1
2	C	2805	PLX	C2-O1-P1-O4
2	C	2808	PLX	C3-O4-P1-O1
2	B	2804	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
2	B	2805	PLX	C3-O4-P1-O1
2	B	2806	PLX	C3-O4-P1-O1
2	B	2807	PLX	C3-O4-P1-O1
2	B	2808	PLX	C2-O1-P1-O4
2	C	2807	PLX	C30-C31-C32-C33
2	A	2806	PLX	C30-C31-C32-C33
2	A	2802	PLX	O6-C6-C7-C8
2	A	2802	PLX	O8-C24-C25-C26
2	D	2802	PLX	O6-C6-C7-C8
2	D	2806	PLX	O8-C24-C25-C26
2	C	2803	PLX	O6-C6-C7-C8
2	B	2802	PLX	O8-C24-C25-C26
2	B	2806	PLX	O6-C6-C7-C8
2	A	2807	PLX	C11-C12-C13-C14
2	C	2805	PLX	C9-C10-C11-C12
2	A	2804	PLX	C9-C10-C11-C12
2	D	2804	PLX	C25-C26-C27-C28
2	C	2805	PLX	C25-C26-C27-C28
2	B	2801	PLX	C9-C10-C11-C12
2	B	2803	PLX	C11-C12-C13-C14
2	B	2804	PLX	C9-C10-C11-C12
2	B	2808	PLX	C25-C26-C27-C28
2	A	2804	PLX	C25-C26-C27-C28
2	A	2808	PLX	C9-C10-C11-C12
2	D	2804	PLX	C9-C10-C11-C12
2	D	2807	PLX	C11-C12-C13-C14
2	C	2801	PLX	C9-C10-C11-C12
2	B	2808	PLX	C9-C10-C11-C12
2	D	2802	PLX	C11-C10-C9-C8
2	C	2808	PLX	C11-C12-C13-C14
2	B	2808	PLX	C11-C10-C9-C8
2	D	2804	PLX	C11-C10-C9-C8
2	C	2805	PLX	C11-C10-C9-C8
2	B	2806	PLX	C11-C10-C9-C8
2	C	2808	PLX	C11-C10-C9-C8
2	C	2808	PLX	C26-C27-C28-C29
2	B	2803	PLX	C11-C10-C9-C8
2	D	2807	PLX	O6-C4-C5-O8
2	A	2804	PLX	C11-C10-C9-C8
2	A	2807	PLX	C11-C10-C9-C8
2	A	2807	PLX	C26-C27-C28-C29
2	D	2807	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	D	2807	PLX	C27-C28-C29-C30
2	C	2803	PLX	C11-C10-C9-C8
2	A	2804	PLX	C26-C27-C28-C29
2	C	2801	PLX	C7-C8-C9-C10
2	B	2804	PLX	C7-C8-C9-C10
2	B	2808	PLX	C26-C27-C28-C29
2	A	2806	PLX	C26-C27-C28-C29
2	A	2807	PLX	C27-C28-C29-C30
2	D	2804	PLX	C26-C27-C28-C29
2	D	2806	PLX	C25-C26-C27-C28
2	D	2806	PLX	C35-C36-C37-C38
2	D	2807	PLX	C26-C27-C28-C29
2	C	2807	PLX	C26-C27-C28-C29
2	C	2808	PLX	C27-C28-C29-C30
2	B	2801	PLX	C7-C8-C9-C10
2	B	2803	PLX	C27-C28-C29-C30
2	A	2808	PLX	C7-C8-C9-C10
2	C	2804	PLX	C26-C27-C28-C29
2	A	2808	PLX	C11-C10-C9-C8
2	D	2806	PLX	C11-C10-C9-C8
2	C	2801	PLX	C11-C10-C9-C8
2	B	2801	PLX	C28-C29-C30-C31
2	B	2802	PLX	C26-C27-C28-C29
2	B	2803	PLX	C26-C27-C28-C29
2	B	2807	PLX	C9-C10-C11-C12
2	A	2801	PLX	C27-C28-C29-C30
2	A	2803	PLX	C9-C10-C11-C12
2	D	2801	PLX	C27-C28-C29-C30
2	D	2803	PLX	C9-C10-C11-C12
2	C	2804	PLX	C11-C10-C9-C8
2	C	2805	PLX	C26-C27-C28-C29
2	B	2801	PLX	C11-C10-C9-C8
2	B	2802	PLX	C35-C36-C37-C38
2	B	2804	PLX	C11-C10-C9-C8
2	B	2804	PLX	C28-C29-C30-C31
2	A	2804	PLX	C2-C1-N1-C1B
2	A	2802	PLX	C11-C10-C9-C8
2	A	2806	PLX	C11-C10-C9-C8
2	C	2802	PLX	C27-C28-C29-C30
2	C	2807	PLX	C11-C10-C9-C8
2	B	2805	PLX	C27-C28-C29-C30
2	A	2806	PLX	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
2	C	2807	PLX	C35-C36-C37-C38
2	D	2801	PLX	C26-C27-C28-C29
2	C	2802	PLX	C26-C27-C28-C29
2	C	2804	PLX	C9-C10-C11-C12
2	C	2808	PLX	C25-C26-C27-C28
2	B	2802	PLX	C11-C10-C9-C8
2	B	2805	PLX	C26-C27-C28-C29
2	B	2807	PLX	C11-C10-C9-C8
2	A	2801	PLX	C26-C27-C28-C29
2	A	2807	PLX	C25-C26-C27-C28
2	B	2802	PLX	C9-C10-C11-C12
2	A	2806	PLX	C9-C10-C11-C12
2	A	2803	PLX	C26-C27-C28-C29
2	D	2803	PLX	C11-C10-C9-C8
2	C	2807	PLX	C9-C10-C11-C12
2	D	2806	PLX	C28-C29-C30-C31
2	D	2806	PLX	C11-C12-C13-C14
2	B	2802	PLX	C11-C12-C13-C14
2	B	2804	PLX	C27-C28-C29-C30
2	D	2803	PLX	C26-C27-C28-C29
2	D	2806	PLX	C9-C10-C11-C12
2	A	2803	PLX	C11-C10-C9-C8
2	D	2807	PLX	C25-C26-C27-C28
2	B	2801	PLX	C27-C28-C29-C30
2	A	2808	PLX	C28-C29-C30-C31
2	C	2803	PLX	C27-C28-C29-C30
2	B	2803	PLX	C25-C26-C27-C28
2	D	2804	PLX	C2-C1-N1-C1B
2	C	2805	PLX	C2-C1-N1-C1B
2	B	2808	PLX	C2-C1-N1-C1B
2	A	2806	PLX	C11-C12-C13-C14
2	D	2802	PLX	C27-C28-C29-C30
2	C	2807	PLX	C11-C12-C13-C14
2	C	2801	PLX	C27-C28-C29-C30
2	B	2801	PLX	C11-C12-C13-C14
2	A	2808	PLX	C11-C12-C13-C14
2	C	2801	PLX	C11-C12-C13-C14
2	C	2801	PLX	C28-C29-C30-C31
2	B	2806	PLX	C27-C28-C29-C30
2	A	2808	PLX	C27-C28-C29-C30
2	B	2804	PLX	C11-C12-C13-C14
2	D	2806	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	A	2802	PLX	C27-C28-C29-C30
2	B	2802	PLX	C32-C33-C34-C35
2	D	2807	PLX	C10-C11-C12-C13
2	B	2807	PLX	C26-C27-C28-C29
2	C	2808	PLX	C10-C11-C12-C13
2	A	2807	PLX	C10-C11-C12-C13
2	B	2803	PLX	C10-C11-C12-C13
2	A	2806	PLX	O4-C3-C4-C5
2	A	2807	PLX	O4-C3-C4-C5
2	D	2806	PLX	O4-C3-C4-C5
2	D	2807	PLX	O4-C3-C4-C5
2	C	2807	PLX	O4-C3-C4-C5
2	C	2808	PLX	O4-C3-C4-C5
2	B	2802	PLX	O4-C3-C4-C5
2	B	2803	PLX	O4-C3-C4-C5
2	D	2803	PLX	C7-C8-C9-C10
2	B	2807	PLX	C7-C8-C9-C10
2	A	2801	PLX	C3-C4-C5-O8
2	A	2804	PLX	C3-C4-C5-O8
2	A	2807	PLX	C3-C4-C5-O8
2	D	2801	PLX	C25-C26-C27-C28
2	D	2803	PLX	C3-C4-C5-O8
2	D	2804	PLX	C3-C4-C5-O8
2	C	2804	PLX	C3-C4-C5-O8
2	C	2805	PLX	C3-C4-C5-O8
2	B	2803	PLX	C3-C4-C5-O8
2	B	2808	PLX	C3-C4-C5-O8
2	B	2805	PLX	C25-C26-C27-C28
2	A	2802	PLX	C4-C5-O8-C24
2	D	2802	PLX	C4-C5-O8-C24
2	C	2803	PLX	C4-C5-O8-C24
2	B	2806	PLX	C4-C5-O8-C24
2	A	2803	PLX	C10-C11-C12-C13
2	C	2802	PLX	C25-C26-C27-C28
2	C	2808	PLX	O6-C6-C7-C8
2	C	2804	PLX	C10-C11-C12-C13
2	C	2802	PLX	C9-C10-C11-C12
2	B	2801	PLX	C13-C14-C15-C16
2	D	2801	PLX	C9-C10-C11-C12
2	B	2805	PLX	C9-C10-C11-C12
2	D	2803	PLX	C10-C11-C12-C13
2	B	2804	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	A	2801	PLX	C9-C10-C11-C12
2	B	2807	PLX	C10-C11-C12-C13
2	A	2804	PLX	C14-C15-C16-C17
2	A	2808	PLX	C13-C14-C15-C16
2	D	2806	PLX	C14-C15-C16-C17
2	C	2801	PLX	C13-C14-C15-C16
2	D	2802	PLX	O4-C3-C4-O6
2	C	2803	PLX	O4-C3-C4-O6
2	B	2806	PLX	O4-C3-C4-O6
2	C	2804	PLX	C7-C8-C9-C10
2	D	2801	PLX	C11-C10-C9-C8
2	D	2804	PLX	C13-C14-C15-C16
2	A	2806	PLX	C13-C14-C15-C16
2	C	2807	PLX	C14-C15-C16-C17
2	C	2807	PLX	C13-C14-C15-C16
2	B	2802	PLX	C14-C15-C16-C17
2	A	2806	PLX	C14-C15-C16-C17
2	B	2808	PLX	C13-C14-C15-C16
2	A	2801	PLX	C11-C10-C9-C8
2	C	2802	PLX	C11-C10-C9-C8
2	B	2805	PLX	C11-C10-C9-C8
2	C	2805	PLX	C13-C14-C15-C16
2	C	2805	PLX	C14-C15-C16-C17
2	B	2808	PLX	C14-C15-C16-C17
2	D	2804	PLX	C14-C15-C16-C17
2	A	2801	PLX	C25-C26-C27-C28
2	A	2802	PLX	C9-C10-C11-C12
2	C	2808	PLX	C14-C15-C16-C17
2	A	2807	PLX	C14-C15-C16-C17
2	D	2807	PLX	C14-C15-C16-C17
2	B	2803	PLX	C14-C15-C16-C17
2	C	2803	PLX	C9-C10-C11-C12
2	C	2803	PLX	C30-C31-C32-C33
2	B	2803	PLX	C30-C31-C32-C33
2	B	2803	PLX	C29-C30-C31-C32
2	D	2803	PLX	C4-C3-O4-P1
2	C	2804	PLX	C4-C3-O4-P1
2	B	2807	PLX	C4-C3-O4-P1
2	D	2802	PLX	C9-C10-C11-C12
2	C	2808	PLX	C32-C33-C34-C35
2	A	2807	PLX	C32-C33-C34-C35
2	B	2806	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	D	2801	PLX	C3-C4-C5-O8
2	D	2807	PLX	C3-C4-C5-O8
2	C	2802	PLX	C3-C4-C5-O8
2	C	2808	PLX	C3-C4-C5-O8
2	B	2805	PLX	C3-C4-C5-O8
2	D	2807	PLX	C30-C31-C32-C33
2	A	2804	PLX	C13-C14-C15-C16
2	B	2806	PLX	C30-C31-C32-C33
2	D	2802	PLX	C30-C31-C32-C33
2	A	2802	PLX	O4-C3-C4-O6
2	D	2807	PLX	C29-C30-C31-C32
2	B	2802	PLX	O6-C4-C5-O8
2	A	2803	PLX	C4-C3-O4-P1
2	A	2807	PLX	C29-C30-C31-C32
2	C	2808	PLX	C29-C30-C31-C32
2	A	2802	PLX	C30-C31-C32-C33
2	B	2802	PLX	C13-C14-C15-C16
2	B	2802	PLX	C24-C25-C26-C27
2	A	2804	PLX	O6-C6-C7-C8
2	A	2806	PLX	O6-C6-C7-C8
2	A	2807	PLX	O6-C6-C7-C8
2	A	2808	PLX	O6-C6-C7-C8
2	D	2804	PLX	O6-C6-C7-C8
2	D	2807	PLX	O6-C6-C7-C8
2	C	2801	PLX	O6-C6-C7-C8
2	C	2805	PLX	O6-C6-C7-C8
2	C	2807	PLX	O6-C6-C7-C8
2	B	2801	PLX	O6-C6-C7-C8
2	B	2802	PLX	O6-C6-C7-C8
2	B	2803	PLX	O6-C6-C7-C8
2	B	2804	PLX	O6-C6-C7-C8
2	B	2808	PLX	O6-C6-C7-C8
2	A	2802	PLX	O4-C3-C4-C5
2	D	2802	PLX	O4-C3-C4-C5
2	C	2803	PLX	O4-C3-C4-C5
2	B	2806	PLX	O4-C3-C4-C5
2	A	2803	PLX	C7-C8-C9-C10
2	A	2807	PLX	C13-C14-C15-C16
2	B	2803	PLX	C13-C14-C15-C16
2	B	2802	PLX	C3-C4-C5-O8
2	A	2806	PLX	O4-C3-C4-O6
2	D	2806	PLX	O4-C3-C4-O6

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Mol	Chain	Res	Type	Atoms
2	C	2807	PLX	O4-C3-C4-O6
2	B	2802	PLX	O4-C3-C4-O6
2	D	2807	PLX	C13-C14-C15-C16
2	C	2808	PLX	C13-C14-C15-C16
2	A	2801	PLX	O6-C4-C5-O8
2	A	2804	PLX	O6-C4-C5-O8
2	A	2806	PLX	O6-C4-C5-O8
2	D	2801	PLX	O6-C4-C5-O8
2	D	2804	PLX	O6-C4-C5-O8
2	C	2802	PLX	O6-C4-C5-O8
2	C	2804	PLX	O6-C4-C5-O8
2	C	2805	PLX	O6-C4-C5-O8
2	C	2807	PLX	O6-C4-C5-O8
2	B	2805	PLX	O6-C4-C5-O8
2	B	2808	PLX	O6-C4-C5-O8
2	A	2804	PLX	C2-C1-N1-C1C
2	B	2801	PLX	C31-C32-C33-C34
2	A	2804	PLX	C24-C25-C26-C27
2	A	2806	PLX	C24-C25-C26-C27
2	D	2804	PLX	C24-C25-C26-C27
2	C	2805	PLX	C24-C25-C26-C27
2	C	2807	PLX	C24-C25-C26-C27
2	B	2808	PLX	C24-C25-C26-C27
2	A	2802	PLX	C6-C7-C8-C9
2	A	2802	PLX	C24-C25-C26-C27
2	C	2803	PLX	C24-C25-C26-C27
2	A	2806	PLX	C3-O4-P1-O1
2	C	2807	PLX	C3-O4-P1-O1
2	B	2801	PLX	C26-C27-C28-C29
2	A	2807	PLX	C3-O4-P1-O2
2	D	2807	PLX	C3-O4-P1-O2
2	C	2805	PLX	C2-C1-N1-C1C
2	C	2808	PLX	C3-O4-P1-O2
2	B	2803	PLX	C3-O4-P1-O2
2	B	2808	PLX	C2-C1-N1-C1C
2	B	2802	PLX	C28-C29-C30-C31
2	A	2801	PLX	C25-C24-O8-C5
2	A	2808	PLX	C25-C24-O8-C5
2	D	2801	PLX	C25-C24-O8-C5
2	C	2801	PLX	C25-C24-O8-C5
2	C	2802	PLX	C25-C24-O8-C5
2	B	2801	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
2	B	2804	PLX	C25-C24-O8-C5
2	B	2805	PLX	C25-C24-O8-C5
2	D	2802	PLX	C24-C25-C26-C27
2	B	2806	PLX	C24-C25-C26-C27
2	B	2807	PLX	C29-C30-C31-C32
2	C	2808	PLX	C30-C31-C32-C33
2	A	2807	PLX	O4-C3-C4-O6
2	A	2808	PLX	O4-C3-C4-O6
2	D	2807	PLX	O4-C3-C4-O6
2	C	2801	PLX	O4-C3-C4-O6
2	B	2801	PLX	O4-C3-C4-O6
2	B	2803	PLX	O4-C3-C4-O6
2	B	2804	PLX	O4-C3-C4-O6
2	A	2807	PLX	C30-C31-C32-C33
2	D	2804	PLX	C2-C1-N1-C1C
2	A	2801	PLX	N1-C1-C2-O1
2	A	2806	PLX	C3-C4-C5-O8
2	A	2806	PLX	N1-C1-C2-O1
2	D	2801	PLX	N1-C1-C2-O1
2	D	2806	PLX	C3-C4-C5-O8
2	C	2802	PLX	N1-C1-C2-O1
2	C	2807	PLX	C3-C4-C5-O8
2	C	2807	PLX	N1-C1-C2-O1
2	B	2802	PLX	N1-C1-C2-O1
2	B	2805	PLX	N1-C1-C2-O1
2	D	2806	PLX	O6-C4-C5-O8
2	C	2807	PLX	C25-C26-C27-C28
2	A	2806	PLX	O8-C24-C25-C26
2	D	2806	PLX	O6-C6-C7-C8
2	C	2807	PLX	O8-C24-C25-C26
2	D	2806	PLX	C13-C14-C15-C16
2	D	2807	PLX	C33-C34-C35-C36
2	D	2804	PLX	C27-C28-C29-C30
2	B	2808	PLX	C27-C28-C29-C30
2	D	2803	PLX	C29-C30-C31-C32
2	C	2804	PLX	C24-C25-C26-C27
2	A	2808	PLX	C4-C3-O4-P1
2	C	2801	PLX	C4-C3-O4-P1
2	B	2804	PLX	C4-C3-O4-P1
2	C	2808	PLX	O4-C3-C4-O6
2	A	2806	PLX	C25-C26-C27-C28
2	D	2803	PLX	O6-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
2	A	2803	PLX	C2-O1-P1-O4
2	D	2803	PLX	C2-O1-P1-O4
2	D	2806	PLX	C3-O4-P1-O1
2	C	2804	PLX	C2-O1-P1-O4
2	B	2807	PLX	C2-O1-P1-O4
2	A	2803	PLX	C3-C4-C5-O8
2	D	2802	PLX	C6-C7-C8-C9
2	C	2803	PLX	C6-C7-C8-C9
2	D	2806	PLX	C26-C27-C28-C29
2	D	2806	PLX	C4-C3-O4-P1
2	B	2801	PLX	C4-C3-O4-P1
2	D	2806	PLX	C24-C25-C26-C27
2	D	2807	PLX	C24-C25-C26-C27
2	B	2806	PLX	C6-C7-C8-C9
2	D	2807	PLX	C32-C33-C34-C35
2	C	2808	PLX	C24-C25-C26-C27
2	B	2803	PLX	C6-C7-C8-C9
2	B	2807	PLX	C24-C25-C26-C27
2	A	2801	PLX	O4-C3-C4-O6
2	B	2801	PLX	C10-C11-C12-C13
2	A	2807	PLX	C6-C7-C8-C9
2	D	2803	PLX	C24-C25-C26-C27
2	D	2807	PLX	C6-C7-C8-C9
2	C	2808	PLX	C6-C7-C8-C9
2	B	2803	PLX	C24-C25-C26-C27
2	D	2802	PLX	O8-C24-C25-C26
2	C	2803	PLX	O8-C24-C25-C26
2	B	2806	PLX	O8-C24-C25-C26
2	B	2807	PLX	C30-C31-C32-C33
2	A	2803	PLX	C24-C25-C26-C27
2	A	2806	PLX	C6-C7-C8-C9
2	A	2807	PLX	C24-C25-C26-C27
2	C	2807	PLX	C6-C7-C8-C9
2	A	2807	PLX	C9-C10-C11-C12
2	B	2802	PLX	C25-C26-C27-C28
2	D	2803	PLX	C30-C31-C32-C33
2	A	2801	PLX	C6-C7-C8-C9
2	D	2801	PLX	C6-C7-C8-C9
2	B	2802	PLX	C6-C7-C8-C9
2	C	2804	PLX	C30-C31-C32-C33
2	D	2801	PLX	C5-C4-O6-C6
2	C	2802	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
2	B	2805	PLX	C5-C4-O6-C6
2	D	2802	PLX	C4-C3-O4-P1
2	C	2803	PLX	C4-C3-O4-P1
2	B	2806	PLX	C4-C3-O4-P1
2	B	2803	PLX	C9-C10-C11-C12
2	C	2801	PLX	C10-C11-C12-C13
2	D	2806	PLX	C30-C31-C32-C33
2	B	2804	PLX	C10-C11-C12-C13
2	C	2802	PLX	C6-C7-C8-C9
2	B	2805	PLX	C6-C7-C8-C9
2	C	2807	PLX	C32-C33-C34-C35
2	A	2808	PLX	C10-C11-C12-C13
2	D	2807	PLX	C9-C10-C11-C12
2	C	2808	PLX	C9-C10-C11-C12
2	A	2803	PLX	C30-C31-C32-C33
2	D	2806	PLX	C6-C7-C8-C9
2	A	2806	PLX	C32-C33-C34-C35
2	D	2803	PLX	C4-C5-O8-C24
2	C	2804	PLX	C4-C5-O8-C24
2	D	2801	PLX	O4-C3-C4-O6
2	C	2802	PLX	O4-C3-C4-O6
2	B	2805	PLX	O4-C3-C4-O6
2	D	2806	PLX	C27-C28-C29-C30
2	A	2808	PLX	O4-C3-C4-C5
2	C	2801	PLX	O4-C3-C4-C5
2	B	2801	PLX	O4-C3-C4-C5
2	B	2804	PLX	O4-C3-C4-C5
2	A	2802	PLX	C4-C3-O4-P1
2	C	2807	PLX	C33-C34-C35-C36
2	D	2803	PLX	C27-C28-C29-C30
2	A	2806	PLX	C33-C34-C35-C36
2	B	2802	PLX	C33-C34-C35-C36
2	A	2804	PLX	O4-C3-C4-O6
2	A	2803	PLX	C6-C7-C8-C9
2	A	2804	PLX	O4-C3-C4-C5
2	A	2808	PLX	O9-C24-C25-C26
2	C	2801	PLX	O9-C24-C25-C26
2	B	2801	PLX	O9-C24-C25-C26
2	B	2804	PLX	O9-C24-C25-C26
2	D	2801	PLX	C24-C25-C26-C27
2	C	2802	PLX	C24-C25-C26-C27
2	B	2805	PLX	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
2	B	2801	PLX	C12-C13-C14-C15
2	B	2804	PLX	C12-C13-C14-C15
2	B	2804	PLX	C26-C27-C28-C29
2	A	2806	PLX	C28-C29-C30-C31
2	A	2802	PLX	C2-O1-P1-O2
2	A	2804	PLX	C2-O1-P1-O3
2	A	2806	PLX	C2-O1-P1-O2
2	D	2802	PLX	C2-O1-P1-O2
2	D	2806	PLX	C3-O4-P1-O2
2	C	2803	PLX	C2-O1-P1-O2
2	C	2807	PLX	C2-O1-P1-O2
2	B	2802	PLX	C2-O1-P1-O2
2	B	2806	PLX	C2-O1-P1-O2
2	A	2801	PLX	O4-C3-C4-C5
2	D	2804	PLX	O4-C3-C4-C5
2	C	2805	PLX	O4-C3-C4-C5
2	B	2808	PLX	O4-C3-C4-C5
2	C	2807	PLX	C28-C29-C30-C31
2	A	2802	PLX	C25-C24-O8-C5
2	D	2802	PLX	C25-C24-O8-C5
2	C	2803	PLX	C25-C24-O8-C5
2	B	2802	PLX	C25-C24-O8-C5
2	B	2806	PLX	C25-C24-O8-C5
2	A	2804	PLX	C27-C28-C29-C30
2	C	2801	PLX	C26-C27-C28-C29
2	D	2803	PLX	C6-C7-C8-C9

There are no ring outliers.

24 monomers are involved in 121 short contacts:

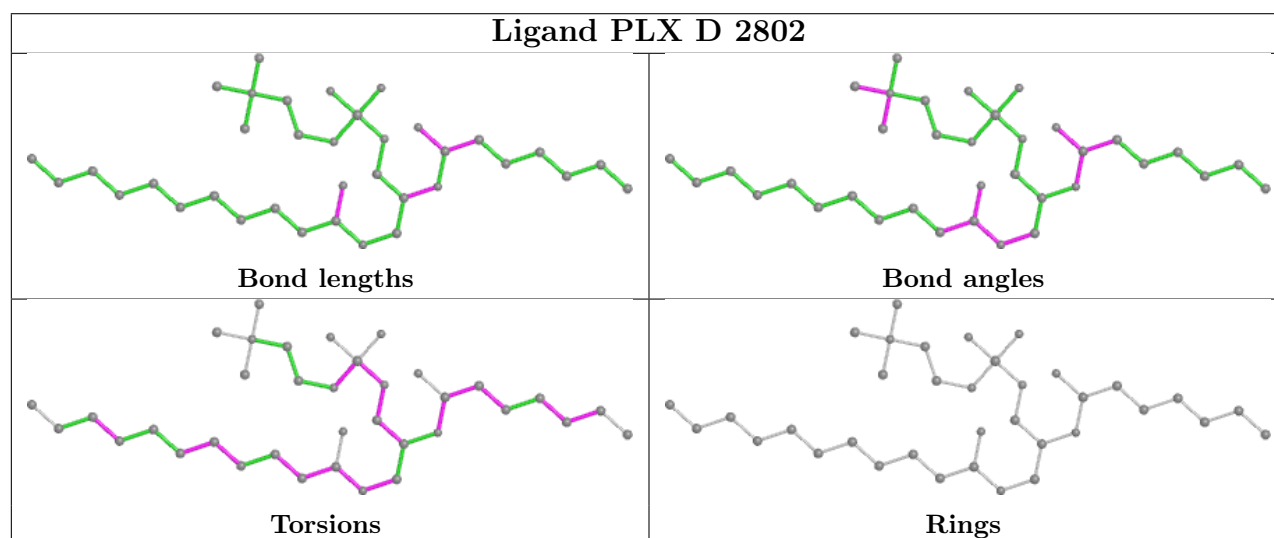
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2802	PLX	1	0
2	B	2808	PLX	2	0
2	A	2804	PLX	2	0
2	C	2805	PLX	1	0
2	A	2801	PLX	1	0
2	C	2802	PLX	2	0
2	A	2807	PLX	1	0
2	C	2804	PLX	18	0
2	B	2807	PLX	20	0
2	B	2803	PLX	1	0
2	B	2802	PLX	7	0

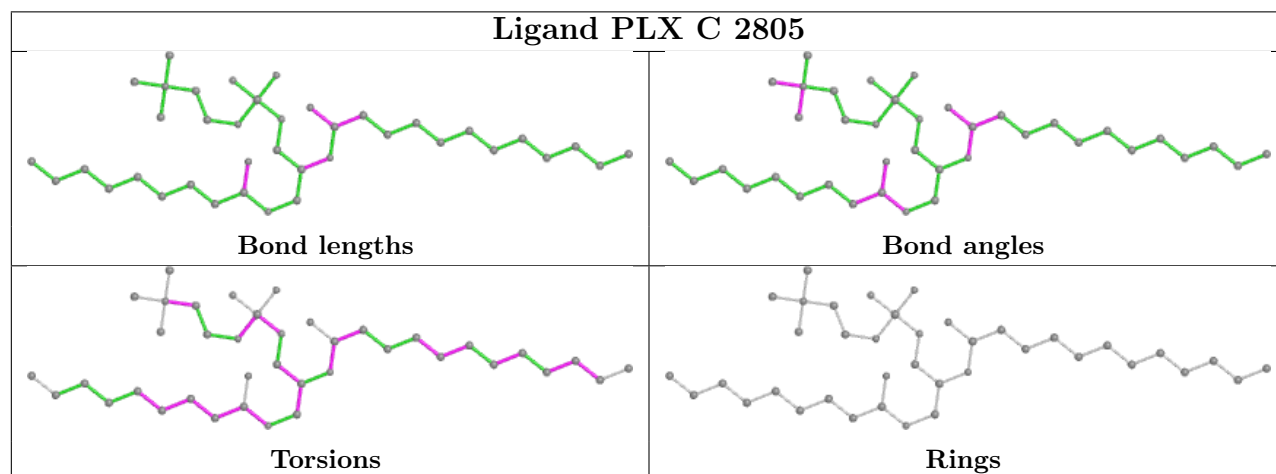
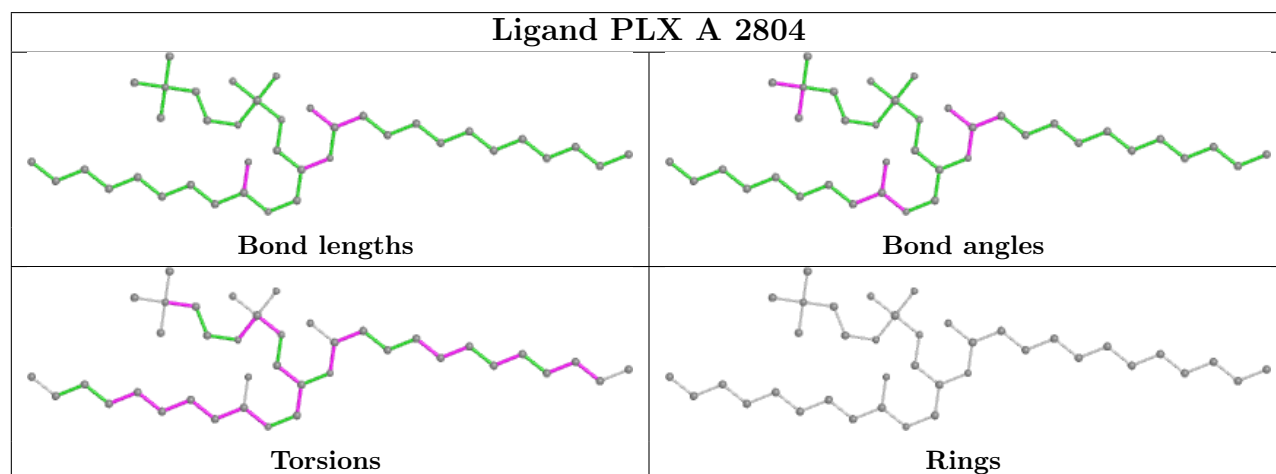
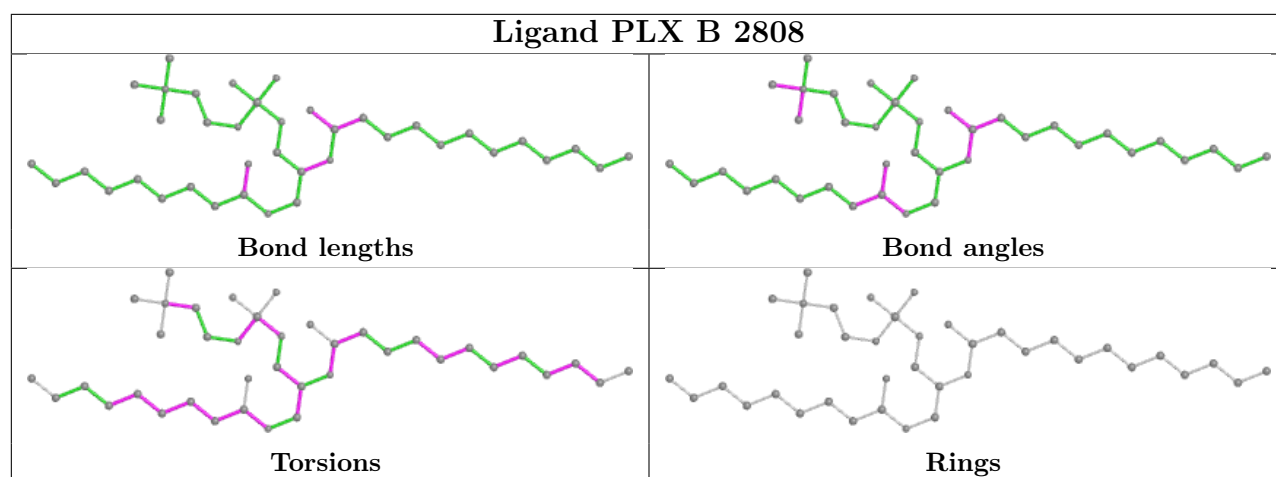
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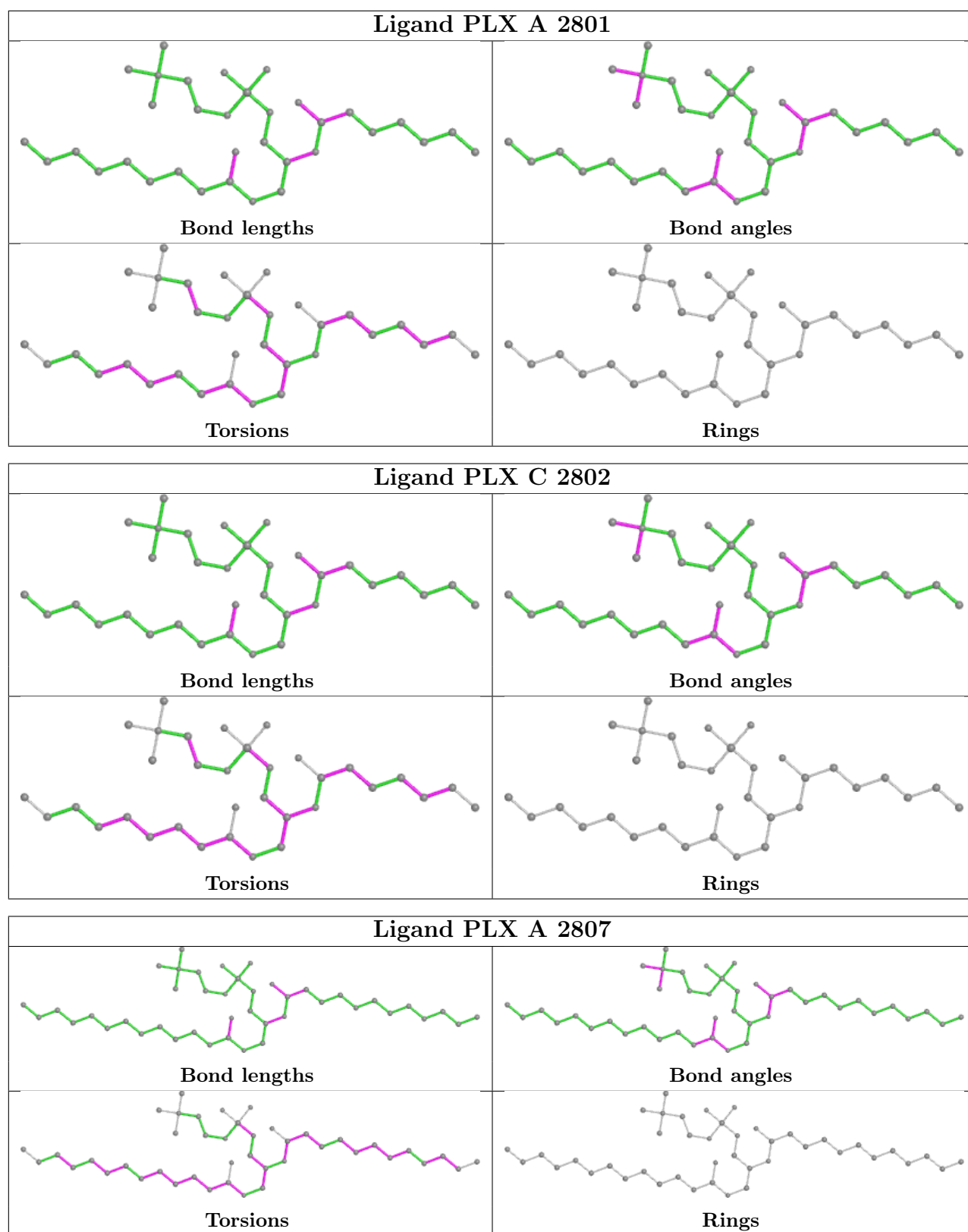
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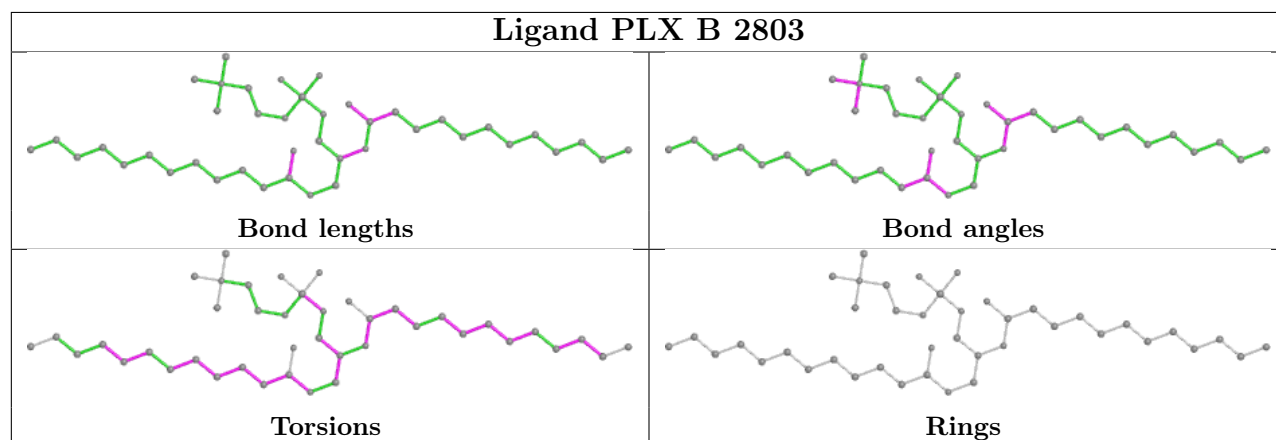
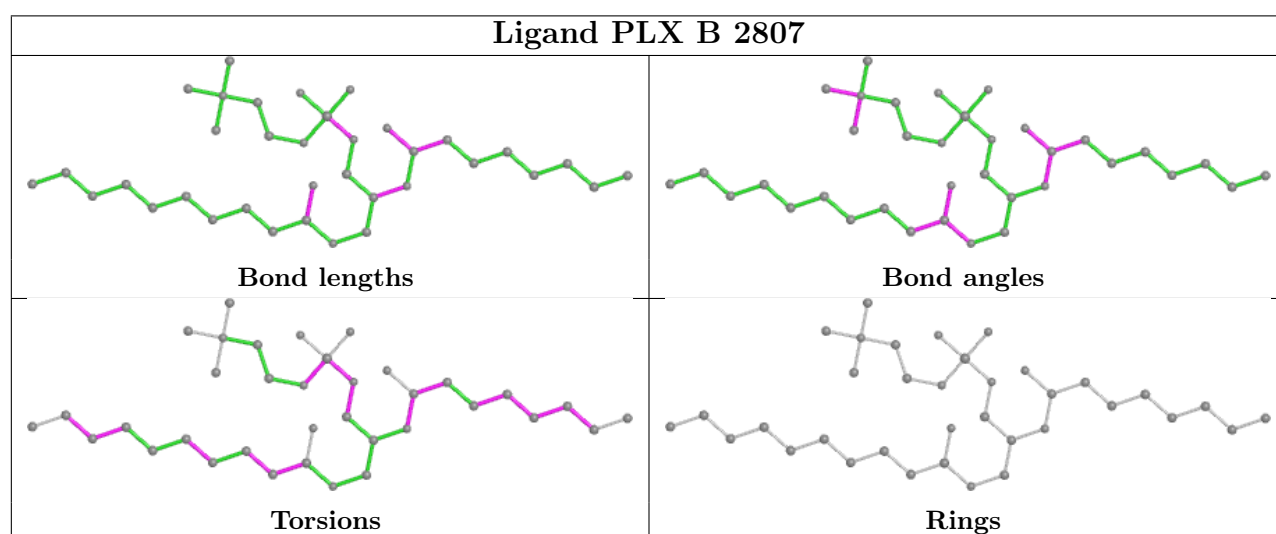
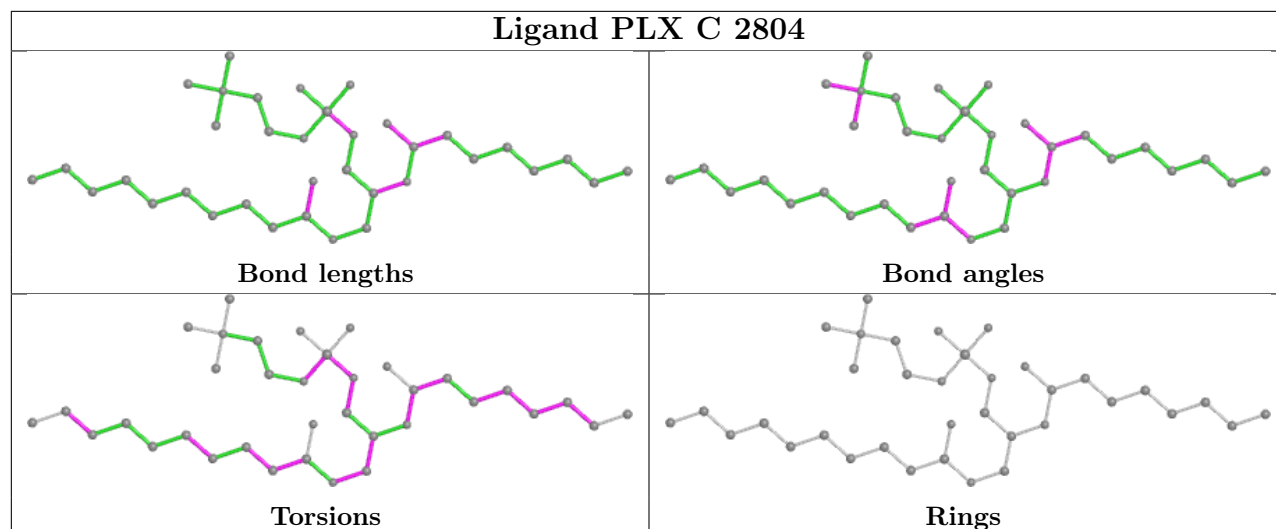
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2807	PLX	7	0
2	D	2803	PLX	18	0
2	C	2808	PLX	1	0
2	C	2803	PLX	3	0
2	D	2804	PLX	2	0
2	B	2806	PLX	3	0
2	A	2806	PLX	6	0
2	A	2803	PLX	18	0
2	D	2807	PLX	2	0
2	B	2805	PLX	2	0
2	D	2801	PLX	2	0
2	D	2806	PLX	5	0
2	A	2802	PLX	2	0

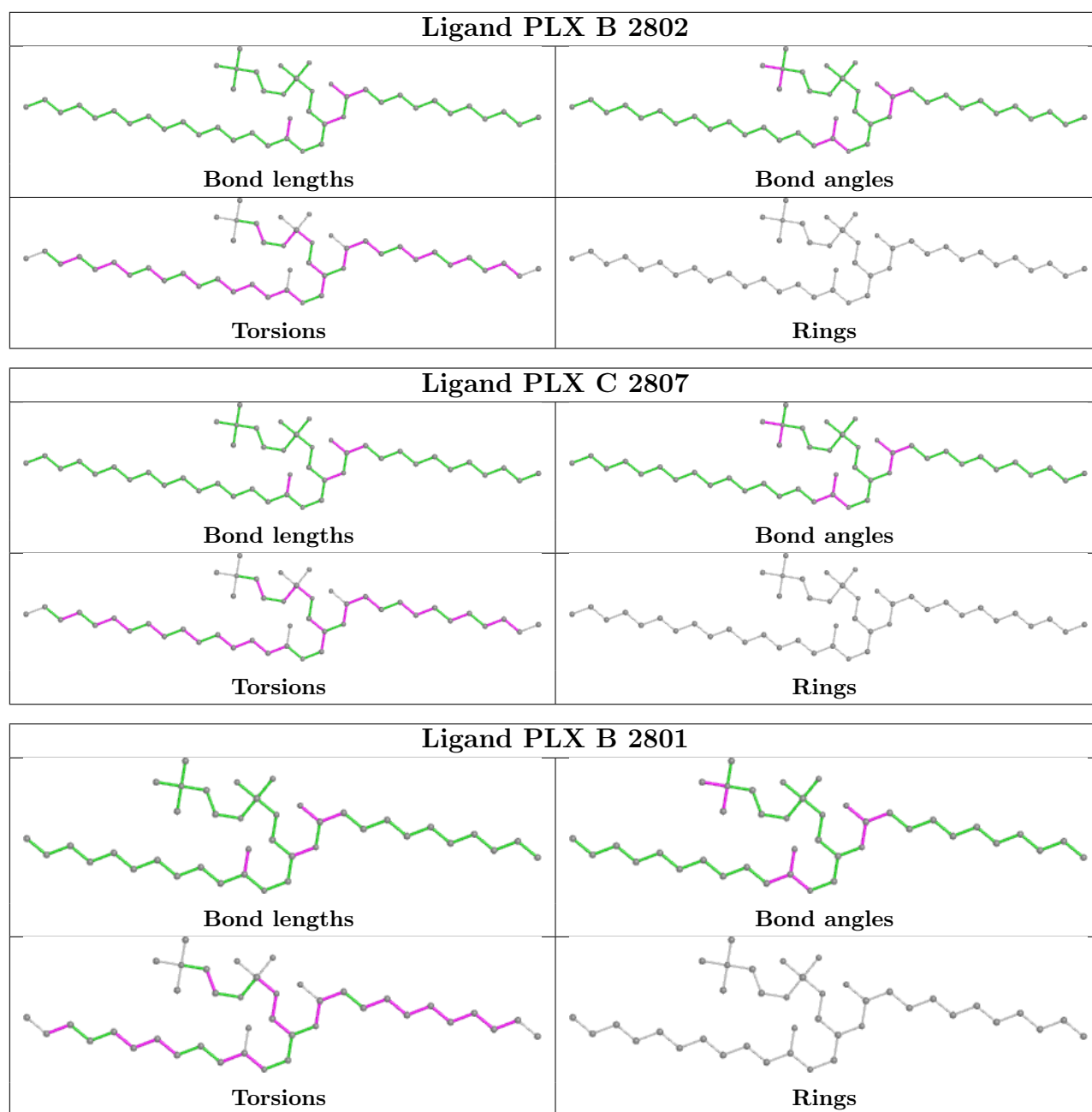
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

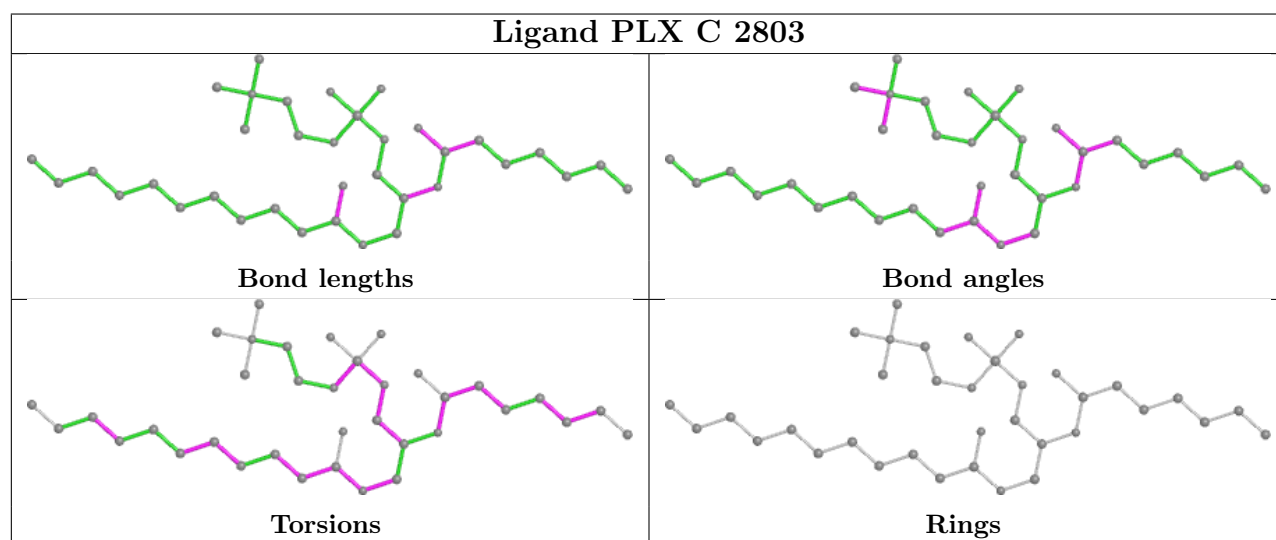
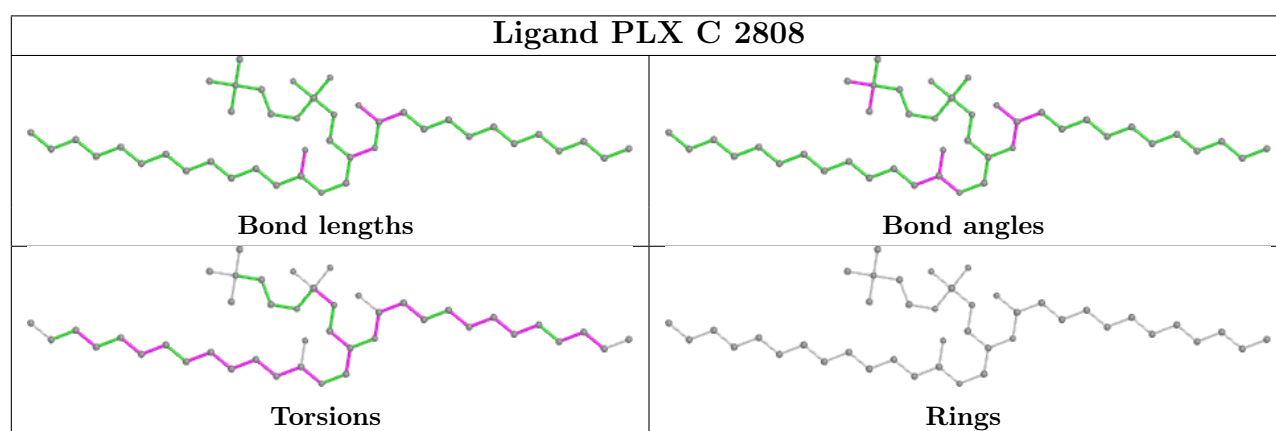
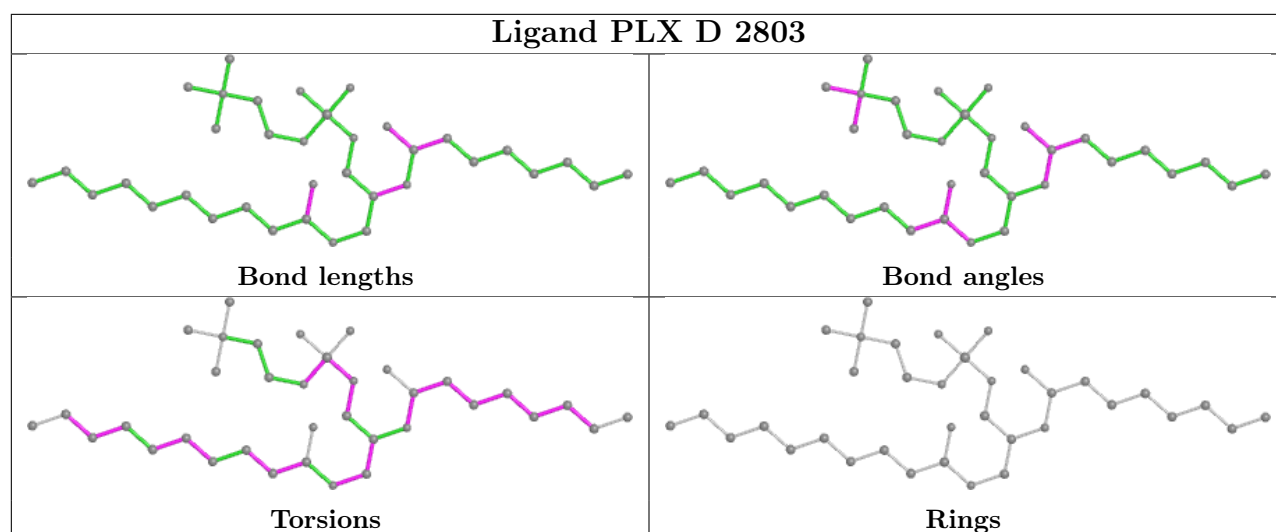


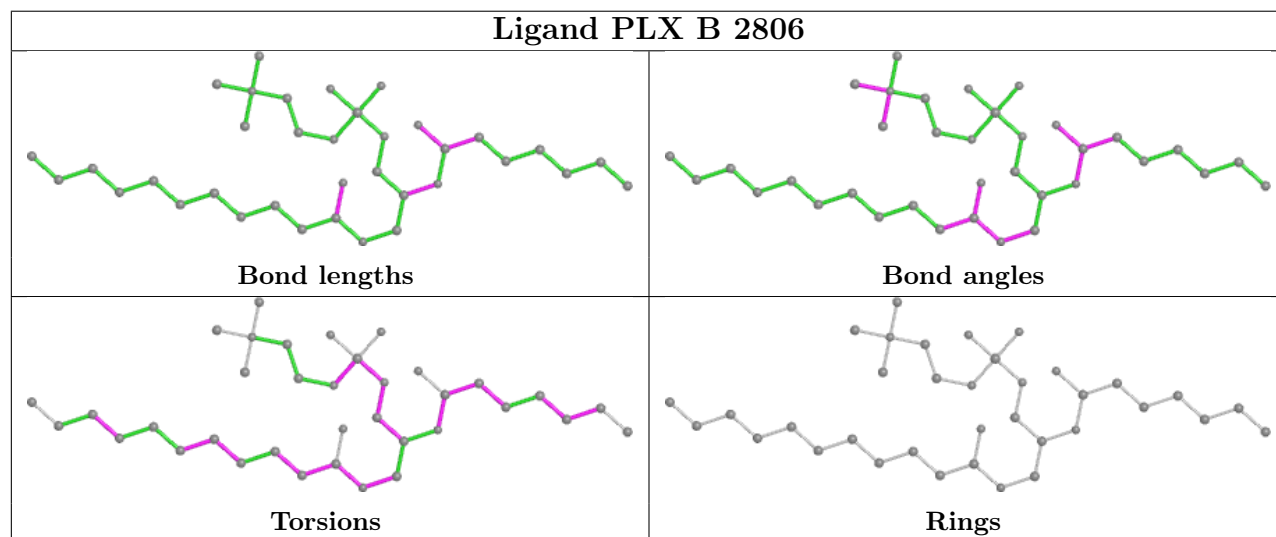
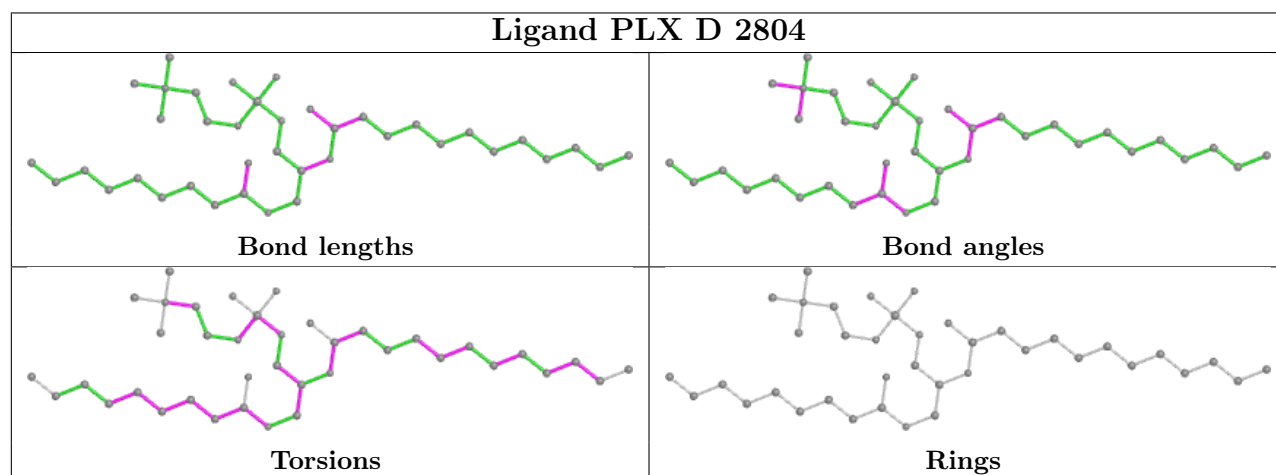
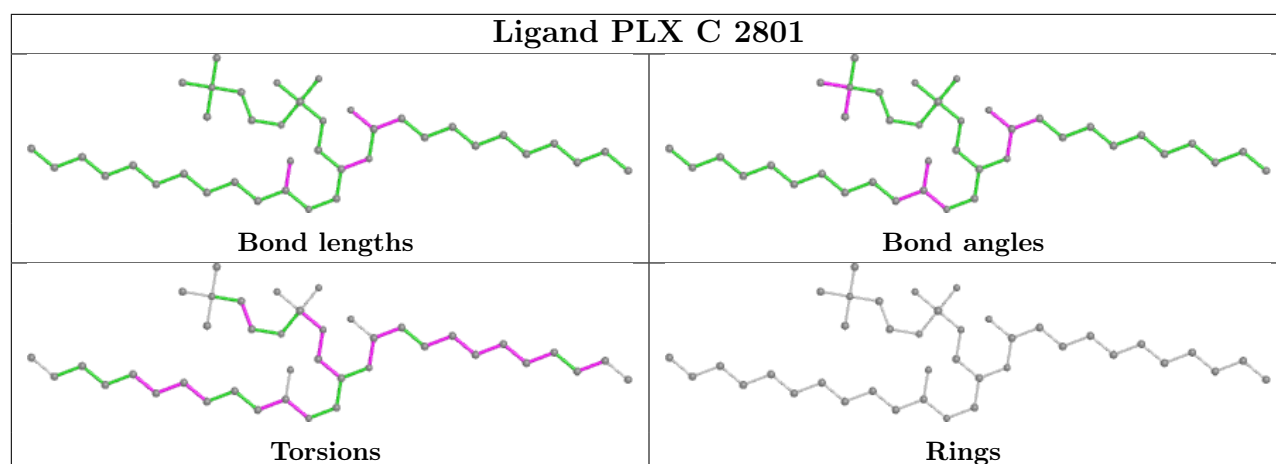


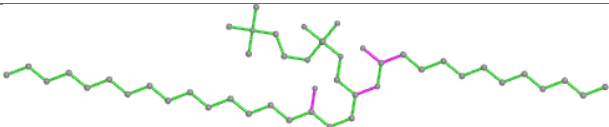
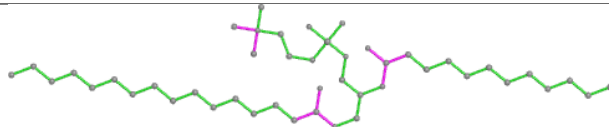
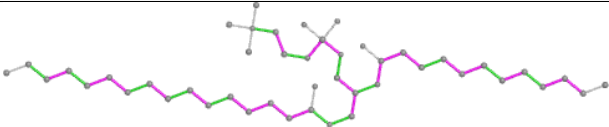
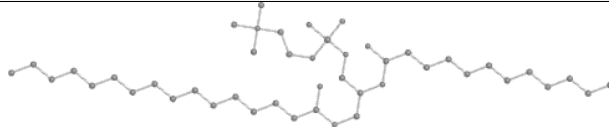


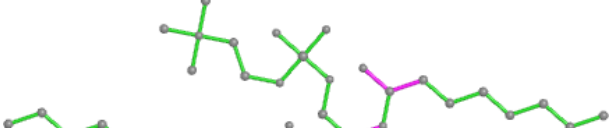
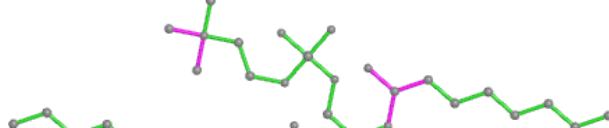
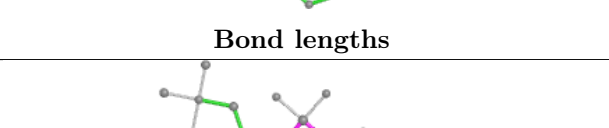
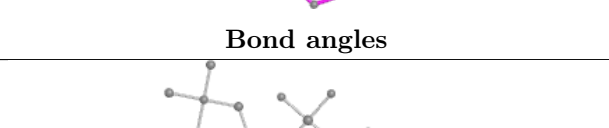


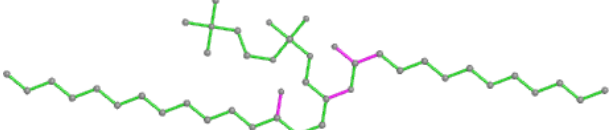
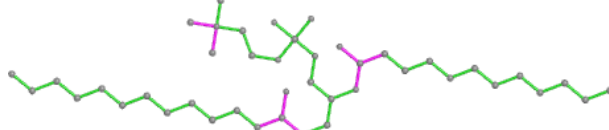
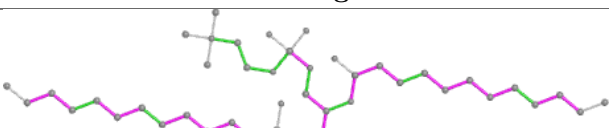
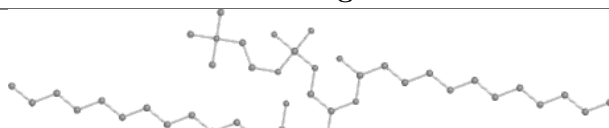


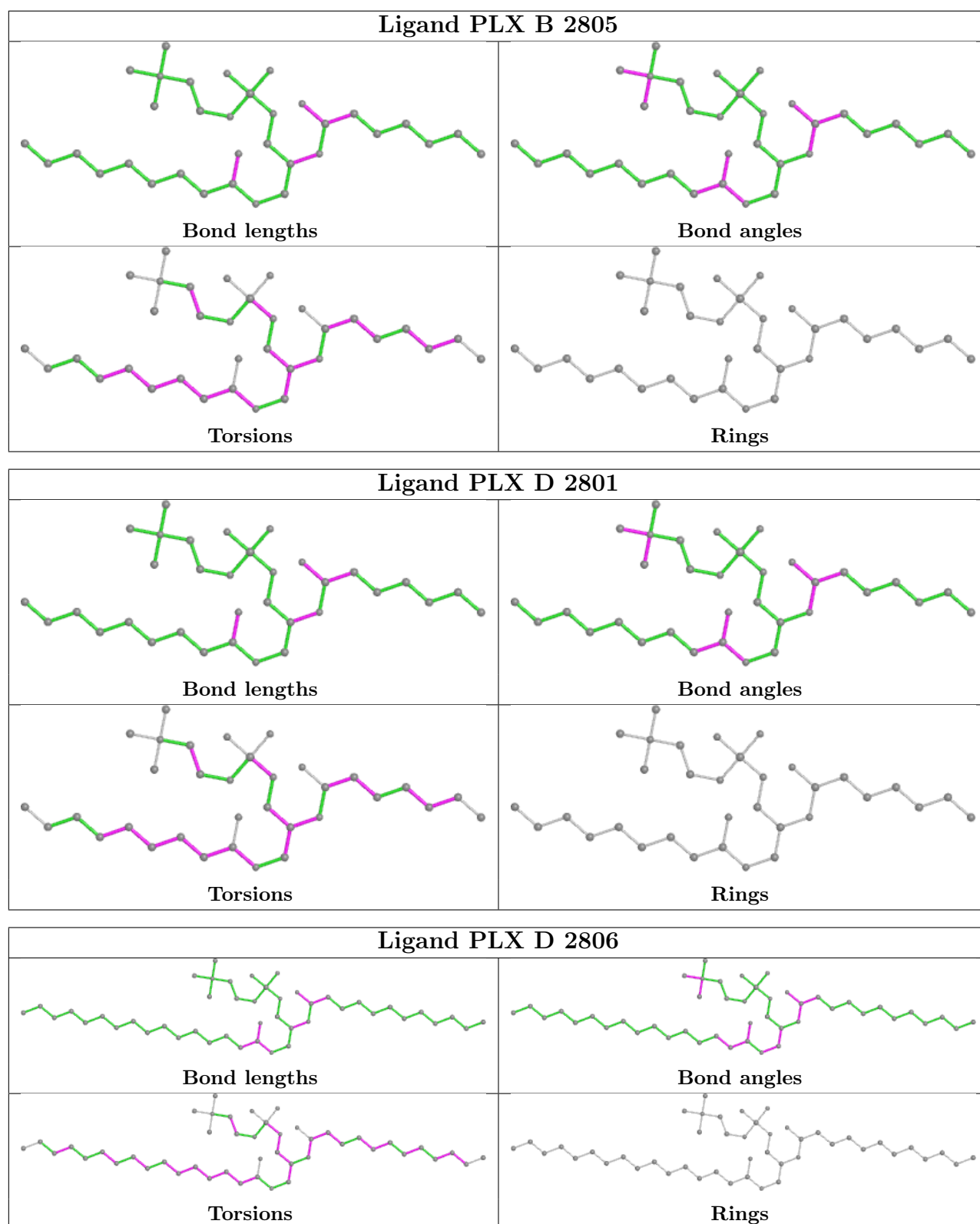


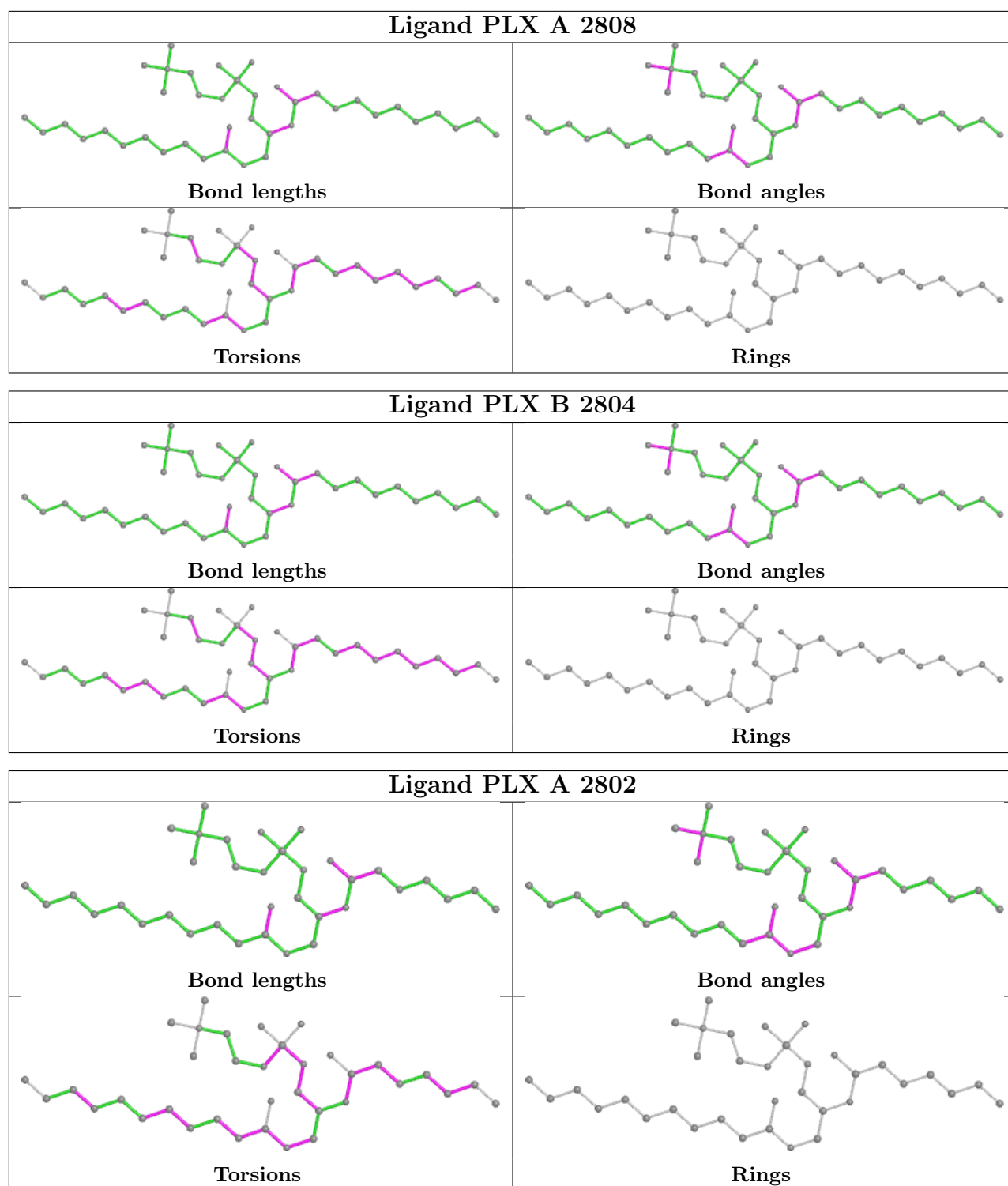


Ligand PLX A 2806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX A 2803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX D 2807	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

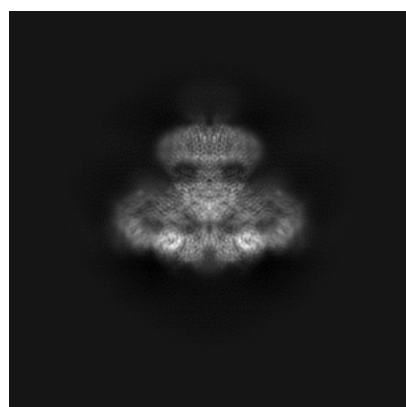
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23337. These allow visual inspection of the internal detail of the map and identification of artifacts.

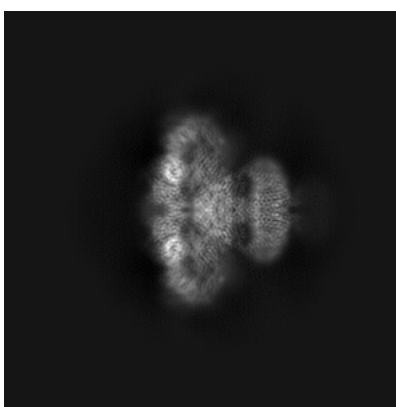
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

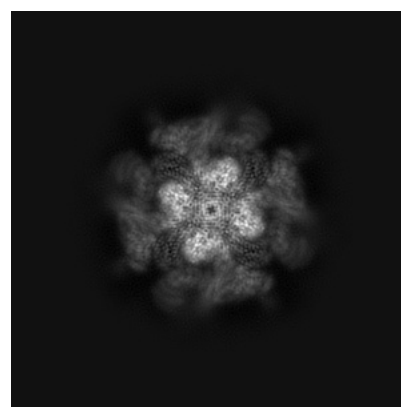
6.1.1 Primary map



X



Y

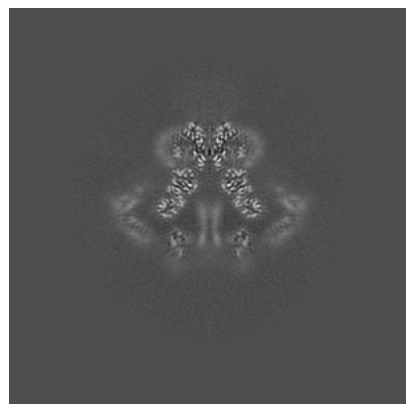


Z

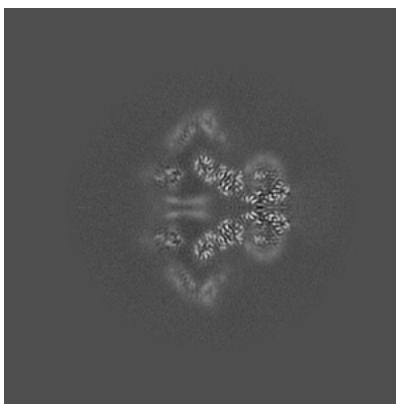
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

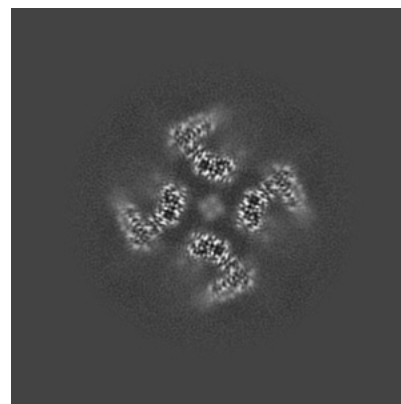
6.2.1 Primary map



X Index: 220



Y Index: 220

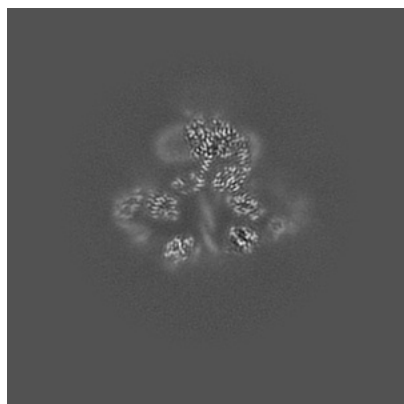


Z Index: 220

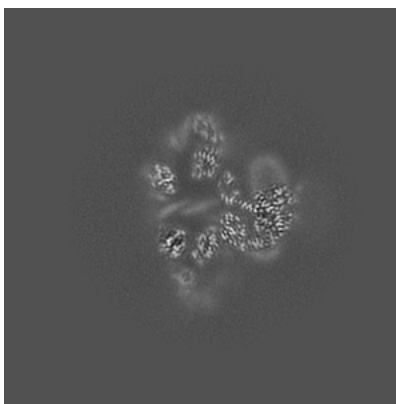
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

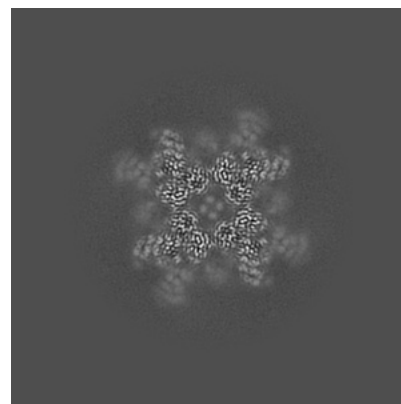
6.3.1 Primary map



X Index: 229



Y Index: 229



Z Index: 182

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

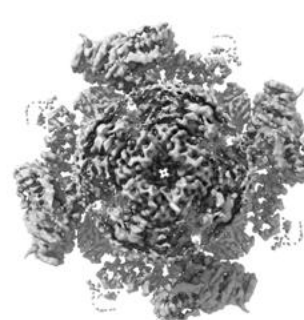
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

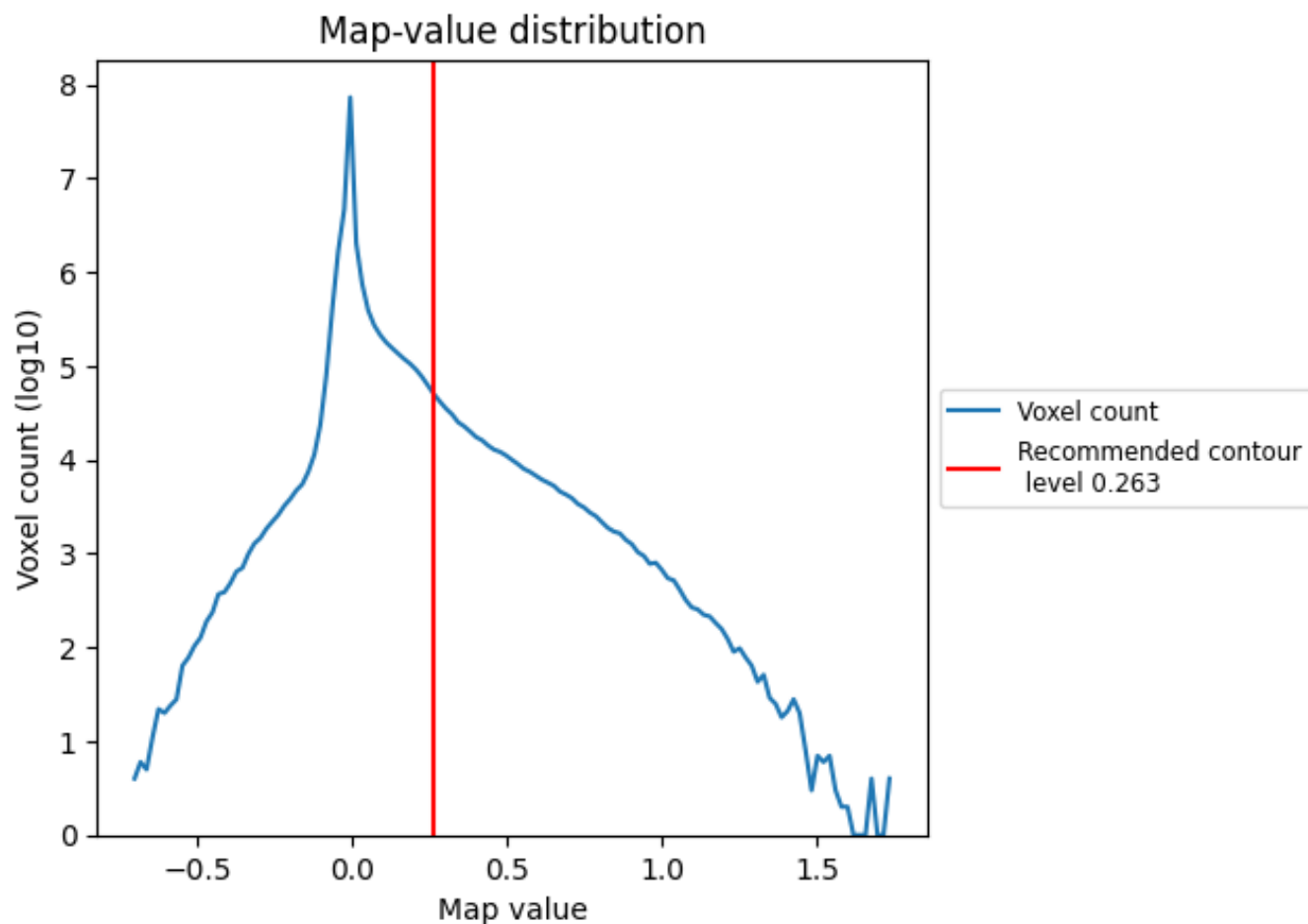
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

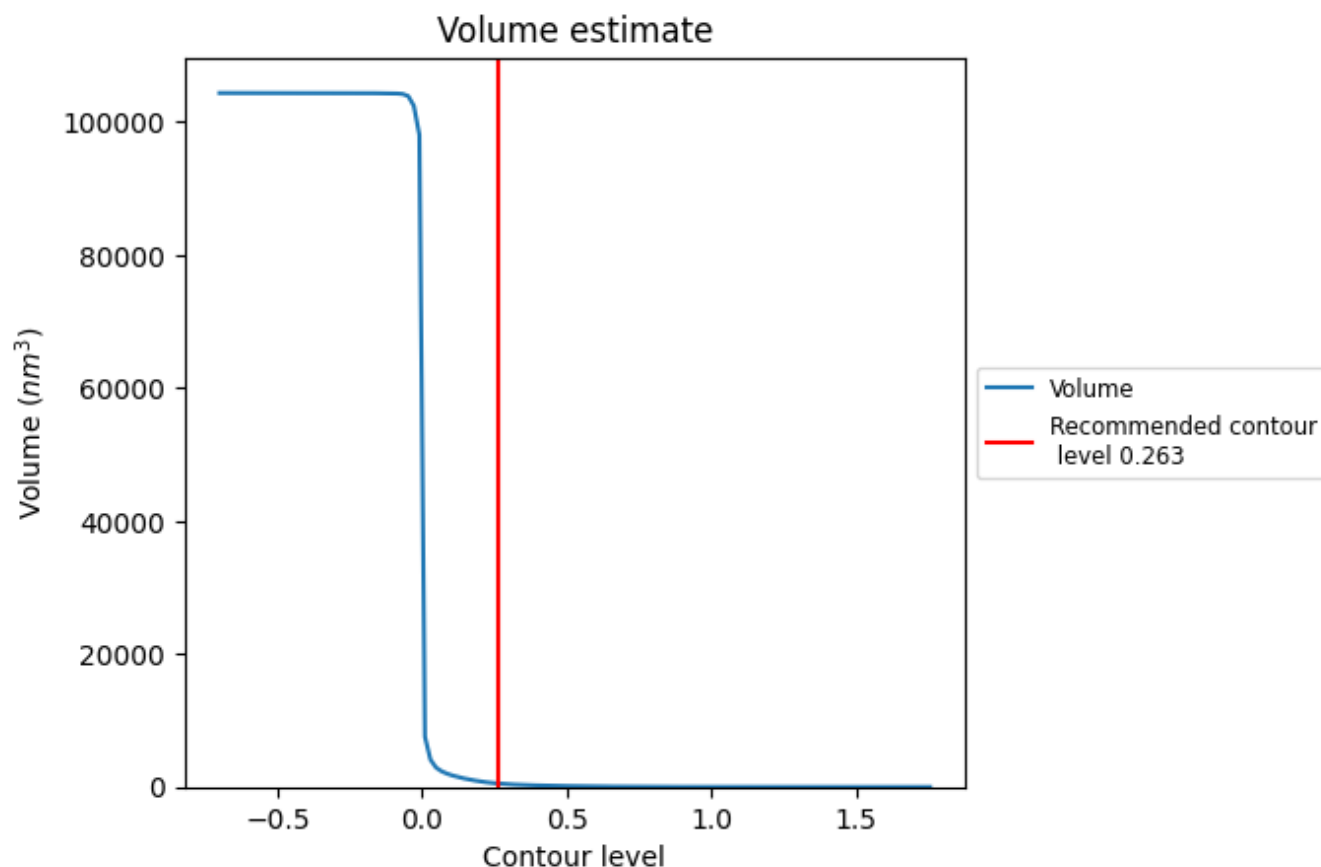
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

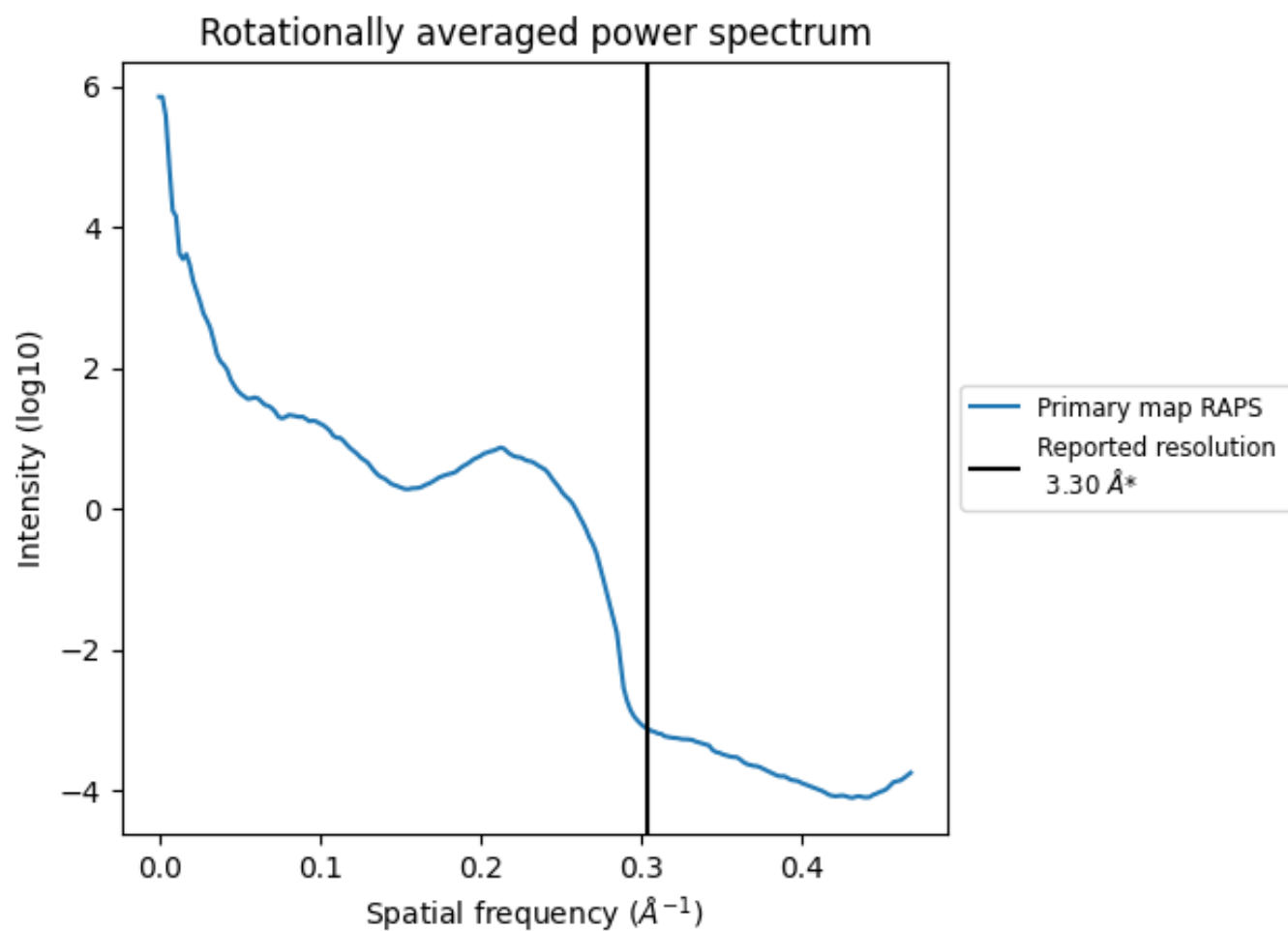
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 514 nm^3 ; this corresponds to an approximate mass of 464 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

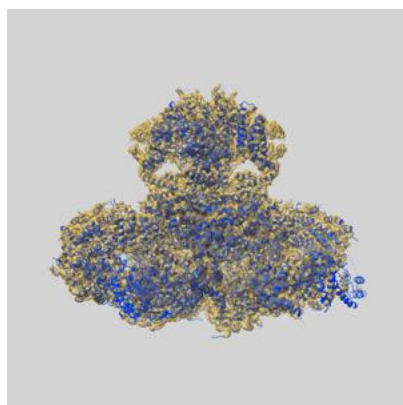
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

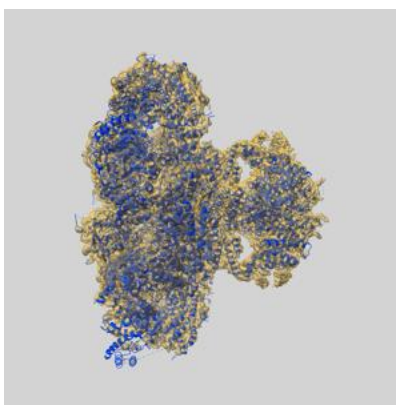
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23337 and PDB model 7LHE. Per-residue inclusion information can be found in section 3 on page 7.

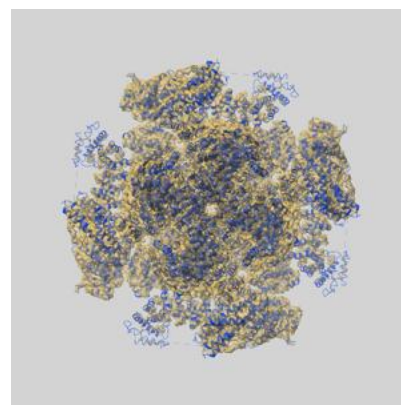
9.1 Map-model overlay [i](#)



X



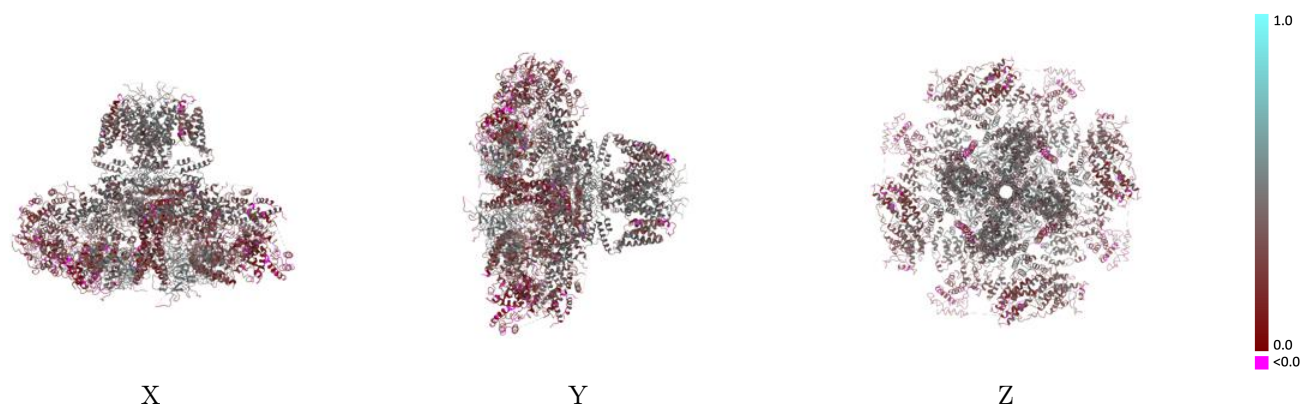
Y



Z

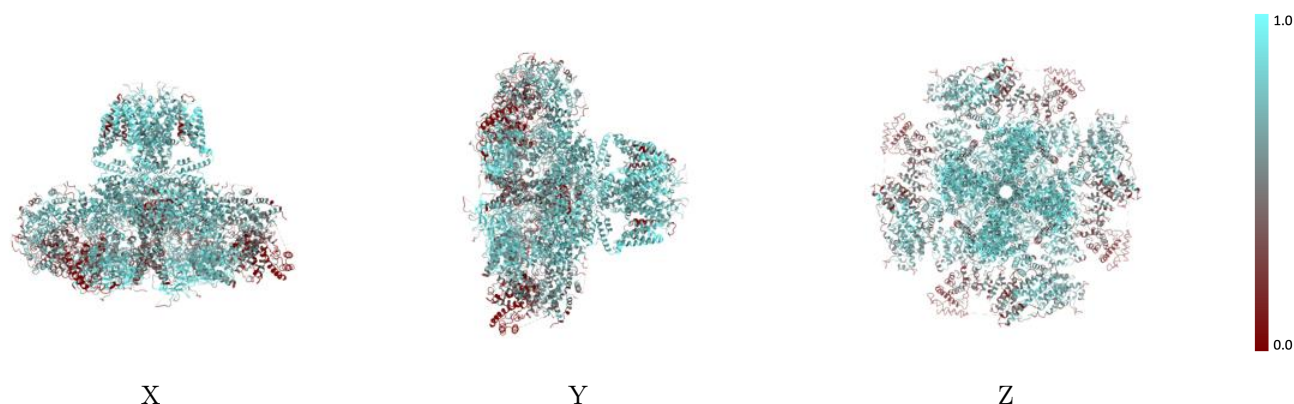
The images above show the 3D surface view of the map at the recommended contour level 0.263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



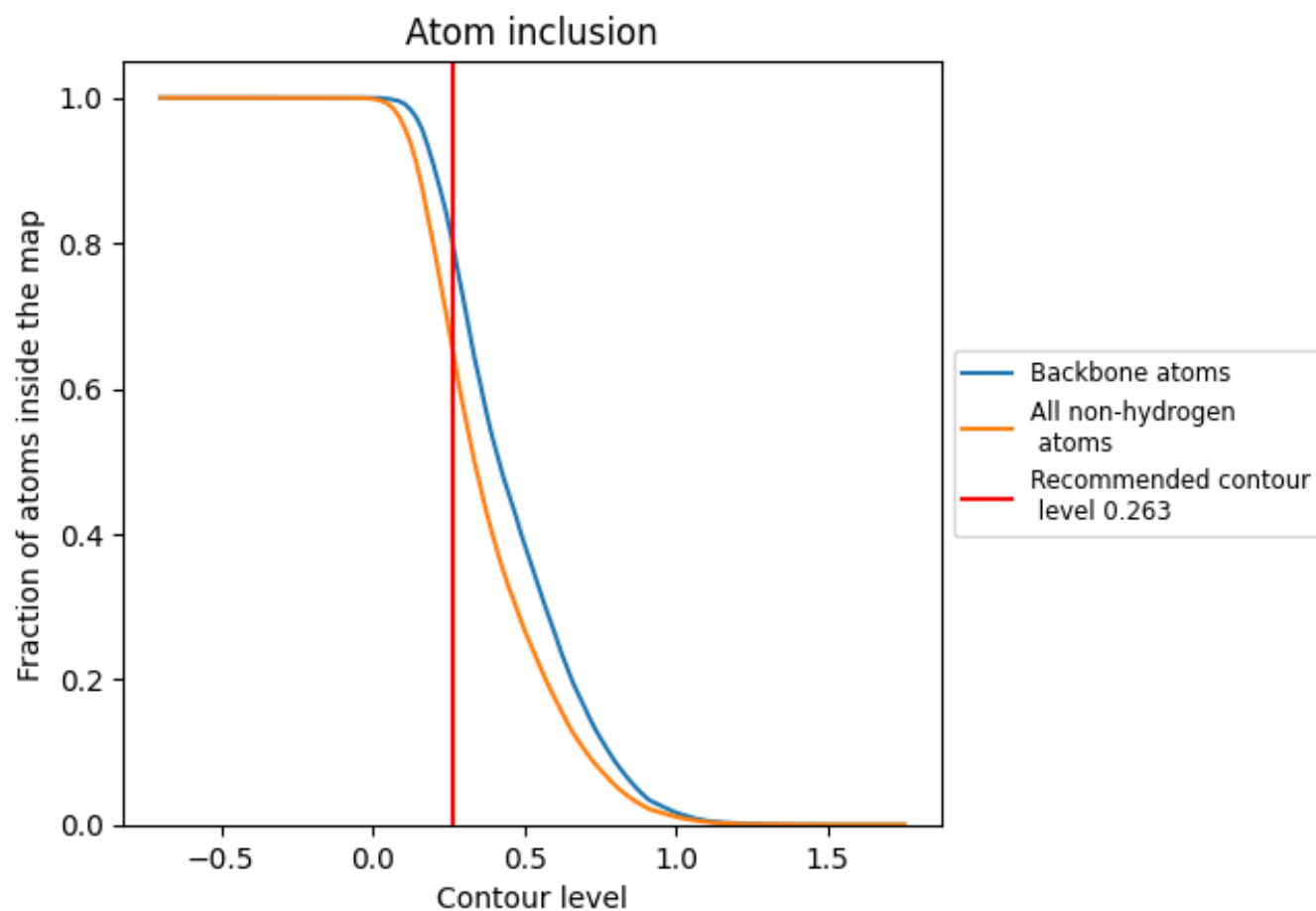
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.263).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6540	<div></div> 0.3460
A	<div></div> 0.6544	<div></div> 0.3460
B	<div></div> 0.6536	<div></div> 0.3460
C	<div></div> 0.6538	<div></div> 0.3460
D	<div></div> 0.6540	<div></div> 0.3450

