



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:18 PM UTC

PDB ID : 7LHF / pdb_00007lhf
EMDB ID : EMD-23338
Title : Structure of full-length IP3R1 channel solubilized in LNMG & lipid in the apo-state
Authors : Baker, M.R.; Fan, G.; Baker, M.L.; Serysheva, I.I.
Deposited on : 2021-01-22
Resolution : 2.96 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:

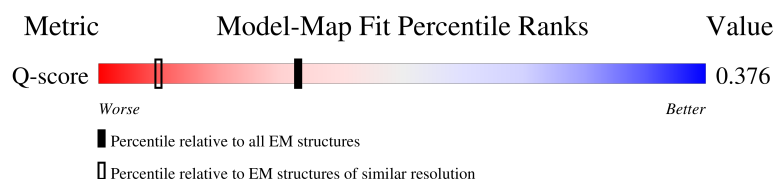
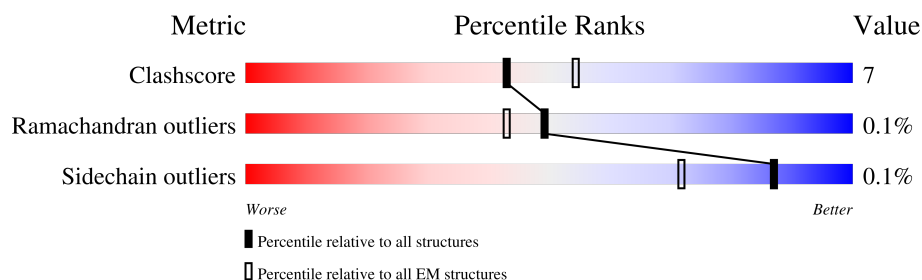
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	2736	
1	B	2736	
1	C	2736	
1	D	2736	

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	-	-	-
2	PLX	A	2802	X	-	-	-
2	PLX	A	2803	X	-	-	-
2	PLX	A	2804	X	-	-	-
2	PLX	A	2805	X	-	-	-
2	PLX	A	2806	X	-	-	-
2	PLX	A	2807	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	C	5102	X	-	-	-
2	PLX	C	5103	X	-	-	-
2	PLX	C	5104	X	-	-	-
2	PLX	C	5105	X	-	-	-
2	PLX	C	5106	X	-	-	-
2	PLX	C	5107	X	-	-	-
2	PLX	C	5108	X	-	-	-
2	PLX	D	5102	X	-	-	-
2	PLX	D	5103	X	-	-	-
2	PLX	D	5104	X	-	-	-
2	PLX	D	5105	X	-	-	-
2	PLX	D	5106	X	-	-	-
2	PLX	D	5107	X	-	-	-
2	PLX	D	5108	X	-	-	-

2 Entry composition [i](#)

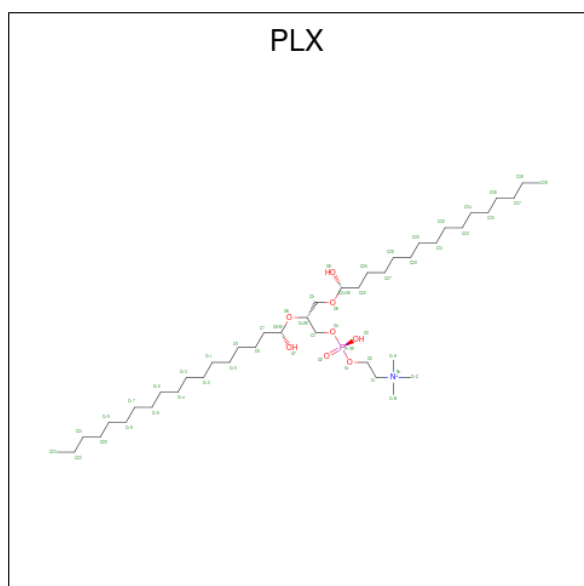
There are 3 unique types of molecules in this entry. The entry contains 72092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	D	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	B	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		
1	C	2300	Total	C	N	O	S	0	0
			17734	11338	3140	3156	100		

- 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 (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	A	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	D	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	D	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	D	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
2	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	B	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	B	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	B	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	B	1	Total	C	N	O	P	0
			40	30	1	8	1	
2	C	1	Total	C	N	O	P	0
			37	27	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
2	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
2	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			46	36	1	8	1	
2	C	1	Total	C	N	O	P	0
			40	30	1	8	1	

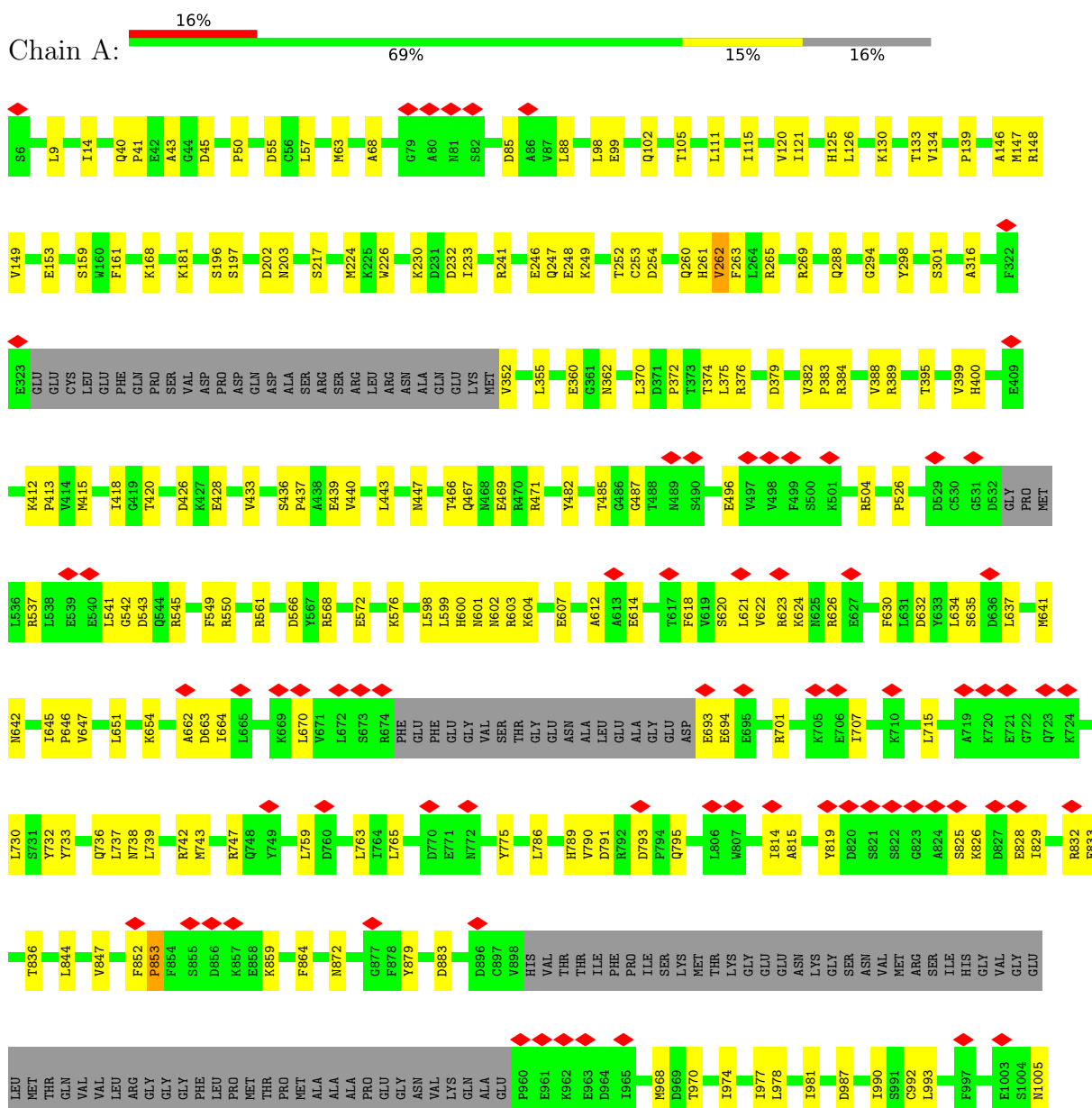
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

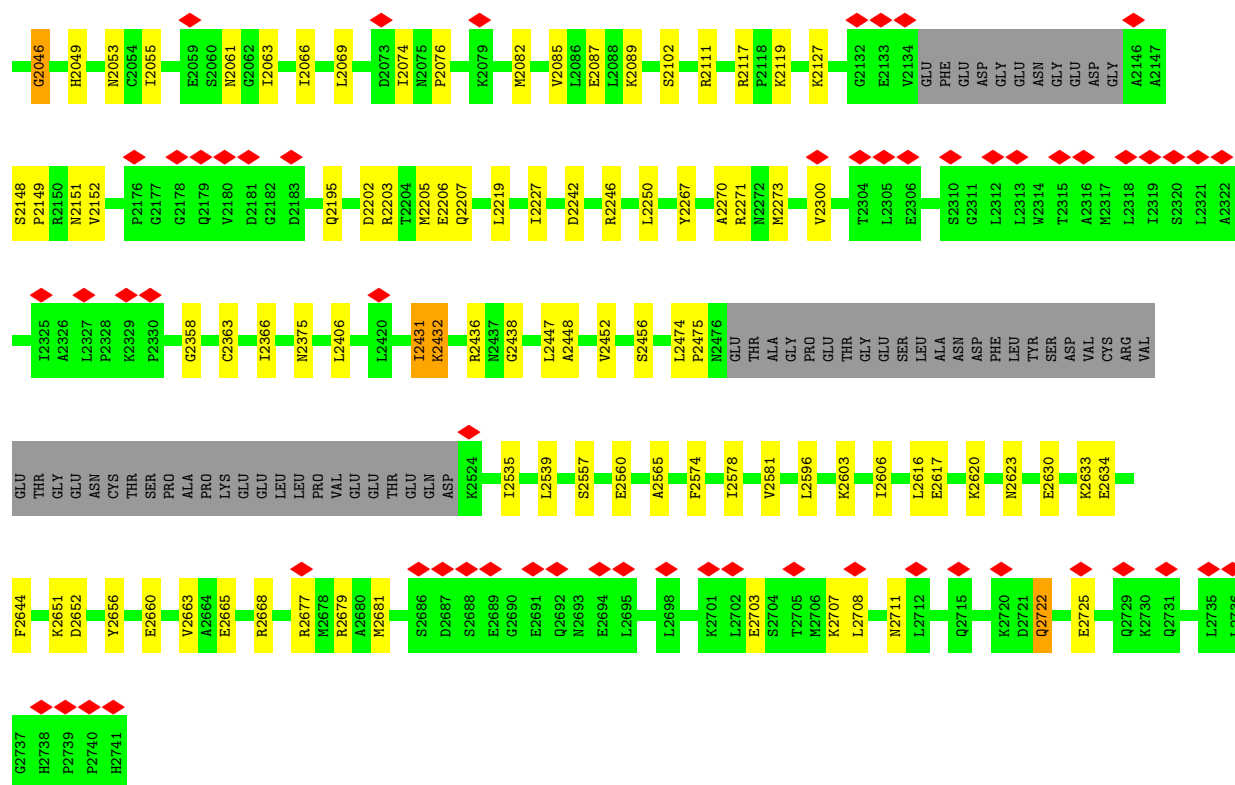
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

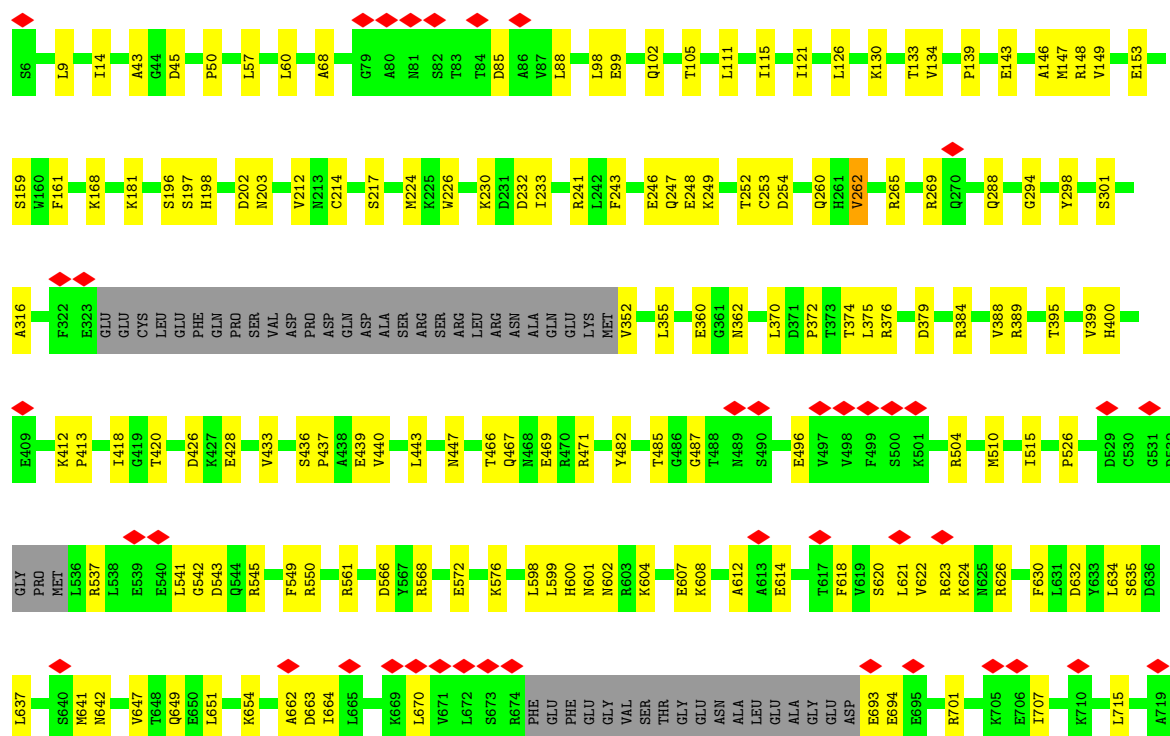
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



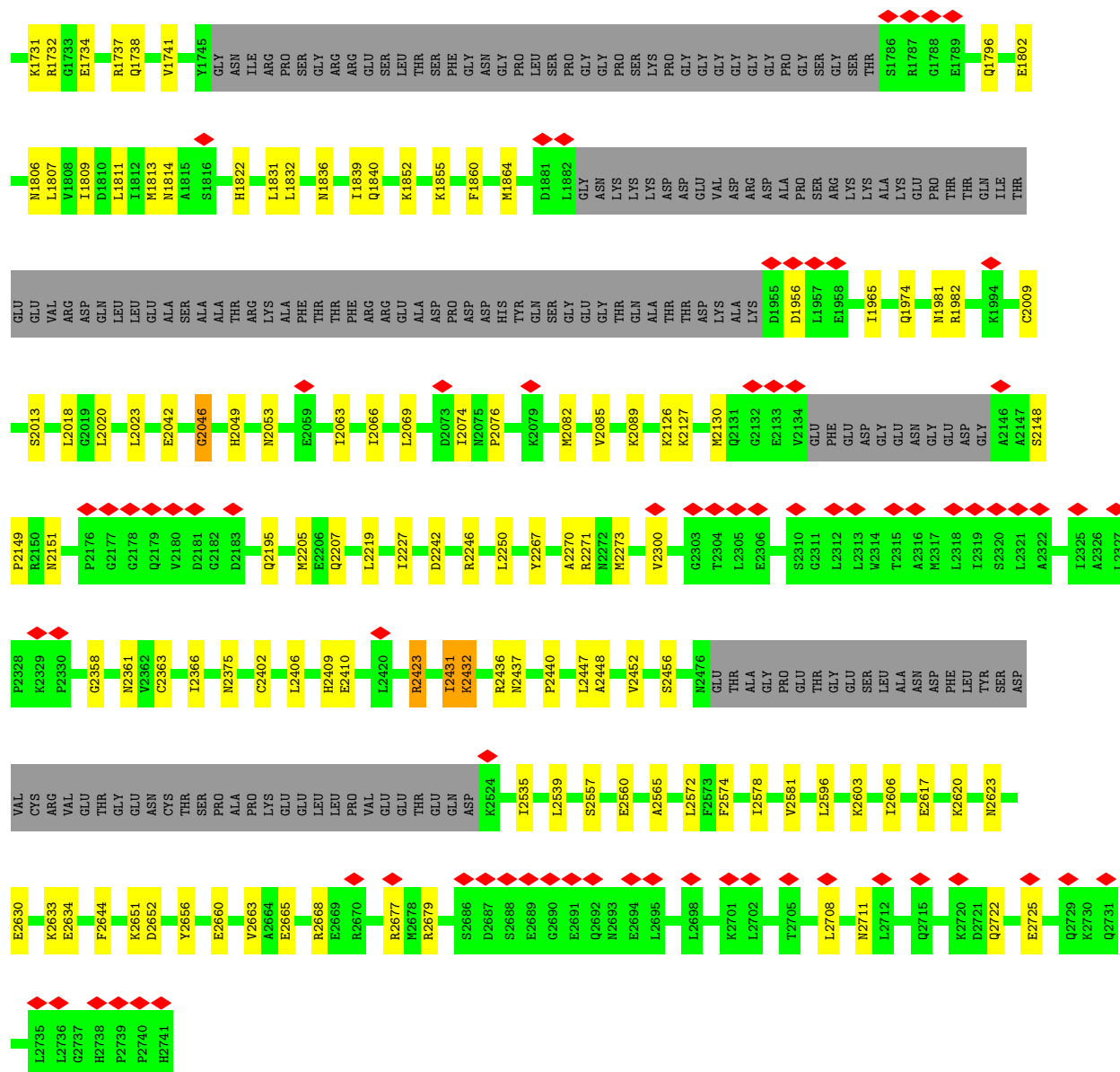




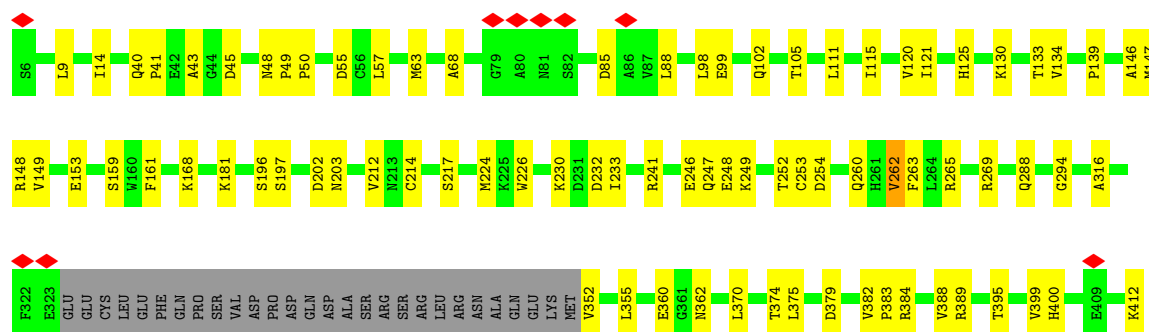
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

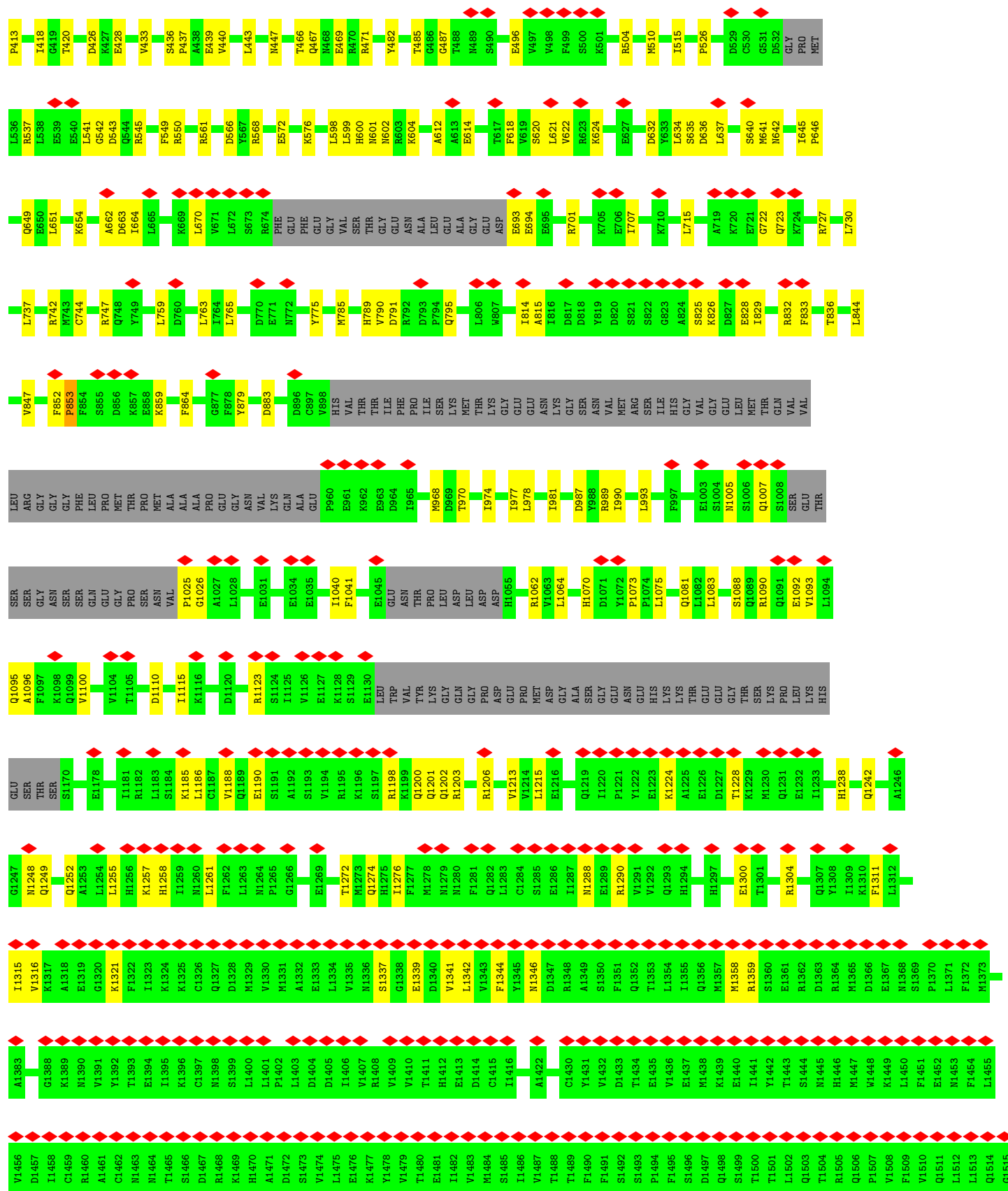




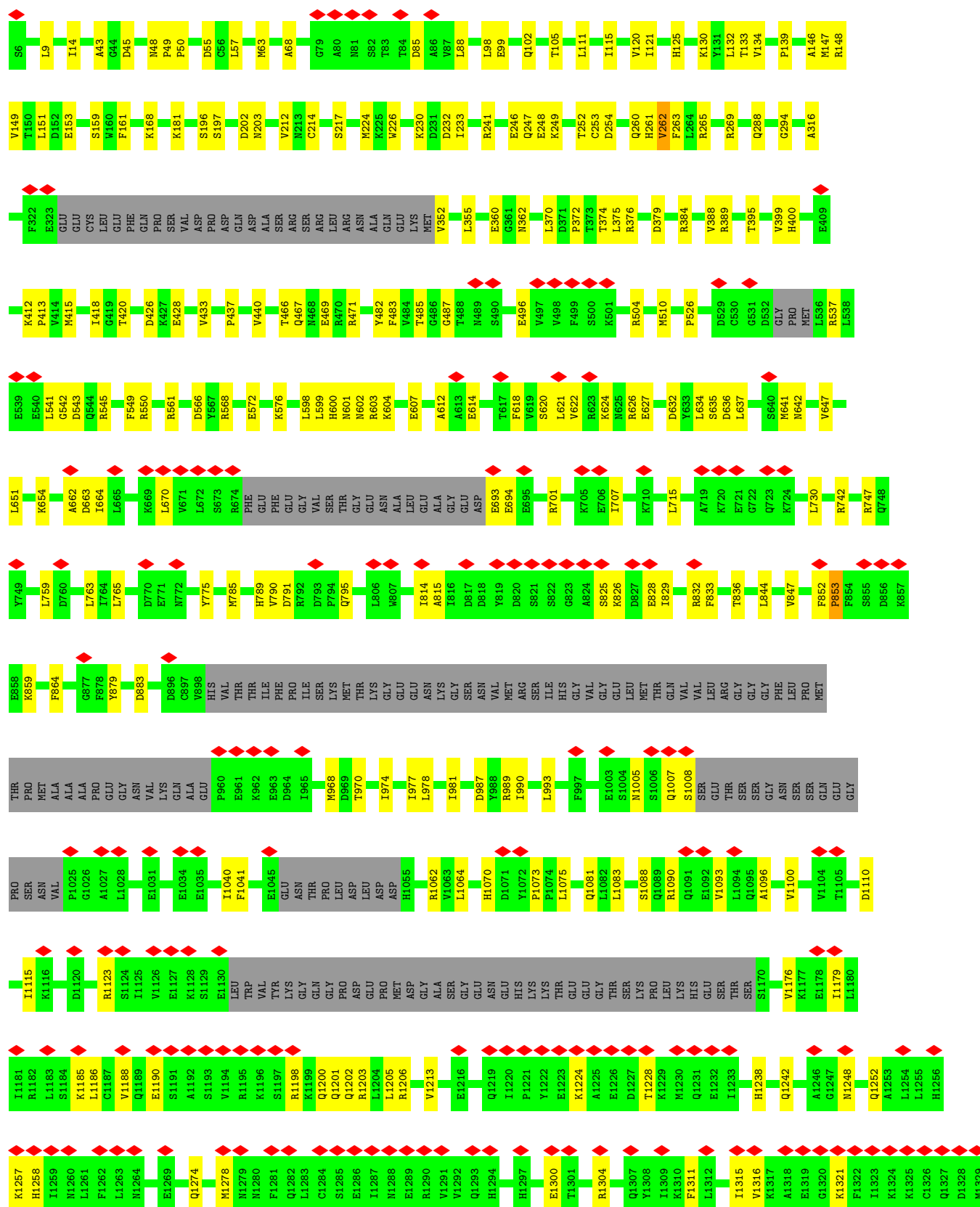


- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

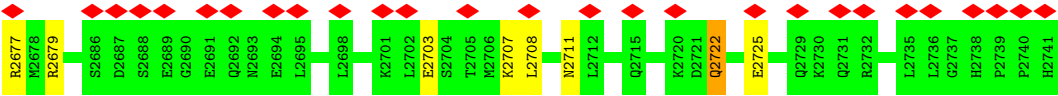












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	303481	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 ($e^-/\text{\AA}^2$)	42	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	0.087	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0112	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	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	0.22	0/18029	0.58	13/24246 (0.1%)
1	B	0.22	0/18029	0.57	11/24246 (0.0%)
1	C	0.22	0/18029	0.58	12/24246 (0.0%)
1	D	0.22	0/18029	0.57	11/24246 (0.0%)
All	All	0.22	0/72116	0.57	47/96984 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	5
1	D	0	6
All	All	0	20

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2432	LYS	CB-CG-CD	-10.94	86.14	111.30
1	B	2432	LYS	CB-CG-CD	-8.10	92.67	111.30
1	D	2432	LYS	CB-CG-CD	-7.69	93.61	111.30
1	C	2432	LYS	CB-CG-CD	-7.60	93.82	111.30
1	A	2432	LYS	N-CA-C	-7.48	104.18	113.38
1	A	2432	LYS	CG-CD-CE	7.09	127.60	111.30
1	C	146	ALA	CA-C-N	6.71	134.36	121.54
1	C	146	ALA	C-N-CA	6.71	134.36	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	ALA	CA-C-N	6.70	134.34	121.54
1	D	146	ALA	C-N-CA	6.70	134.34	121.54
1	B	146	ALA	CA-C-N	6.69	134.31	121.54
1	B	146	ALA	C-N-CA	6.69	134.31	121.54
1	B	2432	LYS	CA-CB-CG	6.65	127.40	114.10
1	D	2432	LYS	CA-CB-CG	6.52	127.13	114.10
1	C	2432	LYS	CA-CB-CG	6.51	127.13	114.10
1	A	2431	ILE	CA-C-N	-6.10	111.70	122.26
1	A	2431	ILE	C-N-CA	-6.10	111.70	122.26
1	C	2722	GLN	N-CA-CB	6.09	119.68	110.30
1	A	2432	LYS	CA-CB-CG	5.99	126.08	114.10
1	A	146	ALA	CA-C-N	5.93	132.86	121.54
1	A	146	ALA	C-N-CA	5.93	132.86	121.54
1	B	2300	VAL	N-CA-C	-5.91	108.09	113.71
1	C	2300	VAL	N-CA-C	-5.85	108.16	113.71
1	A	2300	VAL	N-CA-C	-5.83	108.17	113.71
1	D	2300	VAL	N-CA-C	-5.79	108.20	113.71
1	B	2431	ILE	CA-C-N	-5.70	113.70	122.60
1	B	2431	ILE	C-N-CA	-5.70	113.70	122.60
1	D	2431	ILE	CA-C-N	-5.60	113.86	122.60
1	D	2431	ILE	C-N-CA	-5.60	113.86	122.60
1	C	2431	ILE	CA-C-N	-5.58	113.89	122.60
1	C	2431	ILE	C-N-CA	-5.58	113.89	122.60
1	A	2432	LYS	CD-CE-NZ	-5.50	94.29	111.90
1	C	262	VAL	CA-C-N	5.48	132.01	121.54
1	C	262	VAL	C-N-CA	5.48	132.01	121.54
1	A	262	VAL	CA-C-N	5.48	132.00	121.54
1	A	262	VAL	C-N-CA	5.48	132.00	121.54
1	D	262	VAL	CA-C-N	5.47	131.98	121.54
1	D	262	VAL	C-N-CA	5.47	131.98	121.54
1	B	2432	LYS	CG-CD-CE	5.46	123.86	111.30
1	B	262	VAL	CA-C-N	5.45	131.96	121.54
1	B	262	VAL	C-N-CA	5.45	131.96	121.54
1	D	2432	LYS	CG-CD-CE	5.29	123.47	111.30
1	C	2432	LYS	CG-CD-CE	5.16	123.18	111.30
1	B	2432	LYS	CB-CA-C	5.04	119.24	110.72
1	D	2432	LYS	CB-CA-C	5.03	119.21	110.72
1	C	2432	LYS	CB-CA-C	5.01	119.18	110.72
1	A	2722	GLN	N-CA-CB	5.00	118.04	110.28

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1346	ASN	Peptide
1	A	1637	PHE	Peptide
1	A	2046	GLY	Peptide
1	A	663	ASP	Peptide
1	B	1346	ASN	Peptide
1	B	1637	PHE	Peptide
1	B	2046	GLY	Peptide
1	B	2432	LYS	Peptide
1	B	663	ASP	Peptide
1	C	1346	ASN	Peptide
1	C	1637	PHE	Peptide
1	C	2046	GLY	Peptide
1	C	2432	LYS	Peptide
1	C	663	ASP	Peptide
1	D	1346	ASN	Peptide
1	D	1637	PHE	Peptide
1	D	2046	GLY	Peptide
1	D	2423	ARG	Sidechain
1	D	2432	LYS	Peptide
1	D	663	ASP	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	17734	0	17384	244	0
1	B	17734	0	17383	235	0
1	C	17734	0	17383	227	0
1	D	17734	0	17383	236	0
2	A	288	0	399	12	0
2	B	288	0	395	10	0
2	C	288	0	398	8	0
2	D	288	0	398	9	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	72092	0	71123	946	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 (946) 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:A:1096:ALA:O	1:A:1100:VAL:HB	1.78	0.83
1:D:1096:ALA:O	1:D:1100:VAL:HB	1.79	0.82
1:B:1096:ALA:O	1:B:1100:VAL:HB	1.83	0.78
1:C:1096:ALA:O	1:C:1100:VAL:HB	1.87	0.73
1:D:288:GLN:HG3	1:D:294:GLY:HA2	1.69	0.73
1:B:288:GLN:HG3	1:B:294:GLY:HA2	1.71	0.72
1:A:288:GLN:HG3	1:A:294:GLY:HA2	1.71	0.71
1:D:2361:ASN:ND2	1:D:2402:CYS:SG	2.63	0.71
1:C:288:GLN:HG3	1:C:294:GLY:HA2	1.72	0.70
1:A:111:LEU:HG	1:A:226:TRP:HE1	1.56	0.70
1:D:111:LEU:HG	1:D:226:TRP:HE1	1.56	0.70
1:B:1864:MET:HG3	1:B:1966:MET:HE3	1.74	0.70
1:C:111:LEU:HG	1:C:226:TRP:HE1	1.56	0.70
1:D:232:ASP:HA	1:D:384:ARG:HD2	1.74	0.70
1:C:232:ASP:HA	1:C:384:ARG:HD2	1.74	0.69
1:B:133:THR:HG22	1:B:159:SER:HB3	1.73	0.69
1:D:133:THR:HG22	1:D:159:SER:HB3	1.75	0.69
1:A:232:ASP:HA	1:A:384:ARG:HD2	1.74	0.69
1:C:133:THR:HG22	1:C:159:SER:HB3	1.73	0.69
1:B:111:LEU:HG	1:B:226:TRP:HE1	1.56	0.68
1:B:232:ASP:HA	1:B:384:ARG:HD2	1.74	0.68
1:D:360:GLU:OE2	1:D:362:ASN:ND2	2.27	0.67
1:C:1864:MET:HG3	1:C:1966:MET:HE3	1.74	0.67
1:A:63:MET:HE2	1:A:120:VAL:HG21	1.76	0.67
1:A:360:GLU:OE2	1:A:362:ASN:ND2	2.27	0.66
1:B:360:GLU:OE2	1:B:362:ASN:ND2	2.28	0.66
1:C:360:GLU:OE2	1:C:362:ASN:ND2	2.27	0.66
1:C:599:LEU:HD22	1:C:637:LEU:HB3	1.79	0.65
1:A:2205:MET:HE2	1:A:2679:ARG:HE	1.61	0.64
1:B:599:LEU:HD22	1:B:637:LEU:HB3	1.79	0.64
1:A:1974:GLN:HG3	1:A:2042:GLU:HG3	1.81	0.63
1:D:1974:GLN:HG3	1:D:2042:GLU:HG3	1.81	0.63
1:B:640:SER:OG	1:B:742:ARG:NH1	2.32	0.63
1:A:701:ARG:HB3	1:A:707:ILE:HD12	1.80	0.63
1:D:701:ARG:HB3	1:D:707:ILE:HD12	1.80	0.63
1:C:701:ARG:HB3	1:C:707:ILE:HD12	1.80	0.62
1:C:1974:GLN:HG3	1:C:2042:GLU:HG3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LEU:O	1:A:550:ARG:NH2	2.33	0.62
1:D:541:LEU:O	1:D:550:ARG:NH2	2.33	0.62
1:B:541:LEU:O	1:B:550:ARG:NH2	2.32	0.62
1:B:1796:GLN:OE1	1:B:1836:ASN:ND2	2.31	0.62
1:B:614:GLU:O	1:B:618:PHE:HB2	2.00	0.61
1:B:701:ARG:HB3	1:B:707:ILE:HD12	1.80	0.61
1:C:614:GLU:O	1:C:618:PHE:HB2	1.99	0.61
1:B:1683:MET:HE2	1:B:1831:LEU:HA	1.83	0.61
1:B:1974:GLN:HG3	1:B:2042:GLU:HG3	1.82	0.61
1:D:614:GLU:O	1:D:618:PHE:HB2	1.99	0.61
1:B:542:GLY:HA2	1:B:550:ARG:HH22	1.66	0.61
1:A:1796:GLN:OE1	1:A:1836:ASN:ND2	2.31	0.61
1:C:542:GLY:HA2	1:C:550:ARG:HH22	1.65	0.61
1:A:542:GLY:HA2	1:A:550:ARG:HH22	1.65	0.61
1:A:1683:MET:HE2	1:A:1831:LEU:HA	1.82	0.61
1:C:541:LEU:O	1:C:550:ARG:NH2	2.33	0.61
1:D:693:GLU:HG2	1:D:694:GLU:HG2	1.83	0.61
1:A:693:GLU:HG2	1:A:694:GLU:HG2	1.83	0.60
1:D:542:GLY:HA2	1:D:550:ARG:HH22	1.66	0.60
1:C:2448:ALA:HB2	1:C:2581:VAL:HG11	1.83	0.60
1:D:1683:MET:HE2	1:D:1831:LEU:HA	1.82	0.60
1:A:747:ARG:NH1	1:A:791:ASP:O	2.34	0.60
1:A:790:VAL:HG12	1:A:795:GLN:HE21	1.65	0.60
1:B:693:GLU:HG2	1:B:694:GLU:HG2	1.83	0.60
1:D:1840:GLN:OE1	1:D:1981:ASN:ND2	2.35	0.59
1:B:1840:GLN:OE1	1:B:1981:ASN:ND2	2.36	0.59
1:A:2448:ALA:HB2	1:A:2581:VAL:HG11	1.83	0.59
1:C:693:GLU:HG2	1:C:694:GLU:HG2	1.83	0.59
1:B:2195:GLN:NE2	1:B:2207:GLN:OE1	2.35	0.59
2:B:2803:PLX:H271	2:B:2803:PLX:H101	1.84	0.59
1:C:1840:GLN:OE1	1:C:1981:ASN:ND2	2.36	0.59
1:C:2110:GLU:HA	1:C:2113:LEU:HB2	1.85	0.59
1:A:614:GLU:O	1:A:618:PHE:HB2	2.03	0.59
1:D:2448:ALA:HB2	1:D:2581:VAL:HG11	1.84	0.59
1:B:747:ARG:NH1	1:B:791:ASP:O	2.36	0.59
1:D:249:LYS:HB2	1:D:269:ARG:HH21	1.68	0.59
1:D:1796:GLN:OE1	1:D:1836:ASN:ND2	2.31	0.59
1:B:2651:LYS:HG2	1:B:2652:ASP:H	1.68	0.59
1:C:968:MET:HB3	1:C:1073:PRO:HG3	1.85	0.58
1:D:828:GLU:HG2	1:D:829:ILE:HG23	1.85	0.58
1:C:626:ARG:HG3	1:C:627:GLU:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:GLN:NE2	1:C:1278:MET:SD	2.77	0.58
1:D:1252:GLN:NE2	1:D:1278:MET:SD	2.76	0.58
1:D:1616:ARG:HH22	1:D:1732:ARG:HD3	1.69	0.58
1:C:2651:LYS:HG2	1:C:2652:ASP:H	1.68	0.58
1:A:1840:GLN:OE1	1:A:1981:ASN:ND2	2.35	0.58
1:B:828:GLU:HG2	1:B:829:ILE:HG23	1.84	0.58
1:B:1603:ARG:HG3	1:B:1604:LEU:HD12	1.86	0.58
1:B:2474:LEU:HD12	1:B:2475:PRO:HD2	1.85	0.58
1:A:599:LEU:HD22	1:A:637:LEU:HB3	1.86	0.58
1:A:828:GLU:HG2	1:A:829:ILE:HG23	1.85	0.58
1:D:1603:ARG:HG3	1:D:1604:LEU:HD12	1.86	0.58
1:B:968:MET:HB3	1:B:1073:PRO:HG3	1.85	0.58
1:B:2448:ALA:HB2	1:B:2581:VAL:HG11	1.85	0.58
1:C:828:GLU:HG2	1:C:829:ILE:HG23	1.84	0.58
1:C:1616:ARG:HH22	1:C:1732:ARG:HD3	1.69	0.58
1:C:230:LYS:HB2	1:C:233:ILE:HD12	1.86	0.58
1:C:1603:ARG:HG3	1:C:1604:LEU:HD12	1.86	0.58
1:A:1252:GLN:NE2	1:A:1278:MET:SD	2.76	0.58
1:A:1832:LEU:HA	1:A:1839:ILE:HD11	1.85	0.58
1:B:537:ARG:O	1:B:550:ARG:NH2	2.37	0.58
1:C:1796:GLN:OE1	1:C:1836:ASN:ND2	2.30	0.58
1:C:2205:MET:HE2	1:C:2679:ARG:HE	1.68	0.58
1:D:599:LEU:HD22	1:D:637:LEU:HB3	1.85	0.58
1:D:759:LEU:HA	1:D:763:LEU:HD23	1.86	0.58
1:D:968:MET:HB3	1:D:1073:PRO:HG3	1.84	0.58
1:A:968:MET:HB3	1:A:1073:PRO:HG3	1.85	0.58
1:B:230:LYS:HB2	1:B:233:ILE:HD12	1.86	0.58
1:A:1603:ARG:HG3	1:A:1604:LEU:HD12	1.86	0.57
1:A:2651:LYS:HG2	1:A:2652:ASP:H	1.68	0.57
1:D:2651:LYS:HG2	1:D:2652:ASP:H	1.68	0.57
1:B:1832:LEU:HA	1:B:1839:ILE:HD11	1.85	0.57
1:C:747:ARG:NH1	1:C:791:ASP:O	2.36	0.57
1:C:1832:LEU:HA	1:C:1839:ILE:HD11	1.85	0.57
1:D:253:CYS:SG	1:D:254:ASP:N	2.77	0.57
1:D:600:HIS:ND1	1:D:601:ASN:OD1	2.37	0.57
1:D:1832:LEU:HA	1:D:1839:ILE:HD11	1.85	0.57
1:A:635:SER:OG	1:A:742:ARG:NH2	2.36	0.57
1:A:1088:SER:HB2	1:A:1622:GLU:HB3	1.86	0.57
1:A:2474:LEU:HD12	1:A:2475:PRO:HD2	1.85	0.57
1:D:14:ILE:HG22	1:D:57:LEU:HD12	1.87	0.57
1:D:1092:GLU:HA	1:D:1095:GLN:HG2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1257:LYS:HG3	1:C:1258:HIS:HD2	1.69	0.57
1:C:2195:GLN:NE2	1:C:2207:GLN:OE1	2.38	0.57
1:D:436:SER:OG	1:D:439:GLU:OE1	2.22	0.57
1:D:2195:GLN:NE2	1:D:2207:GLN:OE1	2.38	0.57
1:A:600:HIS:ND1	1:A:601:ASN:OD1	2.35	0.57
1:D:230:LYS:HB2	1:D:233:ILE:HD12	1.86	0.57
1:B:1616:ARG:HH22	1:B:1732:ARG:HD3	1.70	0.57
1:C:537:ARG:O	1:C:550:ARG:NH2	2.36	0.57
1:C:1640:ASN:O	1:C:1645:ARG:NH1	2.38	0.57
1:D:2074:ILE:HG22	1:D:2076:PRO:HD2	1.87	0.56
1:B:1640:ASN:O	1:B:1645:ARG:NH1	2.38	0.56
1:C:2074:ILE:HG22	1:C:2076:PRO:HD2	1.87	0.56
1:A:230:LYS:HB2	1:A:233:ILE:HD12	1.86	0.56
1:A:436:SER:OG	1:A:439:GLU:OE1	2.22	0.56
1:C:389:ARG:NH2	1:C:426:ASP:OD1	2.38	0.56
1:A:1616:ARG:HH22	1:A:1732:ARG:HD3	1.70	0.56
1:B:759:LEU:HA	1:B:763:LEU:HD23	1.86	0.56
1:B:775:TYR:HE2	1:B:859:LYS:HA	1.70	0.56
1:C:775:TYR:HE2	1:C:859:LYS:HA	1.71	0.56
1:A:1640:ASN:O	1:A:1645:ARG:NH1	2.38	0.56
1:D:496:GLU:HG2	1:D:561:ARG:HH21	1.71	0.56
1:D:1238:HIS:O	1:D:1242:GLN:NE2	2.39	0.56
1:B:600:HIS:ND1	1:B:601:ASN:OD1	2.37	0.56
1:B:2074:ILE:HG22	1:B:2076:PRO:HD2	1.87	0.56
1:A:1092:GLU:HA	1:A:1095:GLN:HG2	1.86	0.56
1:A:2074:ILE:HG22	1:A:2076:PRO:HD2	1.87	0.56
1:B:374:THR:HG22	1:B:375:LEU:H	1.71	0.56
1:A:496:GLU:HG2	1:A:561:ARG:HH21	1.71	0.56
1:A:739:LEU:O	1:A:743:MET:HB2	2.05	0.56
1:B:510:MET:HG2	1:B:515:ILE:HD12	1.87	0.56
1:A:1274:GLN:HE21	1:A:1311:PHE:HB2	1.71	0.56
1:C:759:LEU:HA	1:C:763:LEU:HD23	1.86	0.56
1:D:389:ARG:NH2	1:D:426:ASP:OD1	2.39	0.56
1:D:568:ARG:HH22	1:D:604:LYS:HB3	1.69	0.56
1:B:2127:LYS:NZ	1:B:2149:PRO:O	2.38	0.56
1:C:1238:HIS:O	1:C:1242:GLN:NE2	2.38	0.56
1:D:537:ARG:O	1:D:550:ARG:NH2	2.37	0.56
1:B:1088:SER:HB2	1:B:1622:GLU:HB3	1.88	0.56
1:B:2148:SER:OG	1:B:2151:ASN:OD1	2.24	0.56
1:D:374:THR:HG22	1:D:375:LEU:H	1.70	0.56
1:B:568:ARG:HH22	1:B:604:LYS:HB3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ILE:HG22	1:A:57:LEU:HD12	1.88	0.55
1:A:121:ILE:HG22	1:A:161:PHE:HB2	1.88	0.55
1:A:2436:ARG:HG3	2:A:2807:PLX:H1C3	1.88	0.55
1:B:1092:GLU:HA	1:B:1095:GLN:HG2	1.87	0.55
1:A:374:THR:HG22	1:A:375:LEU:H	1.70	0.55
1:B:389:ARG:NH2	1:B:426:ASP:OD1	2.38	0.55
1:C:496:GLU:HG2	1:C:561:ARG:HH21	1.71	0.55
1:C:621:LEU:HA	1:C:624:LYS:HB2	1.87	0.55
1:D:1640:ASN:O	1:D:1645:ARG:NH1	2.38	0.55
1:C:641:MET:SD	1:C:642:ASN:N	2.78	0.55
1:A:253:CYS:SG	1:A:254:ASP:N	2.78	0.55
1:A:389:ARG:NH2	1:A:426:ASP:OD1	2.38	0.55
1:A:537:ARG:O	1:A:550:ARG:NH2	2.36	0.55
1:C:568:ARG:HH22	1:C:604:LYS:HB3	1.71	0.55
1:A:833:PHE:O	1:A:836:THR:OG1	2.25	0.55
1:D:2677:ARG:HH22	1:C:2623:ASN:HA	1.71	0.55
1:B:496:GLU:HG2	1:B:561:ARG:HH21	1.71	0.55
1:A:1681:GLU:O	1:A:1687:ARG:NH2	2.37	0.55
1:A:2195:GLN:NE2	1:A:2207:GLN:OE1	2.39	0.55
1:D:2127:LYS:NZ	1:D:2149:PRO:O	2.39	0.55
1:B:1203:ARG:HH12	1:B:1248:ASN:HB2	1.72	0.55
1:C:374:THR:HG22	1:C:375:LEU:H	1.70	0.55
1:A:139:PRO:O	1:A:148:ARG:NH1	2.39	0.55
1:A:775:TYR:HE2	1:A:859:LYS:HA	1.70	0.55
1:B:181:LYS:HB3	1:B:217:SER:HB2	1.88	0.55
1:B:1681:GLU:O	1:B:1687:ARG:NH2	2.37	0.55
1:C:2148:SER:OG	1:C:2151:ASN:OD1	2.24	0.55
1:A:759:LEU:HA	1:A:763:LEU:HD23	1.88	0.55
1:A:2148:SER:OG	1:A:2151:ASN:OD1	2.24	0.55
1:D:181:LYS:HB3	1:D:217:SER:HB2	1.88	0.55
1:D:246:GLU:HG2	1:D:247:GLN:HG3	1.89	0.55
1:D:775:TYR:HE2	1:D:859:LYS:HA	1.72	0.55
1:D:2205:MET:HE2	1:D:2679:ARG:HE	1.72	0.55
1:A:2677:ARG:HH22	1:D:2623:ASN:HA	1.71	0.54
1:C:181:LYS:HB3	1:C:217:SER:HB2	1.88	0.54
1:C:1088:SER:HB2	1:C:1622:GLU:HB3	1.89	0.54
1:A:641:MET:SD	1:A:642:ASN:N	2.78	0.54
1:A:568:ARG:HH22	1:A:604:LYS:HB3	1.73	0.54
1:A:651:LEU:HA	1:A:654:LYS:HZ3	1.73	0.54
1:D:747:ARG:NH1	1:D:749:TYR:OH	2.37	0.54
1:D:2148:SER:OG	1:D:2151:ASN:OD1	2.24	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:ILE:HA	1:C:977:ILE:HG22	1.90	0.54
1:A:181:LYS:HB3	1:A:217:SER:HB2	1.88	0.54
1:D:974:ILE:HA	1:D:977:ILE:HG22	1.90	0.54
1:C:1090:ARG:HA	1:C:1093:VAL:HG12	1.90	0.54
1:B:1274:GLN:HE21	1:B:1311:PHE:HB2	1.72	0.54
1:A:504:ARG:NH2	1:A:566:ASP:O	2.41	0.54
1:A:974:ILE:HA	1:A:977:ILE:HG22	1.90	0.54
1:C:635:SER:OG	1:C:742:ARG:NH2	2.36	0.54
1:D:1088:SER:HB2	1:D:1622:GLU:HB3	1.90	0.54
1:C:600:HIS:ND1	1:C:601:ASN:OD1	2.37	0.54
1:A:14:ILE:HB	1:A:224:MET:HB3	1.90	0.54
1:A:1238:HIS:O	1:A:1242:GLN:NE2	2.40	0.54
1:D:98:LEU:HD21	1:C:2018:LEU:HD22	1.89	0.54
1:D:2270:ALA:HB1	1:D:2375:ASN:HB3	1.89	0.54
1:B:102:GLN:HA	1:B:105:THR:HG22	1.90	0.54
1:C:504:ARG:NH2	1:C:566:ASP:O	2.41	0.54
1:B:14:ILE:HB	1:B:224:MET:HB3	1.90	0.53
1:B:436:SER:OG	1:B:439:GLU:OE1	2.22	0.53
1:A:2623:ASN:HA	1:B:2677:ARG:HH22	1.72	0.53
1:B:2270:ALA:HB1	1:B:2375:ASN:HB3	1.90	0.53
1:C:102:GLN:HA	1:C:105:THR:HG22	1.90	0.53
1:C:253:CYS:SG	1:C:254:ASP:N	2.79	0.53
1:A:1007:GLN:HG3	1:A:1599:ASN:HD21	1.74	0.53
1:D:102:GLN:HA	1:D:105:THR:HG22	1.90	0.53
1:B:139:PRO:O	1:B:148:ARG:NH1	2.41	0.53
1:B:974:ILE:HA	1:B:977:ILE:HG22	1.90	0.53
1:C:1274:GLN:HE21	1:C:1311:PHE:HB2	1.73	0.53
1:D:504:ARG:NH2	1:D:566:ASP:O	2.42	0.53
1:C:139:PRO:O	1:C:148:ARG:NH1	2.41	0.53
1:C:14:ILE:HG22	1:C:57:LEU:HD12	1.89	0.53
1:A:241:ARG:HG3	1:A:433:VAL:HG13	1.91	0.53
1:D:1624:SER:HB2	1:D:1737:ARG:HE	1.73	0.53
1:B:641:MET:SD	1:B:642:ASN:N	2.82	0.53
1:B:2018:LEU:HD22	1:C:98:LEU:HD21	1.89	0.53
1:A:2665:GLU:OE1	1:A:2668:ARG:NH2	2.39	0.53
1:D:14:ILE:HB	1:D:224:MET:HB3	1.91	0.53
1:B:14:ILE:HG22	1:B:57:LEU:HD12	1.89	0.53
1:B:253:CYS:SG	1:B:254:ASP:N	2.78	0.53
1:B:1249:GLN:HA	1:B:1252:GLN:HB2	1.89	0.53
1:C:2009:CYS:HA	1:C:2013:SER:HB3	1.90	0.53
1:A:1090:ARG:HA	1:A:1093:VAL:HG12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1007:GLN:HG3	1:D:1599:ASN:HD21	1.74	0.53
1:B:1090:ARG:HA	1:B:1093:VAL:HG12	1.91	0.53
1:B:1238:HIS:O	1:B:1242:GLN:NE2	2.42	0.53
1:C:265:ARG:HH22	1:C:412:LYS:HG3	1.74	0.53
1:B:265:ARG:HH22	1:B:412:LYS:HG3	1.73	0.53
1:B:504:ARG:NH2	1:B:566:ASP:O	2.41	0.53
1:B:2009:CYS:HA	1:B:2013:SER:HB3	1.90	0.53
1:C:14:ILE:HB	1:C:224:MET:HB3	1.90	0.53
1:C:651:LEU:HA	1:C:654:LYS:HZ3	1.74	0.53
1:A:2009:CYS:HA	1:A:2013:SER:HB3	1.90	0.52
1:C:1342:LEU:HD12	1:C:1344:PHE:HB2	1.91	0.52
1:A:265:ARG:HH22	1:A:412:LYS:HG3	1.74	0.52
1:A:1307:GLN:O	1:A:1310:LYS:NZ	2.40	0.52
1:D:1342:LEU:HD12	1:D:1344:PHE:HB2	1.92	0.52
1:C:1007:GLN:HG3	1:C:1599:ASN:HD21	1.74	0.52
1:C:2270:ALA:HB1	1:C:2375:ASN:HB3	1.91	0.52
1:A:98:LEU:HD21	1:D:2018:LEU:HD22	1.89	0.52
1:B:2126:LYS:HG2	1:B:2130:MET:HE3	1.92	0.52
1:C:715:LEU:HB3	1:C:730:LEU:HD21	1.91	0.52
1:A:102:GLN:HA	1:A:105:THR:HG22	1.90	0.52
1:D:139:PRO:O	1:D:148:ARG:NH1	2.41	0.52
1:B:2623:ASN:HA	1:C:2677:ARG:HH22	1.73	0.52
1:D:2009:CYS:HA	1:D:2013:SER:HB3	1.91	0.52
1:A:2270:ALA:HB1	1:A:2375:ASN:HB3	1.91	0.52
1:A:352:VAL:O	1:A:420:THR:OG1	2.28	0.52
1:B:790:VAL:HG12	1:B:795:GLN:HE21	1.75	0.52
1:B:1007:GLN:HG3	1:B:1599:ASN:HD21	1.74	0.52
1:D:241:ARG:HG3	1:D:433:VAL:HG13	1.92	0.52
1:D:2069:LEU:O	1:D:2089:LYS:NZ	2.39	0.52
1:B:482:TYR:HA	1:B:485:THR:HG22	1.92	0.52
1:D:621:LEU:HA	1:D:624:LYS:HB2	1.91	0.52
1:D:1274:GLN:HE21	1:D:1311:PHE:HB2	1.74	0.52
1:B:1200:GLN:HA	1:B:1203:ARG:HB3	1.92	0.52
1:B:1342:LEU:HD12	1:B:1344:PHE:HB2	1.92	0.52
1:C:352:VAL:O	1:C:420:THR:OG1	2.28	0.52
1:C:1624:SER:HB2	1:C:1737:ARG:HE	1.75	0.52
1:A:1342:LEU:HD12	1:A:1344:PHE:HB2	1.92	0.51
1:B:352:VAL:O	1:B:420:THR:OG1	2.28	0.51
1:A:2018:LEU:HD22	1:B:98:LEU:HD21	1.90	0.51
1:D:649:GLN:NE2	1:D:744:CYS:O	2.43	0.51
1:D:715:LEU:HB3	1:D:730:LEU:HD21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2126:LYS:HG2	1:D:2130:MET:HE3	1.92	0.51
2:D:5103:PLX:H271	1:B:2565:ALA:HB2	1.93	0.51
1:C:241:ARG:HG3	1:C:433:VAL:HG13	1.92	0.51
1:B:121:ILE:HG22	1:B:161:PHE:HB2	1.93	0.51
1:A:2565:ALA:HB2	2:C:5107:PLX:H271	1.93	0.51
1:D:814:ILE:HG13	1:D:815:ALA:H	1.75	0.51
1:B:651:LEU:HA	1:B:654:LYS:HZ3	1.75	0.51
1:B:715:LEU:HB3	1:B:730:LEU:HD21	1.92	0.51
1:A:786:LEU:HD21	1:A:872:ASN:HD22	1.75	0.51
1:A:1200:GLN:HA	1:A:1203:ARG:HB3	1.93	0.51
1:D:1081:GLN:NE2	1:D:1668:GLU:OE1	2.44	0.51
1:C:121:ILE:HG22	1:C:161:PHE:HB2	1.93	0.51
1:B:485:THR:HG23	1:B:487:GLY:H	1.75	0.51
1:B:2063:ILE:HG13	1:B:2066:ILE:HD11	1.93	0.51
1:C:1200:GLN:HA	1:C:1203:ARG:HB3	1.93	0.51
1:C:1734:GLU:HA	1:C:1737:ARG:HG2	1.93	0.51
1:A:621:LEU:HA	1:A:624:LYS:HB2	1.91	0.51
1:A:133:THR:HG22	1:A:159:SER:HB3	1.94	0.50
1:A:1081:GLN:NE2	1:A:1668:GLU:OE1	2.44	0.50
1:D:196:SER:OG	1:D:197:SER:N	2.43	0.50
1:D:352:VAL:O	1:D:420:THR:OG1	2.29	0.50
1:D:2565:ALA:HB2	2:B:2806:PLX:H271	1.93	0.50
1:B:196:SER:OG	1:B:197:SER:N	2.44	0.50
1:B:1081:GLN:NE2	1:B:1668:GLU:OE1	2.44	0.50
1:C:2242:ASP:OD2	1:C:2246:ARG:NE	2.39	0.50
1:A:485:THR:HG23	1:A:487:GLY:H	1.77	0.50
1:D:2227:ILE:HG13	1:D:2250:LEU:HD11	1.93	0.50
1:D:2630:GLU:HA	1:D:2633:LYS:HG2	1.93	0.50
1:B:467:GLN:OE1	1:B:471:ARG:NH2	2.45	0.50
1:C:2063:ILE:HG13	1:C:2066:ILE:HD11	1.93	0.50
1:D:1090:ARG:HA	1:D:1093:VAL:HG12	1.92	0.50
1:C:790:VAL:HG12	1:C:795:GLN:HE21	1.75	0.50
1:C:2049:HIS:O	1:C:2053:ASN:ND2	2.44	0.50
1:A:624:LYS:HD3	1:A:662:ALA:HA	1.94	0.50
2:A:2802:PLX:H271	1:C:2565:ALA:HB2	1.92	0.50
1:D:2049:HIS:O	1:D:2053:ASN:ND2	2.45	0.50
1:B:2049:HIS:O	1:B:2053:ASN:ND2	2.45	0.50
1:A:2069:LEU:O	1:A:2089:LYS:NZ	2.38	0.50
1:A:2242:ASP:OD2	1:A:2246:ARG:NE	2.38	0.50
1:D:467:GLN:OE1	1:D:471:ARG:NH2	2.45	0.50
1:B:241:ARG:HG3	1:B:433:VAL:HG13	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2205:MET:HE2	1:B:2679:ARG:HE	1.76	0.50
1:C:1081:GLN:NE2	1:C:1668:GLU:OE1	2.44	0.50
1:C:2069:LEU:O	1:C:2089:LYS:NZ	2.39	0.50
1:D:168:LYS:HD2	1:C:246:GLU:HA	1.94	0.50
1:D:1185:LYS:HA	1:D:1188:VAL:HG12	1.92	0.50
1:D:2436:ARG:HG3	2:D:5108:PLX:H1C3	1.93	0.50
1:C:467:GLN:OE1	1:C:471:ARG:NH2	2.45	0.50
1:C:1185:LYS:HA	1:C:1188:VAL:HG12	1.93	0.50
1:A:1638:PRO:HG2	1:A:1640:ASN:HB2	1.94	0.50
1:A:2063:ILE:HG13	1:A:2066:ILE:HD11	1.94	0.50
1:D:1200:GLN:HA	1:D:1203:ARG:HB3	1.93	0.50
1:B:624:LYS:HD3	1:B:662:ALA:HA	1.94	0.50
1:B:632:ASP:HA	1:B:635:SER:HB3	1.94	0.50
1:B:2242:ASP:OD2	1:B:2246:ARG:NE	2.38	0.50
1:B:1638:PRO:HG2	1:B:1640:ASN:HB2	1.94	0.50
1:A:612:ALA:HB2	1:A:651:LEU:HD11	1.94	0.50
1:A:2227:ILE:HG13	1:A:2250:LEU:HD11	1.94	0.50
1:B:621:LEU:HA	1:B:624:LYS:HB2	1.93	0.50
1:B:2069:LEU:O	1:B:2089:LYS:NZ	2.38	0.50
1:A:246:GLU:HA	1:B:168:LYS:HD2	1.94	0.49
1:D:1734:GLU:HA	1:D:1737:ARG:HG2	1.93	0.49
1:C:2227:ILE:HG13	1:C:2250:LEU:HD11	1.93	0.49
1:D:2633:LYS:HG3	1:D:2634:GLU:HG3	1.93	0.49
1:B:765:LEU:HD13	1:B:836:THR:HG22	1.94	0.49
1:C:2102:SER:OG	1:C:2206:GLU:OE1	2.26	0.49
1:A:1813:MET:SD	1:A:1852:LYS:NZ	2.85	0.49
1:D:1638:PRO:HG2	1:D:1640:ASN:HB2	1.94	0.49
1:B:246:GLU:HA	1:C:168:LYS:HD2	1.93	0.49
1:C:196:SER:OG	1:C:197:SER:N	2.44	0.49
1:C:2574:PHE:O	1:C:2578:ILE:HB	2.13	0.49
1:A:1315:ILE:HG23	1:A:1316:VAL:HG23	1.93	0.49
1:B:2227:ILE:HG13	1:B:2250:LEU:HD11	1.93	0.49
1:B:2358:GLY:HA3	1:B:2406:LEU:HD13	1.93	0.49
1:A:55:ASP:O	1:A:125:HIS:NE2	2.45	0.49
1:A:467:GLN:OE1	1:A:471:ARG:NH2	2.45	0.49
1:B:833:PHE:O	1:B:836:THR:OG1	2.25	0.49
1:A:598:LEU:O	1:A:602:ASN:ND2	2.45	0.49
1:A:2630:GLU:HA	1:A:2633:LYS:HG2	1.94	0.49
1:D:790:VAL:HG12	1:D:795:GLN:HE21	1.76	0.49
1:D:2358:GLY:HA3	1:D:2406:LEU:HD13	1.94	0.49
1:B:246:GLU:HG2	1:B:247:GLN:HG3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1300:GLU:OE2	1:B:1337:SER:OG	2.31	0.49
1:B:1814:ASN:OD1	1:B:1855:LYS:NZ	2.46	0.49
1:C:1315:ILE:HG23	1:C:1316:VAL:HG23	1.94	0.49
1:C:2665:GLU:OE1	1:C:2668:ARG:NH2	2.42	0.49
1:D:43:ALA:HB1	1:D:50:PRO:HB3	1.93	0.49
1:D:1073:PRO:HD2	1:D:1075:LEU:HD22	1.95	0.49
1:B:618:PHE:HE2	1:B:634:LEU:HB2	1.78	0.49
1:C:1300:GLU:OE2	1:C:1337:SER:OG	2.31	0.49
1:C:1638:PRO:HG2	1:C:1640:ASN:HB2	1.94	0.49
1:A:715:LEU:HB3	1:A:730:LEU:HD21	1.94	0.49
1:D:664:ILE:H	1:D:664:ILE:HD12	1.78	0.49
1:D:747:ARG:NH2	1:D:792:ARG:O	2.41	0.49
1:A:196:SER:OG	1:A:197:SER:N	2.44	0.49
1:A:2049:HIS:O	1:A:2053:ASN:ND2	2.45	0.49
1:C:1814:ASN:OD1	1:C:1855:LYS:NZ	2.46	0.49
1:A:147:MET:SD	1:A:147:MET:N	2.86	0.48
1:D:624:LYS:HD3	1:D:662:ALA:HA	1.94	0.48
1:B:1813:MET:SD	1:B:1852:LYS:NZ	2.86	0.48
1:C:249:LYS:HB2	1:C:269:ARG:HH21	1.78	0.48
1:C:1813:MET:SD	1:C:1852:LYS:NZ	2.86	0.48
1:A:246:GLU:HG2	1:A:247:GLN:HG3	1.95	0.48
1:A:765:LEU:HD13	1:A:836:THR:HG22	1.95	0.48
1:A:1814:ASN:OD1	1:A:1855:LYS:NZ	2.46	0.48
1:D:265:ARG:NE	1:D:413:PRO:O	2.45	0.48
1:D:485:THR:HG23	1:D:487:GLY:H	1.78	0.48
1:D:2665:GLU:OE1	1:D:2668:ARG:NH2	2.42	0.48
1:B:2574:PHE:O	1:B:2578:ILE:HB	2.13	0.48
1:C:130:LYS:HG2	1:C:153:GLU:HG2	1.96	0.48
1:C:1982:ARG:NH1	1:C:2046:GLY:O	2.47	0.48
1:C:2126:LYS:HG2	1:C:2130:MET:HE3	1.95	0.48
1:A:379:ASP:N	1:A:379:ASP:OD1	2.46	0.48
1:A:747:ARG:NH1	1:A:793:ASP:OD2	2.46	0.48
1:A:2127:LYS:HZ2	1:A:2149:PRO:HB3	1.79	0.48
1:D:2574:PHE:O	1:D:2578:ILE:HB	2.13	0.48
1:A:2574:PHE:O	1:A:2578:ILE:HB	2.13	0.48
1:D:626:ARG:HH22	1:D:732:TYR:HB2	1.77	0.48
1:B:55:ASP:O	1:B:125:HIS:NE2	2.46	0.48
1:D:641:MET:HG2	1:D:642:ASN:H	1.78	0.48
1:D:1813:MET:SD	1:D:1852:LYS:NZ	2.85	0.48
1:D:2063:ILE:HG13	1:D:2066:ILE:HD11	1.94	0.48
1:B:2219:LEU:HD11	1:B:2250:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ASP:N	1:C:379:ASP:OD1	2.46	0.48
1:C:833:PHE:O	1:C:836:THR:OG1	2.26	0.48
1:C:1681:GLU:O	1:C:1687:ARG:NH2	2.41	0.48
1:A:249:LYS:HB2	1:A:269:ARG:HH21	1.78	0.48
1:A:1185:LYS:HA	1:A:1188:VAL:HG12	1.94	0.48
1:D:819:TYR:OH	1:D:992:CYS:SG	2.71	0.48
1:D:1814:ASN:OD1	1:D:1855:LYS:NZ	2.47	0.48
1:D:1982:ARG:NH1	1:D:2046:GLY:O	2.47	0.48
1:A:99:GLU:HA	1:A:102:GLN:HG3	1.95	0.48
1:A:252:THR:HB	1:A:260:GLN:HG2	1.96	0.48
1:B:379:ASP:OD1	1:B:379:ASP:N	2.46	0.48
1:B:1123:ARG:HH21	1:B:1213:VAL:HG22	1.78	0.48
1:B:2665:GLU:OE1	1:B:2668:ARG:NH2	2.42	0.48
1:A:466:THR:HG23	1:A:469:GLU:H	1.79	0.48
1:A:1300:GLU:OE2	1:A:1337:SER:OG	2.31	0.48
1:B:1185:LYS:HA	1:B:1188:VAL:HG12	1.94	0.48
1:A:2219:LEU:HD11	1:A:2250:LEU:HD22	1.96	0.48
1:A:2633:LYS:HG3	1:A:2634:GLU:HG3	1.94	0.48
1:D:379:ASP:OD1	1:D:379:ASP:N	2.46	0.48
1:B:993:LEU:HD11	1:B:1040:ILE:HG21	1.95	0.48
1:C:624:LYS:HD3	1:C:662:ALA:HA	1.95	0.48
1:A:1203:ARG:HH12	1:A:1248:ASN:HB2	1.77	0.48
1:A:1654:CYS:HB2	1:A:1802:GLU:HB2	1.96	0.48
1:D:370:LEU:HB2	1:D:388:VAL:HG13	1.96	0.48
1:D:1123:ARG:HH21	1:D:1213:VAL:HG22	1.78	0.48
1:B:249:LYS:HB2	1:B:269:ARG:HH21	1.78	0.48
1:C:612:ALA:HB2	1:C:651:LEU:HD11	1.95	0.48
1:A:2363:CYS:HA	1:A:2366:ILE:HG12	1.96	0.47
1:B:598:LEU:O	1:B:602:ASN:ND2	2.46	0.47
1:B:1982:ARG:NH1	1:B:2046:GLY:O	2.47	0.47
1:C:246:GLU:HG2	1:C:247:GLN:HG3	1.95	0.47
1:D:1203:ARG:HH12	1:D:1248:ASN:HB2	1.78	0.47
1:D:1681:GLU:O	1:D:1687:ARG:NH2	2.37	0.47
1:B:248:GLU:HB2	1:B:263:PHE:HB3	1.96	0.47
1:B:612:ALA:HB2	1:B:651:LEU:HD11	1.95	0.47
1:A:664:ILE:HD12	1:A:664:ILE:H	1.79	0.47
1:D:99:GLU:HA	1:D:102:GLN:HG3	1.96	0.47
1:B:635:SER:OG	1:B:742:ARG:NH2	2.47	0.47
1:C:372:PRO:HG2	1:C:376:ARG:HD3	1.96	0.47
1:C:2127:LYS:HZ2	1:C:2149:PRO:HB3	1.79	0.47
1:A:1123:ARG:HH21	1:A:1213:VAL:HG22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:LYS:HG2	1:D:153:GLU:HG2	1.96	0.47
1:D:747:ARG:NH1	1:D:793:ASP:OD1	2.47	0.47
1:B:252:THR:HB	1:B:260:GLN:HG2	1.96	0.47
1:C:265:ARG:NE	1:C:413:PRO:O	2.48	0.47
1:D:482:TYR:HA	1:D:485:THR:HG22	1.96	0.47
1:D:785:MET:O	1:D:789:HIS:ND1	2.48	0.47
1:D:1300:GLU:OE2	1:D:1337:SER:OG	2.32	0.47
1:D:1304:ARG:HD3	1:D:1341:VAL:HG22	1.97	0.47
1:B:99:GLU:HA	1:B:102:GLN:HG3	1.95	0.47
1:C:1203:ARG:HH12	1:C:1248:ASN:HB2	1.78	0.47
1:D:399:VAL:HG12	1:D:420:THR:HG22	1.97	0.47
1:D:443:LEU:O	1:D:447:ASN:ND2	2.47	0.47
1:D:466:THR:HG23	1:D:469:GLU:H	1.79	0.47
1:B:2630:GLU:HA	1:B:2633:LYS:HG2	1.96	0.47
1:B:2656:TYR:HD2	1:B:2660:GLU:HB2	1.80	0.47
1:C:43:ALA:HB1	1:C:50:PRO:HB3	1.97	0.47
1:C:99:GLU:HA	1:C:102:GLN:HG3	1.95	0.47
1:C:1123:ARG:HH21	1:C:1213:VAL:HG22	1.79	0.47
1:C:2219:LEU:HD11	1:C:2250:LEU:HD22	1.95	0.47
1:C:2436:ARG:HG3	2:C:5105:PLX:H1C3	1.97	0.47
1:A:1274:GLN:HG2	1:A:1311:PHE:HD1	1.79	0.47
1:D:1215:LEU:HD11	1:D:1261:LEU:HD11	1.96	0.47
1:B:466:THR:HG23	1:B:469:GLU:H	1.79	0.47
1:D:618:PHE:HE2	1:D:634:LEU:HB2	1.80	0.47
1:D:2020:LEU:HD12	1:D:2023:LEU:HD23	1.97	0.47
1:B:130:LYS:HG2	1:B:153:GLU:HG2	1.96	0.47
1:C:55:ASP:O	1:C:125:HIS:NE2	2.46	0.47
1:C:485:THR:HG23	1:C:487:GLY:H	1.79	0.47
1:D:572:GLU:OE1	1:D:576:LYS:NZ	2.48	0.47
1:B:2603:LYS:HA	1:B:2606:ILE:HG22	1.97	0.47
1:C:252:THR:HB	1:C:260:GLN:HG2	1.96	0.47
1:C:370:LEU:HB2	1:C:388:VAL:HG13	1.97	0.47
1:C:466:THR:HG23	1:C:469:GLU:H	1.79	0.47
1:C:1073:PRO:HD2	1:C:1075:LEU:HD22	1.97	0.47
1:A:626:ARG:HD2	1:A:626:ARG:HA	1.71	0.46
1:A:990:ILE:HG13	1:A:1097:PHE:CE2	2.50	0.46
1:D:252:THR:HB	1:D:260:GLN:HG2	1.96	0.46
1:D:765:LEU:HD13	1:D:836:THR:HG22	1.97	0.46
1:D:1654:CYS:HB2	1:D:1802:GLU:HB2	1.98	0.46
1:C:598:LEU:O	1:C:602:ASN:ND2	2.48	0.46
1:C:879:TYR:HB3	1:C:883:ASP:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD23	1:A:115:ILE:HD11	1.98	0.46
1:A:316:ALA:HB2	1:A:355:LEU:HD23	1.97	0.46
1:A:1073:PRO:HD2	1:A:1075:LEU:HD22	1.96	0.46
1:D:316:ALA:HB2	1:D:355:LEU:HD23	1.98	0.46
2:D:5102:PLX:H101	2:D:5102:PLX:H72	1.62	0.46
1:B:9:LEU:HD23	1:B:115:ILE:HD11	1.97	0.46
2:C:5104:PLX:H101	2:C:5104:PLX:H271	1.97	0.46
1:A:370:LEU:HB2	1:A:388:VAL:HG13	1.97	0.46
1:A:879:TYR:HB3	1:A:883:ASP:HB2	1.96	0.46
1:A:130:LYS:HG2	1:A:153:GLU:HG2	1.98	0.46
2:A:2801:PLX:H72	2:A:2801:PLX:H101	1.61	0.46
1:D:632:ASP:HA	1:D:635:SER:HB3	1.98	0.46
1:B:2273:MET:SD	1:B:2375:ASN:ND2	2.84	0.46
1:C:632:ASP:HA	1:C:635:SER:HB3	1.98	0.46
1:C:2656:TYR:HD2	1:C:2660:GLU:HB2	1.80	0.46
1:A:372:PRO:HG2	1:A:376:ARG:HD3	1.96	0.46
1:A:482:TYR:HA	1:A:485:THR:HG22	1.97	0.46
1:A:1224:LYS:HD2	1:A:1228:THR:HG21	1.98	0.46
1:D:372:PRO:HG2	1:D:376:ARG:HD3	1.96	0.46
1:B:43:ALA:HB1	1:B:50:PRO:HB3	1.97	0.46
1:B:1073:PRO:HD2	1:B:1075:LEU:HD22	1.97	0.46
1:B:2281:PHE:HD1	1:B:2420:LEU:HG	1.80	0.46
2:B:2805:PLX:H101	2:B:2805:PLX:H72	1.62	0.46
1:C:543:ASP:OD2	1:C:545:ARG:NH1	2.49	0.46
1:A:1982:ARG:NH1	1:A:2046:GLY:O	2.46	0.46
1:B:265:ARG:NE	1:B:413:PRO:O	2.48	0.46
1:B:2708:LEU:HA	1:B:2711:ASN:ND2	2.31	0.46
1:C:670:LEU:HD23	1:C:763:LEU:HB2	1.98	0.46
1:C:2557:SER:OG	1:C:2560:GLU:OE1	2.34	0.46
1:A:399:VAL:HG12	1:A:420:THR:HG22	1.97	0.46
1:A:789:HIS:HD1	1:A:790:VAL:HG13	1.79	0.46
1:A:2596:LEU:HD23	1:A:2596:LEU:HA	1.78	0.46
1:B:400:HIS:HA	1:B:428:GLU:HG2	1.98	0.46
1:C:2603:LYS:HA	1:C:2606:ILE:HG22	1.97	0.46
1:A:43:ALA:HB1	1:A:50:PRO:HB3	1.97	0.46
1:A:626:ARG:HH22	1:A:732:TYR:HB2	1.80	0.46
1:D:134:VAL:HB	1:D:149:VAL:HG12	1.98	0.46
1:B:670:LEU:HD23	1:B:763:LEU:HB2	1.98	0.46
1:B:1224:LYS:HD2	1:B:1228:THR:HG21	1.98	0.46
1:C:9:LEU:HD23	1:C:115:ILE:HD11	1.97	0.46
1:C:1321:LYS:HE2	1:C:1321:LYS:HB3	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2020:LEU:HD12	1:A:2023:LEU:HD23	1.97	0.46
1:A:2273:MET:SD	1:A:2375:ASN:ND2	2.84	0.46
1:A:2656:TYR:HD2	1:A:2660:GLU:HB2	1.79	0.46
1:D:670:LEU:HD23	1:D:763:LEU:HB2	1.98	0.46
1:D:990:ILE:HG13	1:D:1097:PHE:CE2	2.51	0.46
1:B:1304:ARG:HD3	1:B:1341:VAL:HG22	1.97	0.46
1:B:2363:CYS:HA	1:B:2366:ILE:HG12	1.97	0.46
1:C:483:PHE:HD2	1:C:510:MET:HE1	1.80	0.46
1:C:2363:CYS:HA	1:C:2366:ILE:HG12	1.97	0.46
1:C:2452:VAL:HG13	1:C:2539:LEU:HB3	1.98	0.46
1:D:85:ASP:HB2	1:D:88:LEU:HB3	1.98	0.46
1:D:1860:PHE:HB3	1:D:1864:MET:HE2	1.98	0.46
1:B:370:LEU:HB2	1:B:388:VAL:HG13	1.97	0.46
1:B:649:GLN:NE2	1:B:744:CYS:O	2.48	0.46
1:B:879:TYR:HB3	1:B:883:ASP:HB2	1.96	0.46
1:B:2452:VAL:HG13	1:B:2539:LEU:HB3	1.97	0.46
1:C:1257:LYS:HG3	1:C:1258:HIS:CD2	2.51	0.46
1:C:2630:GLU:HA	1:C:2633:LYS:HG2	1.97	0.46
1:A:543:ASP:OD2	1:A:545:ARG:NH1	2.49	0.45
2:A:2802:PLX:H122	2:A:2802:PLX:H272	1.98	0.45
1:D:1257:LYS:HG3	1:D:1258:HIS:CD2	2.51	0.45
1:B:572:GLU:OE1	1:B:576:LYS:NZ	2.49	0.45
1:B:2267:TYR:O	1:B:2271:ARG:HB2	2.16	0.45
1:C:1304:ARG:HD3	1:C:1341:VAL:HG22	1.97	0.45
1:C:2020:LEU:HD12	1:C:2023:LEU:HD23	1.97	0.45
1:A:85:ASP:HB2	1:A:88:LEU:HB3	1.98	0.45
1:A:265:ARG:NE	1:A:413:PRO:O	2.48	0.45
1:C:572:GLU:OE1	1:C:576:LYS:NZ	2.49	0.45
1:C:785:MET:O	1:C:789:HIS:ND1	2.49	0.45
1:C:2708:LEU:HA	1:C:2711:ASN:ND2	2.31	0.45
1:A:572:GLU:OE1	1:A:576:LYS:NZ	2.49	0.45
1:D:879:TYR:HB3	1:D:883:ASP:HB2	1.97	0.45
1:D:2452:VAL:HG13	1:D:2539:LEU:HB3	1.98	0.45
1:D:2656:TYR:HD2	1:D:2660:GLU:HB2	1.80	0.45
2:D:5107:PLX:H271	2:D:5107:PLX:H101	1.97	0.45
1:C:765:LEU:HD13	1:C:836:THR:HG22	1.98	0.45
1:C:987:ASP:HA	1:C:990:ILE:HG22	1.98	0.45
1:C:993:LEU:HD11	1:C:1040:ILE:HG21	1.98	0.45
1:D:607:GLU:HB2	1:D:647:VAL:HG11	1.98	0.45
1:D:987:ASP:HA	1:D:990:ILE:HG22	1.97	0.45
1:D:2267:TYR:O	1:D:2271:ARG:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5103:PLX:H122	2:D:5103:PLX:H272	1.99	0.45
1:A:2708:LEU:HA	1:A:2711:ASN:ND2	2.31	0.45
1:D:2557:SER:OG	1:D:2560:GLU:OE1	2.34	0.45
1:B:785:MET:O	1:B:789:HIS:ND1	2.49	0.45
1:B:2020:LEU:HD12	1:B:2023:LEU:HD23	1.97	0.45
1:B:2557:SER:OG	1:B:2560:GLU:OE1	2.34	0.45
1:C:400:HIS:HA	1:C:428:GLU:HG2	1.99	0.45
1:C:603:ARG:HH11	1:C:641:MET:HE2	1.80	0.45
1:C:1274:GLN:HG2	1:C:1311:PHE:HD1	1.82	0.45
1:A:400:HIS:HA	1:A:428:GLU:HG2	1.98	0.45
1:A:844:LEU:HA	1:A:847:VAL:HG12	1.99	0.45
1:D:262:VAL:HG21	1:D:418:ILE:HB	1.99	0.45
1:B:85:ASP:HB2	1:B:88:LEU:HB3	1.98	0.45
1:B:316:ALA:HB2	1:B:355:LEU:HD23	1.98	0.45
1:C:399:VAL:HG12	1:C:420:THR:HG22	1.98	0.45
1:A:2616:LEU:HD22	1:A:2620:LYS:HG3	1.99	0.45
1:D:9:LEU:HD23	1:D:115:ILE:HD11	1.98	0.45
1:D:265:ARG:HH22	1:D:412:LYS:HG3	1.82	0.45
1:D:1224:LYS:HD2	1:D:1228:THR:HG21	1.98	0.45
1:D:2603:LYS:HA	1:D:2606:ILE:HG22	1.98	0.45
1:D:2708:LEU:HA	1:D:2711:ASN:ND2	2.31	0.45
1:C:134:VAL:HB	1:C:149:VAL:HG12	1.98	0.45
1:A:1304:ARG:HD3	1:A:1341:VAL:HG22	1.99	0.45
1:D:670:LEU:HB3	1:D:763:LEU:HD13	1.99	0.45
1:D:852:PHE:CG	1:D:853:PRO:HD3	2.52	0.45
1:D:2363:CYS:HA	1:D:2366:ILE:HG12	1.98	0.45
1:B:399:VAL:HG12	1:B:420:THR:HG22	1.98	0.45
1:B:437:PRO:HA	1:B:440:VAL:HG12	1.99	0.45
1:B:543:ASP:OD2	1:B:545:ARG:NH1	2.50	0.45
1:B:2622:ASP:O	1:C:2677:ARG:NH1	2.34	0.45
2:C:5107:PLX:H272	2:C:5107:PLX:H122	1.99	0.45
1:A:437:PRO:HA	1:A:440:VAL:HG12	1.99	0.45
1:D:265:ARG:NH2	1:D:412:LYS:HG3	2.32	0.45
1:D:543:ASP:OD2	1:D:545:ARG:NH1	2.50	0.45
1:D:1274:GLN:HG2	1:D:1311:PHE:HD1	1.82	0.45
1:B:1190:GLU:HG3	1:B:1198:ARG:HD3	1.99	0.45
1:B:1215:LEU:HD11	1:B:1261:LEU:HD11	1.99	0.45
1:A:789:HIS:ND1	1:A:790:VAL:HG13	2.32	0.45
1:A:1822:HIS:HB2	1:A:1965:ILE:HD11	1.99	0.45
1:D:978:LEU:HD23	1:D:981:ILE:HD11	1.98	0.45
1:D:2242:ASP:OD2	1:D:2246:ARG:NE	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ALA:HB2	1:C:355:LEU:HD23	1.98	0.45
1:C:1822:HIS:HB2	1:C:1965:ILE:HD11	1.99	0.45
1:A:603:ARG:HH11	1:A:641:MET:HE2	1.82	0.44
1:A:2603:LYS:HA	1:A:2606:ILE:HG22	1.97	0.44
1:D:978:LEU:HA	1:D:981:ILE:HG12	1.99	0.44
1:D:2273:MET:SD	1:D:2375:ASN:ND2	2.86	0.44
1:B:526:PRO:HB3	1:B:549:PHE:HZ	1.82	0.44
1:B:844:LEU:HA	1:B:847:VAL:HG12	1.99	0.44
1:B:2618:ARG:NH1	1:B:2629:GLU:OE2	2.37	0.44
1:C:85:ASP:HB2	1:C:88:LEU:HB3	1.98	0.44
1:C:248:GLU:HB2	1:C:263:PHE:HB3	2.00	0.44
1:C:978:LEU:HA	1:C:981:ILE:HG12	1.99	0.44
1:A:1201:GLN:NE2	1:A:1202:GLN:OE1	2.51	0.44
1:A:1203:ARG:HA	1:A:1206:ARG:HG2	2.00	0.44
1:D:243:PHE:HE1	1:D:248:GLU:HA	1.82	0.44
1:B:134:VAL:HB	1:B:149:VAL:HG12	1.99	0.44
1:B:1203:ARG:HA	1:B:1206:ARG:HG2	1.99	0.44
2:B:2801:PLX:H1B2	2:B:2801:PLX:H22	1.79	0.44
1:C:1224:LYS:HD2	1:C:1228:THR:HG21	1.98	0.44
1:C:2199:VAL:O	1:C:2662:TYR:OH	2.36	0.44
1:C:2267:TYR:O	1:C:2271:ARG:HB2	2.16	0.44
1:A:2267:TYR:O	1:A:2271:ARG:HB2	2.16	0.44
1:D:437:PRO:HA	1:D:440:VAL:HG12	1.99	0.44
1:B:1822:HIS:HB2	1:B:1965:ILE:HD11	1.99	0.44
1:C:121:ILE:HD12	1:C:121:ILE:HA	1.87	0.44
1:C:852:PHE:CG	1:C:853:PRO:HD3	2.52	0.44
1:A:526:PRO:HB3	1:A:549:PHE:HZ	1.82	0.44
1:A:618:PHE:HE2	1:A:634:LEU:HB2	1.82	0.44
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.83	0.44
1:A:2452:VAL:HG13	1:A:2539:LEU:HB3	1.98	0.44
1:D:1203:ARG:HA	1:D:1206:ARG:HG2	1.98	0.44
1:D:1624:SER:HA	1:D:1627:VAL:HG22	1.97	0.44
1:B:852:PHE:CG	1:B:853:PRO:HD3	2.52	0.44
1:B:1257:LYS:HG3	1:B:1258:HIS:CD2	2.52	0.44
1:A:121:ILE:HD12	1:A:121:ILE:HA	1.84	0.44
1:A:1617:PRO:HA	1:A:1620:GLN:HG3	1.99	0.44
1:B:1064:LEU:HD21	1:B:1083:LEU:HB2	1.99	0.44
1:B:1272:THR:O	1:B:1276:ILE:HG12	2.17	0.44
2:B:2806:PLX:H122	2:B:2806:PLX:H272	2.00	0.44
1:A:262:VAL:HG21	1:A:418:ILE:HB	2.00	0.44
1:A:352:VAL:HG12	1:A:395:THR:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:LEU:O	1:A:447:ASN:ND2	2.47	0.44
1:D:1110:ASP:OD1	1:D:1110:ASP:N	2.50	0.44
1:D:2617:GLU:OE2	1:D:2620:LYS:NZ	2.41	0.44
2:D:5107:PLX:H101	2:D:5107:PLX:H72	1.84	0.44
1:B:262:VAL:HG21	1:B:418:ILE:HB	2.00	0.44
1:B:1624:SER:HA	1:B:1627:VAL:HG22	1.99	0.44
1:C:48:ASN:HA	1:C:49:PRO:HD3	1.85	0.44
1:C:2118:PRO:HB3	1:C:2170:LEU:HD13	1.99	0.44
1:A:621:LEU:HD12	1:A:624:LYS:HB2	2.00	0.44
1:A:978:LEU:HA	1:A:981:ILE:HG12	1.99	0.44
1:D:60:LEU:HD12	1:D:121:ILE:HD11	1.99	0.44
1:D:2423:ARG:HD2	2:D:5104:PLX:H12	1.98	0.44
1:B:1321:LYS:HE2	1:B:1321:LYS:HB3	1.81	0.44
1:C:482:TYR:HA	1:C:485:THR:HG22	2.00	0.44
1:A:1064:LEU:HD21	1:A:1083:LEU:HB2	1.99	0.44
1:D:744:CYS:SG	1:D:748:GLN:HB3	2.58	0.44
1:D:2447:LEU:HD22	1:C:2431:ILE:HD11	2.00	0.44
1:B:202:ASP:OD1	1:B:203:ASN:N	2.51	0.44
1:B:352:VAL:HG12	1:B:395:THR:HG21	2.00	0.44
1:B:621:LEU:HD12	1:B:624:LYS:HB2	1.99	0.44
1:B:1255:LEU:HD11	1:B:1276:ILE:HD12	2.00	0.44
1:B:2409:HIS:HE1	1:B:2411:PHE:CD2	2.36	0.44
1:B:2617:GLU:HG2	1:B:2620:LYS:HG2	2.00	0.44
1:C:621:LEU:HD12	1:C:624:LYS:HB2	1.99	0.44
1:C:844:LEU:HA	1:C:847:VAL:HG12	1.99	0.44
1:A:168:LYS:HD2	1:D:246:GLU:HA	2.00	0.44
1:A:852:PHE:CG	1:A:853:PRO:HD3	2.52	0.44
1:A:1624:SER:HA	1:A:1627:VAL:HG22	1.98	0.44
1:A:2127:LYS:HE3	1:A:2152:VAL:HB	2.00	0.44
1:A:2358:GLY:HA3	1:A:2406:LEU:HD13	2.00	0.44
1:A:2617:GLU:HG2	1:A:2620:LYS:HG2	2.00	0.44
1:D:526:PRO:HB3	1:D:549:PHE:HZ	1.83	0.44
1:D:2219:LEU:HD11	1:D:2250:LEU:HD22	2.00	0.44
1:B:2437:ASN:HB3	1:B:2440:PRO:HG2	2.00	0.44
1:C:2127:LYS:HE3	1:C:2152:VAL:HB	1.98	0.44
1:A:1685:LYS:HD2	1:A:1685:LYS:HA	1.75	0.43
1:A:2557:SER:OG	1:A:2560:GLU:OE1	2.35	0.43
1:D:626:ARG:HD2	1:D:626:ARG:HA	1.72	0.43
1:B:1617:PRO:HA	1:B:1620:GLN:HG3	1.99	0.43
1:C:1064:LEU:HD21	1:C:1083:LEU:HB2	2.00	0.43
1:C:1110:ASP:OD1	1:C:1110:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1679:LEU:O	1:C:1683:MET:HB2	2.18	0.43
1:A:733:TYR:HD1	1:A:736:GLN:HE21	1.66	0.43
1:B:978:LEU:HD23	1:B:981:ILE:HD11	2.00	0.43
1:B:1274:GLN:HG2	1:B:1311:PHE:HD1	1.83	0.43
1:B:2703:GLU:HB3	1:B:2707:LYS:NZ	2.33	0.43
2:C:5106:PLX:H101	2:C:5106:PLX:H72	1.62	0.43
1:A:40:GLN:HA	1:A:41:PRO:HD3	1.87	0.43
1:A:202:ASP:OD1	1:A:203:ASN:N	2.51	0.43
1:A:1190:GLU:HG3	1:A:1198:ARG:HD3	2.00	0.43
1:A:2004:LEU:HD22	1:A:2055:ILE:HG23	2.01	0.43
1:A:2205:MET:HE3	1:A:2681:MET:HB3	2.00	0.43
1:D:121:ILE:HG22	1:D:161:PHE:HB2	1.99	0.43
1:D:749:TYR:HD1	1:D:752:ILE:HG21	1.83	0.43
1:B:987:ASP:HA	1:B:990:ILE:HG22	1.99	0.43
1:C:262:VAL:HG21	1:C:418:ILE:HB	2.00	0.43
1:C:1190:GLU:HG3	1:C:1198:ARG:HD3	2.00	0.43
1:C:1203:ARG:HA	1:C:1206:ARG:HG2	1.99	0.43
1:A:248:GLU:HB2	1:A:263:PHE:HB3	2.00	0.43
1:C:526:PRO:HB3	1:C:549:PHE:HZ	1.82	0.43
1:C:618:PHE:HE2	1:C:634:LEU:HB2	1.83	0.43
1:D:352:VAL:HG12	1:D:395:THR:HG21	1.99	0.43
1:D:737:LEU:HD23	1:D:737:LEU:HA	1.85	0.43
1:B:443:LEU:O	1:B:447:ASN:ND2	2.47	0.43
1:C:1005:ASN:HB2	1:C:1007:GLN:H	1.84	0.43
1:A:978:LEU:HD23	1:A:981:ILE:HD11	2.01	0.43
1:D:621:LEU:HD12	1:D:624:LYS:HB2	2.00	0.43
1:D:1064:LEU:HD21	1:D:1083:LEU:HB2	1.99	0.43
1:D:1617:PRO:HA	1:D:1620:GLN:HG3	1.99	0.43
1:D:202:ASP:OD1	1:D:203:ASN:N	2.51	0.43
1:D:2722:GLN:HA	1:D:2725:GLU:HG2	2.00	0.43
1:B:48:ASN:HA	1:B:49:PRO:HD3	1.85	0.43
1:B:620:SER:C	1:B:622:VAL:H	2.27	0.43
2:C:5107:PLX:H251	2:C:5107:PLX:H282	1.76	0.43
2:A:2803:PLX:H111	1:B:2450:ILE:HG22	2.01	0.43
1:D:2437:ASN:HB3	1:D:2440:PRO:HG2	2.01	0.43
2:B:2802:PLX:H1C2	2:B:2802:PLX:H22	1.80	0.43
1:C:1617:PRO:HA	1:C:1620:GLN:HG3	2.00	0.43
2:C:5102:PLX:H22	2:C:5102:PLX:H1B2	1.79	0.43
1:A:632:ASP:HA	1:A:635:SER:HB3	2.00	0.43
2:A:2806:PLX:H101	2:A:2806:PLX:H72	1.83	0.43
1:D:623:ARG:HH22	1:D:630:PHE:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2722:GLN:HA	1:B:2725:GLU:HG2	2.00	0.43
1:A:2432:LYS:HB2	2:A:2807:PLX:H292	2.00	0.43
1:D:844:LEU:HA	1:D:847:VAL:HG12	2.00	0.43
1:D:1806:ASN:HA	1:D:1809:ILE:HG22	2.01	0.43
1:D:2572:LEU:HD23	2:B:2805:PLX:H362	2.01	0.43
1:B:978:LEU:HA	1:B:981:ILE:HG12	1.99	0.43
1:C:664:ILE:HD12	1:C:664:ILE:H	1.84	0.43
1:A:2087:GLU:OE1	1:A:2087:GLU:N	2.50	0.42
1:D:976:GLU:HA	1:D:979:GLN:HB3	2.01	0.42
1:D:1005:ASN:HB2	1:D:1007:GLN:H	1.84	0.42
1:D:1728:GLU:HA	1:D:1731:LYS:HG2	2.00	0.42
1:D:1822:HIS:HB2	1:D:1965:ILE:HD11	2.01	0.42
1:C:1807:LEU:O	1:C:1811:LEU:HB2	2.19	0.42
1:C:2617:GLU:HG2	1:C:2620:LYS:HG2	2.00	0.42
1:A:620:SER:C	1:A:622:VAL:H	2.28	0.42
1:D:143:GLU:OE2	1:D:198:HIS:ND1	2.46	0.42
1:B:1005:ASN:HB2	1:B:1007:GLN:H	1.85	0.42
1:B:1806:ASN:HA	1:B:1809:ILE:HG22	2.01	0.42
1:C:202:ASP:OD1	1:C:203:ASN:N	2.51	0.42
1:C:2358:GLY:HA3	1:C:2406:LEU:HD13	2.01	0.42
1:A:670:LEU:HD23	1:A:763:LEU:HB2	2.00	0.42
1:A:819:TYR:OH	1:A:992:CYS:SG	2.74	0.42
1:A:1005:ASN:HB2	1:A:1007:GLN:H	1.85	0.42
1:A:1728:GLU:HA	1:A:1731:LYS:HG2	2.02	0.42
1:A:2438:GLY:HA3	2:A:2805:PLX:H81	2.01	0.42
1:D:471:ARG:NH2	1:C:1339:GLU:OE1	2.52	0.42
1:D:1190:GLU:HG3	1:D:1198:ARG:HD3	2.00	0.42
1:D:1257:LYS:HG3	1:D:1258:HIS:HD2	1.84	0.42
1:B:664:ILE:HD12	1:B:664:ILE:H	1.84	0.42
1:C:978:LEU:HD23	1:C:981:ILE:HD11	2.01	0.42
1:C:1728:GLU:HA	1:C:1731:LYS:HG2	2.00	0.42
1:C:2703:GLU:HB3	1:C:2707:LYS:NZ	2.34	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.88	0.42
1:A:1807:LEU:O	1:A:1811:LEU:HB2	2.20	0.42
1:A:2431:ILE:HD13	1:A:2431:ILE:HA	1.90	0.42
1:D:45:ASP:OD1	1:D:45:ASP:N	2.53	0.42
1:D:400:HIS:HA	1:D:428:GLU:HG2	2.00	0.42
1:D:723:GLN:O	1:D:727:ARG:N	2.52	0.42
1:D:1807:LEU:O	1:D:1811:LEU:HB2	2.19	0.42
1:B:635:SER:O	1:B:742:ARG:NH1	2.46	0.42
1:B:1956:ASP:OD1	1:B:1956:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2805:PLX:H393	2:B:2807:PLX:H312	2.01	0.42
1:C:352:VAL:HG12	1:C:395:THR:HG21	2.01	0.42
1:C:1738:GLN:HA	1:C:1741:VAL:HG12	2.01	0.42
1:A:471:ARG:NH2	1:D:1339:GLU:OE1	2.52	0.42
1:D:598:LEU:O	1:D:602:ASN:ND2	2.51	0.42
1:D:864:PHE:HD1	1:D:970:THR:HB	1.85	0.42
1:B:723:GLN:O	1:B:727:ARG:N	2.52	0.42
1:B:1115:ILE:HD11	1:B:1186:LEU:HD23	2.01	0.42
1:B:1201:GLN:NE2	1:B:1202:GLN:OE1	2.53	0.42
1:A:987:ASP:HA	1:A:990:ILE:HG22	2.00	0.42
1:A:1956:ASP:N	1:A:1956:ASP:OD1	2.53	0.42
1:A:2447:LEU:HD22	1:D:2431:ILE:HD11	2.00	0.42
1:A:2722:GLN:HA	1:A:2725:GLU:HG2	2.00	0.42
2:D:5103:PLX:H21	2:D:5103:PLX:H1B2	1.82	0.42
1:B:382:VAL:HA	1:B:383:PRO:HD3	1.90	0.42
1:B:1339:GLU:OE1	1:C:471:ARG:NH2	2.52	0.42
1:B:2202:ASP:OD1	1:B:2202:ASP:N	2.53	0.42
1:C:2281:PHE:HD1	1:C:2420:LEU:HG	1.84	0.42
1:C:2437:ASN:HB3	1:C:2440:PRO:HG2	2.02	0.42
1:A:968:MET:HE1	1:A:1070:HIS:CE1	2.55	0.42
1:A:1738:GLN:HA	1:A:1741:VAL:HG12	2.01	0.42
1:D:126:LEU:HD23	1:D:126:LEU:HA	1.88	0.42
1:D:1603:ARG:O	1:D:1607:ILE:HG12	2.20	0.42
1:D:1738:GLN:HA	1:D:1741:VAL:HG12	2.01	0.42
2:B:2806:PLX:H21	2:B:2806:PLX:H1B2	1.82	0.42
1:A:1110:ASP:OD1	1:A:1110:ASP:N	2.50	0.42
1:D:651:LEU:HA	1:D:654:LYS:HE3	2.01	0.42
1:B:670:LEU:HB3	1:B:763:LEU:HD13	2.01	0.42
1:B:968:MET:HE1	1:B:1070:HIS:CE1	2.54	0.42
1:C:607:GLU:HB2	1:C:647:VAL:HG11	2.01	0.42
1:C:864:PHE:HD1	1:C:970:THR:HB	1.84	0.42
1:C:2002:GLU:HA	1:C:2005:GLN:HB2	2.02	0.42
1:A:1806:ASN:HA	1:A:1809:ILE:HG22	2.01	0.42
1:A:2202:ASP:OD1	1:A:2202:ASP:N	2.53	0.42
1:A:2431:ILE:HG21	2:A:2807:PLX:H342	2.02	0.42
1:D:612:ALA:HB2	1:D:651:LEU:HD11	2.02	0.42
1:B:212:VAL:HG23	1:B:214:CYS:H	1.85	0.42
1:B:825:SER:OG	1:B:826:LYS:N	2.53	0.42
1:B:1685:LYS:HD2	1:B:1685:LYS:HA	1.75	0.42
1:B:1728:GLU:HA	1:B:1731:LYS:HG2	2.02	0.42
1:B:1807:LEU:O	1:B:1811:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:SER:C	1:C:622:VAL:H	2.27	0.42
1:A:738:ASN:HD21	1:A:742:ARG:HH12	1.68	0.42
1:A:1115:ILE:HD11	1:A:1186:LEU:HD23	2.01	0.42
1:D:968:MET:HE1	1:D:1070:HIS:CE1	2.55	0.42
1:D:1005:ASN:HD22	1:D:1007:GLN:HB3	1.85	0.42
1:D:1315:ILE:HG23	1:D:1316:VAL:HG23	2.02	0.42
1:C:670:LEU:HB3	1:C:763:LEU:HD13	2.02	0.42
1:C:2722:GLN:HA	1:C:2725:GLU:HG2	2.01	0.42
1:A:261:HIS:CG	1:A:415:MET:HG2	2.54	0.41
1:A:298:TYR:N	1:A:301:SER:OG	2.49	0.41
1:A:864:PHE:HD1	1:A:970:THR:HB	1.85	0.41
1:B:1738:GLN:HA	1:B:1741:VAL:HG12	2.01	0.41
1:C:63:MET:SD	1:C:120:VAL:HG21	2.60	0.41
1:C:1115:ILE:HD11	1:C:1186:LEU:HD23	2.01	0.41
1:C:1201:GLN:NE2	1:C:1202:GLN:OE1	2.53	0.41
1:C:1603:ARG:O	1:C:1607:ILE:HG12	2.19	0.41
1:A:607:GLU:HB2	1:A:647:VAL:HG11	2.02	0.41
1:A:2117:ARG:O	1:A:2119:LYS:N	2.52	0.41
1:D:1062:ARG:NH1	1:D:1636:LEU:O	2.53	0.41
1:D:1201:GLN:NE2	1:D:1202:GLN:OE1	2.53	0.41
1:B:1603:ARG:O	1:B:1607:ILE:HG12	2.19	0.41
1:C:261:HIS:CG	1:C:415:MET:HG2	2.55	0.41
1:C:968:MET:HE1	1:C:1070:HIS:CE1	2.54	0.41
1:A:670:LEU:HB3	1:A:763:LEU:HD13	2.02	0.41
1:A:993:LEU:HD11	1:A:1040:ILE:HG21	2.02	0.41
1:A:1215:LEU:HD11	1:A:1261:LEU:HD11	2.01	0.41
1:A:1603:ARG:O	1:A:1607:ILE:HG12	2.20	0.41
1:A:2102:SER:HB2	1:A:2206:GLU:HB3	2.02	0.41
1:D:825:SER:HB3	1:D:829:ILE:HD11	2.02	0.41
1:B:1315:ILE:HG23	1:B:1316:VAL:HG23	2.02	0.41
1:A:825:SER:OG	1:A:826:LYS:N	2.53	0.41
1:B:68:ALA:HB3	1:B:99:GLU:HG2	2.03	0.41
1:B:1062:ARG:NH1	1:B:1636:LEU:O	2.54	0.41
1:C:45:ASP:OD1	1:C:45:ASP:N	2.53	0.41
1:A:68:ALA:HB3	1:A:99:GLU:HG2	2.03	0.41
1:A:382:VAL:HA	1:A:383:PRO:HD3	1.91	0.41
1:A:1339:GLU:OE1	1:B:471:ARG:NH2	2.54	0.41
1:A:1636:LEU:HA	1:A:1639:GLU:HG2	2.02	0.41
1:A:2456:SER:HB2	1:A:2535:ILE:HG22	2.03	0.41
1:B:45:ASP:OD1	1:B:45:ASP:N	2.53	0.41
1:B:2431:ILE:HD11	1:C:2447:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1636:LEU:HA	1:C:1639:GLU:HG2	2.01	0.41
1:D:68:ALA:HB3	1:D:99:GLU:HG2	2.03	0.41
1:D:247:GLN:HB3	1:D:248:GLU:OE1	2.21	0.41
1:D:620:SER:C	1:D:622:VAL:H	2.27	0.41
1:D:1636:LEU:HA	1:D:1639:GLU:HG2	2.01	0.41
1:B:722:GLY:H	1:B:727:ARG:HH21	1.68	0.41
1:B:828:GLU:O	1:B:832:ARG:NH2	2.53	0.41
1:B:1005:ASN:HD22	1:B:1007:GLN:HB3	1.86	0.41
1:A:134:VAL:HB	1:A:149:VAL:HG12	2.02	0.41
1:A:2703:GLU:HB3	1:A:2707:LYS:NZ	2.35	0.41
1:D:2082:MET:HA	1:D:2085:VAL:HG12	2.02	0.41
1:B:814:ILE:HG13	1:B:815:ALA:H	1.86	0.41
1:B:1288:ASN:HB3	1:B:1290:ARG:HD2	2.03	0.41
1:B:2644:PHE:HE2	1:B:2663:VAL:HG11	1.85	0.41
1:C:212:VAL:HG23	1:C:214:CYS:H	1.85	0.41
1:C:825:SER:OG	1:C:826:LYS:N	2.53	0.41
1:C:1062:ARG:NH1	1:C:1636:LEU:O	2.53	0.41
1:C:1176:VAL:HA	1:C:1179:ILE:HG22	2.02	0.41
1:A:1966:MET:HA	1:A:1969:ILE:HB	2.02	0.41
1:D:1956:ASP:N	1:D:1956:ASP:OD1	2.53	0.41
1:B:63:MET:SD	1:B:120:VAL:HG21	2.60	0.41
1:B:825:SER:HB3	1:B:829:ILE:HD11	2.03	0.41
1:B:1110:ASP:OD1	1:B:1110:ASP:N	2.50	0.41
1:B:1636:LEU:HA	1:B:1639:GLU:HG2	2.02	0.41
1:C:828:GLU:O	1:C:832:ARG:NH2	2.54	0.41
1:C:989:ARG:HD3	1:C:1041:PHE:HE1	1.86	0.41
1:A:1005:ASN:HD22	1:A:1007:GLN:HB3	1.86	0.41
1:A:1062:ARG:NH1	1:A:1636:LEU:O	2.54	0.41
1:A:2203:ARG:HH21	1:D:2623:ASN:HB3	1.86	0.41
1:A:2644:PHE:HE2	1:A:2663:VAL:HG11	1.85	0.41
2:A:2802:PLX:H21	2:A:2802:PLX:H1B2	1.81	0.41
2:A:2805:PLX:H1C2	2:A:2805:PLX:H22	1.79	0.41
1:D:510:MET:HG2	1:D:515:ILE:HD12	2.02	0.41
1:D:833:PHE:O	1:D:836:THR:OG1	2.26	0.41
1:D:1115:ILE:HD11	1:D:1186:LEU:HD23	2.01	0.41
1:D:1176:VAL:HA	1:D:1179:ILE:HG22	2.02	0.41
1:D:2456:SER:HB2	1:D:2535:ILE:HG22	2.02	0.41
1:D:2596:LEU:HD23	1:D:2596:LEU:HA	1.92	0.41
1:D:2644:PHE:HE2	1:D:2663:VAL:HG11	1.85	0.41
1:B:989:ARG:HD3	1:B:1041:PHE:HE1	1.86	0.41
1:B:1025:PRO:HB2	1:B:1026:GLY:H	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2082:MET:HA	1:B:2085:VAL:HG12	2.03	0.41
1:C:68:ALA:HB3	1:C:99:GLU:HG2	2.03	0.41
1:C:262:VAL:HG11	1:C:418:ILE:HD12	2.03	0.41
1:C:814:ILE:HG13	1:C:815:ALA:H	1.85	0.41
1:C:1008:SER:O	1:C:1008:SER:OG	2.39	0.41
1:C:1624:SER:HA	1:C:1627:VAL:HG22	2.02	0.41
1:C:1806:ASN:HA	1:C:1809:ILE:HG22	2.01	0.41
1:C:1956:ASP:OD1	1:C:1956:ASP:N	2.53	0.41
1:C:2082:MET:HA	1:C:2085:VAL:HG12	2.02	0.41
1:C:2456:SER:HB2	1:C:2535:ILE:HG22	2.02	0.41
1:A:45:ASP:OD1	1:A:45:ASP:N	2.53	0.41
1:D:298:TYR:N	1:D:301:SER:OG	2.49	0.41
1:D:604:LYS:HG2	1:D:608:LYS:HE3	2.02	0.41
2:D:5105:PLX:H1B2	2:D:5105:PLX:H22	1.79	0.41
1:B:636:ASP:OD2	1:B:636:ASP:N	2.55	0.41
2:B:2801:PLX:H111	2:B:2801:PLX:H271	2.03	0.41
1:C:825:SER:HB3	1:C:829:ILE:HD11	2.03	0.41
1:C:1202:GLN:HA	1:C:1205:LEU:HB2	2.03	0.41
1:A:623:ARG:HH22	1:A:630:PHE:HB3	1.86	0.40
1:A:825:SER:HB3	1:A:829:ILE:HD11	2.03	0.40
1:A:2082:MET:HA	1:A:2085:VAL:HG12	2.03	0.40
1:A:2431:ILE:HD11	1:B:2447:LEU:HD22	2.03	0.40
1:B:645:ILE:HA	1:B:646:PRO:HD3	1.90	0.40
1:C:1005:ASN:HD22	1:C:1007:GLN:HB3	1.85	0.40
2:C:5103:PLX:H22	2:C:5103:PLX:H1C2	1.80	0.40
1:D:1288:ASN:HB3	1:D:1290:ARG:HD2	2.03	0.40
1:D:2409:HIS:HD1	1:D:2410:GLU:H	1.69	0.40
1:B:40:GLN:HA	1:B:41:PRO:HD3	1.86	0.40
1:B:737:LEU:HD23	1:B:737:LEU:HA	1.88	0.40
1:B:864:PHE:HD1	1:B:970:THR:HB	1.85	0.40
1:B:2002:GLU:HA	1:B:2005:GLN:HB2	2.02	0.40
1:A:828:GLU:O	1:A:832:ARG:NH2	2.55	0.40
1:A:2061:ASN:HB3	1:A:2111:ARG:HH21	1.86	0.40
1:D:212:VAL:HG23	1:D:214:CYS:H	1.86	0.40
1:D:833:PHE:O	1:D:837:MET:HG2	2.22	0.40
1:B:1862:ASP:OD1	1:B:1863:ARG:N	2.55	0.40
1:A:814:ILE:HG13	1:A:815:ALA:H	1.85	0.40
1:B:1358:MET:HE3	1:B:1359:ARG:HH12	1.86	0.40
1:B:2616:LEU:HD22	1:B:2620:LYS:HG3	2.03	0.40
1:C:636:ASP:OD2	1:C:636:ASP:N	2.54	0.40
1:A:645:ILE:HA	1:A:646:PRO:HD3	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2804:PLX:H1B2	2:A:2804:PLX:H22	1.79	0.40
1:D:884:LEU:HD12	1:D:981:ILE:HG22	2.02	0.40
1:B:1674:LYS:HA	1:B:1677:GLN:HG3	2.03	0.40
1:B:2061:ASN:HB3	1:B:2111:ARG:HH21	1.86	0.40
1:C:132:LEU:HA	1:C:151:LEU:HD23	2.04	0.40
1:C:437:PRO:HA	1:C:440:VAL:HG12	2.03	0.40
1:C:2644:PHE:HE2	1:C:2663:VAL:HG11	1.85	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	2272/2736 (83%)	2038 (90%)	233 (10%)	1 (0%)	100	100
1	B	2272/2736 (83%)	2038 (90%)	232 (10%)	2 (0%)	48	72
1	C	2272/2736 (83%)	2034 (90%)	236 (10%)	2 (0%)	48	72
1	D	2272/2736 (83%)	2037 (90%)	233 (10%)	2 (0%)	48	72
All	All	9088/10944 (83%)	8147 (90%)	934 (10%)	7 (0%)	49	72

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	147	MET
1	B	147	MET
1	C	147	MET
1	D	853	PRO
1	A	853	PRO
1	B	853	PRO
1	C	853	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1877/2446 (77%)	1876 (100%)	1 (0%)	88	95
1	B	1877/2446 (77%)	1876 (100%)	1 (0%)	88	95
1	C	1877/2446 (77%)	1876 (100%)	1 (0%)	88	95
1	D	1877/2446 (77%)	1876 (100%)	1 (0%)	88	95
All	All	7508/9784 (77%)	7504 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1620	GLN
1	D	1620	GLN
1	B	1620	GLN
1	C	1620	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	71	GLN
1	A	107	ASN
1	A	362	ASN
1	A	649	GLN
1	A	717	GLN
1	A	1219	GLN
1	A	1248	ASN
1	A	1250	GLN
1	A	1279	ASN
1	A	1302	HIS
1	A	1742	ASN
1	A	1868	GLN
1	A	1869	GLN
1	A	1981	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2035	GLN
1	A	2058	HIS
1	A	2061	ASN
1	A	2155	ASN
1	A	2195	GLN
1	A	2476	ASN
1	A	2623	ASN
1	A	2738	HIS
1	D	71	GLN
1	D	191	GLN
1	D	362	ASN
1	D	544	GLN
1	D	546	HIS
1	D	717	GLN
1	D	1219	GLN
1	D	1248	ASN
1	D	1250	GLN
1	D	1302	HIS
1	D	1742	ASN
1	D	1869	GLN
1	D	1981	ASN
1	D	2035	GLN
1	D	2104	HIS
1	D	2171	GLN
1	D	2192	HIS
1	D	2195	GLN
1	D	2361	ASN
1	D	2476	ASN
1	D	2526	HIS
1	D	2623	ASN
1	D	2738	HIS
1	B	64	ASN
1	B	71	GLN
1	B	107	ASN
1	B	191	GLN
1	B	362	ASN
1	B	544	GLN
1	B	582	GLN
1	B	717	GLN
1	B	758	GLN
1	B	797	GLN
1	B	1219	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1250	GLN
1	B	1279	ASN
1	B	1302	HIS
1	B	1742	ASN
1	B	1869	GLN
1	B	1981	ASN
1	B	2035	GLN
1	B	2171	GLN
1	B	2192	HIS
1	B	2195	GLN
1	B	2361	ASN
1	B	2476	ASN
1	B	2526	HIS
1	B	2623	ASN
1	B	2738	HIS
1	C	64	ASN
1	C	71	GLN
1	C	107	ASN
1	C	362	ASN
1	C	564	GLN
1	C	649	GLN
1	C	717	GLN
1	C	797	GLN
1	C	1219	GLN
1	C	1250	GLN
1	C	1302	HIS
1	C	1742	ASN
1	C	1869	GLN
1	C	1981	ASN
1	C	2035	GLN
1	C	2155	ASN
1	C	2192	HIS
1	C	2195	GLN
1	C	2361	ASN
1	C	2476	ASN
1	C	2526	HIS
1	C	2623	ASN
1	C	2738	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	5105	-	36,36,51	1.74	5 (13%)	38,44,59	1.35	5 (13%)
2	PLX	D	5106	-	35,35,51	1.76	5 (14%)	37,43,59	1.37	5 (13%)
2	PLX	A	2807	-	43,43,51	1.65	6 (13%)	45,51,59	1.53	6 (13%)
2	PLX	C	5105	-	43,43,51	1.65	5 (11%)	45,51,59	1.24	5 (11%)
2	PLX	A	2806	-	38,38,51	1.70	4 (10%)	40,46,59	1.34	5 (12%)
2	PLX	C	5107	-	45,45,51	1.59	5 (11%)	47,53,59	1.25	5 (10%)
2	PLX	C	5102	-	36,36,51	1.74	4 (11%)	38,44,59	1.35	5 (13%)
2	PLX	D	5103	-	45,45,51	1.59	5 (11%)	47,53,59	1.24	5 (10%)
2	PLX	B	2805	-	45,45,51	1.59	4 (8%)	47,53,59	1.23	5 (10%)
2	PLX	D	5107	-	38,38,51	1.71	4 (10%)	40,46,59	1.34	5 (12%)
2	PLX	D	5108	-	43,43,51	1.65	5 (11%)	45,51,59	1.24	5 (11%)
2	PLX	B	2802	-	35,35,51	1.76	5 (14%)	37,43,59	1.37	5 (13%)
2	PLX	B	2807	-	39,39,51	1.68	5 (12%)	41,47,59	1.28	5 (12%)
2	PLX	C	5103	-	35,35,51	1.76	5 (14%)	37,43,59	1.37	5 (13%)
2	PLX	D	5102	-	45,45,51	1.59	4 (8%)	47,53,59	1.23	5 (10%)
2	PLX	A	2802	-	45,45,51	1.59	5 (11%)	47,53,59	1.24	5 (10%)
2	PLX	B	2803	-	38,38,51	1.71	5 (13%)	40,46,59	1.34	5 (12%)
2	PLX	A	2805	-	35,35,51	1.76	5 (14%)	37,43,59	1.38	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLX	D	5104	-	39,39,51	1.68	5 (12%)	41,47,59	1.31	5 (12%)
2	PLX	A	2803	-	39,39,51	1.68	5 (12%)	41,47,59	1.29	5 (12%)
2	PLX	C	5108	-	39,39,51	1.68	5 (12%)	41,47,59	1.31	5 (12%)
2	PLX	A	2801	-	45,45,51	1.59	4 (8%)	47,53,59	1.23	5 (10%)
2	PLX	A	2804	-	36,36,51	1.74	4 (11%)	38,44,59	1.35	5 (13%)
2	PLX	C	5106	-	45,45,51	1.59	4 (8%)	47,53,59	1.23	5 (10%)
2	PLX	B	2804	-	43,43,51	1.65	6 (13%)	45,51,59	1.24	5 (11%)
2	PLX	C	5104	-	38,38,51	1.71	4 (10%)	40,46,59	1.34	5 (12%)
2	PLX	B	2801	-	36,36,51	1.75	4 (11%)	38,44,59	1.37	6 (15%)
2	PLX	B	2806	-	45,45,51	1.59	5 (11%)	47,53,59	1.24	5 (10%)

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	5105	-	3/3/5/5	25/40/40/55	-
2	PLX	D	5106	-	3/3/5/5	25/39/39/55	-
2	PLX	A	2807	-	3/3/5/5	23/47/47/55	-
2	PLX	C	5105	-	3/3/5/5	22/47/47/55	-
2	PLX	A	2806	-	3/3/5/5	27/42/42/55	-
2	PLX	C	5107	-	3/3/5/5	27/49/49/55	-
2	PLX	C	5102	-	3/3/5/5	25/40/40/55	-
2	PLX	D	5103	-	3/3/5/5	27/49/49/55	-
2	PLX	B	2805	-	3/3/5/5	24/49/49/55	-
2	PLX	D	5107	-	3/3/5/5	27/42/42/55	-
2	PLX	D	5108	-	3/3/5/5	21/47/47/55	-
2	PLX	B	2802	-	3/3/5/5	25/39/39/55	-
2	PLX	B	2807	-	3/3/5/5	27/43/43/55	-
2	PLX	C	5103	-	3/3/5/5	25/39/39/55	-
2	PLX	D	5102	-	3/3/5/5	26/49/49/55	-
2	PLX	A	2802	-	3/3/5/5	27/49/49/55	-
2	PLX	B	2803	-	3/3/5/5	25/42/42/55	-
2	PLX	A	2805	-	3/3/5/5	25/39/39/55	-
2	PLX	D	5104	-	3/3/5/5	24/43/43/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLX	A	2803	-	3/3/5/5	23/43/43/55	-
2	PLX	C	5108	-	3/3/5/5	24/43/43/55	-
2	PLX	A	2801	-	3/3/5/5	24/49/49/55	-
2	PLX	A	2804	-	3/3/5/5	25/40/40/55	-
2	PLX	C	5106	-	3/3/5/5	26/49/49/55	-
2	PLX	B	2804	-	3/3/5/5	21/47/47/55	-
2	PLX	C	5104	-	3/3/5/5	27/42/42/55	-
2	PLX	B	2801	-	3/3/5/5	21/40/40/55	-
2	PLX	B	2806	-	3/3/5/5	28/49/49/55	-

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2801	PLX	O7-C6	-5.81	1.18	1.39
2	A	2805	PLX	O7-C6	-5.80	1.18	1.39
2	B	2802	PLX	O7-C6	-5.80	1.18	1.39
2	B	2803	PLX	O7-C6	-5.80	1.18	1.39
2	B	2806	PLX	O7-C6	-5.80	1.19	1.39
2	D	5108	PLX	O9-C24	-5.79	1.19	1.39
2	D	5106	PLX	O7-C6	-5.79	1.19	1.39
2	B	2801	PLX	O9-C24	-5.79	1.19	1.39
2	A	2803	PLX	O7-C6	-5.78	1.19	1.39
2	A	2804	PLX	O9-C24	-5.78	1.19	1.39
2	C	5107	PLX	O7-C6	-5.78	1.19	1.39
2	C	5104	PLX	O7-C6	-5.78	1.19	1.39
2	C	5103	PLX	O7-C6	-5.78	1.19	1.39
2	B	2807	PLX	O7-C6	-5.78	1.19	1.39
2	D	5107	PLX	O7-C6	-5.78	1.19	1.39
2	D	5103	PLX	O7-C6	-5.78	1.19	1.39
2	A	2801	PLX	O7-C6	-5.77	1.19	1.39
2	C	5102	PLX	O9-C24	-5.77	1.19	1.39
2	D	5105	PLX	O7-C6	-5.77	1.19	1.39
2	B	2805	PLX	O7-C6	-5.77	1.19	1.39
2	C	5108	PLX	O7-C6	-5.77	1.19	1.39
2	D	5102	PLX	O7-C6	-5.77	1.19	1.39
2	C	5106	PLX	O7-C6	-5.77	1.19	1.39
2	A	2806	PLX	O7-C6	-5.77	1.19	1.39
2	B	2803	PLX	O9-C24	-5.76	1.19	1.39
2	A	2802	PLX	O7-C6	-5.76	1.19	1.39
2	A	2804	PLX	O7-C6	-5.76	1.19	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5105	PLX	O7-C6	-5.76	1.19	1.39
2	D	5105	PLX	O9-C24	-5.76	1.19	1.39
2	C	5102	PLX	O7-C6	-5.75	1.19	1.39
2	B	2804	PLX	O7-C6	-5.75	1.19	1.39
2	D	5108	PLX	O7-C6	-5.75	1.19	1.39
2	C	5105	PLX	O9-C24	-5.75	1.19	1.39
2	D	5104	PLX	O7-C6	-5.74	1.19	1.39
2	A	2806	PLX	O9-C24	-5.74	1.19	1.39
2	C	5104	PLX	O9-C24	-5.74	1.19	1.39
2	B	2804	PLX	O9-C24	-5.73	1.19	1.39
2	D	5106	PLX	O9-C24	-5.73	1.19	1.39
2	D	5103	PLX	O9-C24	-5.73	1.19	1.39
2	D	5107	PLX	O9-C24	-5.73	1.19	1.39
2	B	2806	PLX	O9-C24	-5.72	1.19	1.39
2	B	2805	PLX	O9-C24	-5.72	1.19	1.39
2	D	5102	PLX	O9-C24	-5.72	1.19	1.39
2	C	5103	PLX	O9-C24	-5.71	1.19	1.39
2	C	5107	PLX	O9-C24	-5.71	1.19	1.39
2	A	2802	PLX	O9-C24	-5.70	1.19	1.39
2	A	2801	PLX	O9-C24	-5.70	1.19	1.39
2	B	2802	PLX	O9-C24	-5.70	1.19	1.39
2	C	5106	PLX	O9-C24	-5.70	1.19	1.39
2	A	2805	PLX	O9-C24	-5.69	1.19	1.39
2	D	5104	PLX	O9-C24	-5.67	1.19	1.39
2	B	2807	PLX	O9-C24	-5.67	1.19	1.39
2	C	5108	PLX	O9-C24	-5.67	1.19	1.39
2	A	2803	PLX	O9-C24	-5.67	1.19	1.39
2	A	2807	PLX	O7-C6	-5.57	1.19	1.39
2	A	2807	PLX	O9-C24	-5.26	1.20	1.39
2	C	5106	PLX	O6-C4	-3.48	1.40	1.44
2	C	5104	PLX	O6-C4	-3.47	1.40	1.44
2	A	2801	PLX	O6-C4	-3.46	1.40	1.44
2	D	5102	PLX	O6-C4	-3.46	1.40	1.44
2	B	2805	PLX	O6-C4	-3.46	1.40	1.44
2	D	5107	PLX	O6-C4	-3.45	1.40	1.44
2	A	2806	PLX	O6-C4	-3.40	1.40	1.44
2	D	5105	PLX	O6-C4	-3.39	1.40	1.44
2	C	5103	PLX	O6-C4	-3.39	1.40	1.44
2	B	2803	PLX	O6-C4	-3.38	1.40	1.44
2	A	2805	PLX	O6-C4	-3.38	1.40	1.44
2	B	2802	PLX	O6-C4	-3.36	1.40	1.44
2	A	2804	PLX	O6-C4	-3.33	1.40	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5106	PLX	O6-C4	-3.33	1.40	1.44
2	C	5102	PLX	O6-C4	-3.30	1.40	1.44
2	A	2803	PLX	O6-C4	-3.26	1.40	1.44
2	D	5103	PLX	O6-C4	-3.23	1.40	1.44
2	C	5108	PLX	O6-C4	-3.21	1.40	1.44
2	B	2807	PLX	O6-C4	-3.20	1.40	1.44
2	D	5104	PLX	O6-C4	-3.20	1.40	1.44
2	A	2802	PLX	O6-C4	-3.19	1.40	1.44
2	B	2806	PLX	O6-C4	-3.19	1.40	1.44
2	C	5105	PLX	O6-C4	-3.17	1.40	1.44
2	C	5107	PLX	O6-C4	-3.15	1.40	1.44
2	B	2804	PLX	O6-C4	-3.14	1.40	1.44
2	D	5108	PLX	O6-C4	-3.14	1.40	1.44
2	B	2801	PLX	O6-C4	-3.12	1.40	1.44
2	A	2807	PLX	C7-C6	2.62	1.56	1.50
2	A	2807	PLX	O6-C4	-2.40	1.41	1.44
2	A	2807	PLX	O8-C24	2.35	1.44	1.40
2	A	2807	PLX	C25-C24	2.35	1.55	1.50
2	D	5103	PLX	C7-C6	2.32	1.55	1.50
2	B	2806	PLX	C7-C6	2.30	1.55	1.50
2	A	2802	PLX	C7-C6	2.29	1.55	1.50
2	C	5107	PLX	C7-C6	2.27	1.55	1.50
2	B	2803	PLX	C7-C6	2.26	1.55	1.50
2	C	5105	PLX	C7-C6	2.23	1.55	1.50
2	C	5108	PLX	C7-C6	2.22	1.55	1.50
2	A	2803	PLX	C7-C6	2.21	1.55	1.50
2	B	2807	PLX	C7-C6	2.20	1.55	1.50
2	B	2804	PLX	C7-C6	2.19	1.55	1.50
2	D	5102	PLX	C7-C6	2.18	1.55	1.50
2	C	5104	PLX	C7-C6	2.18	1.55	1.50
2	D	5104	PLX	C7-C6	2.17	1.55	1.50
2	D	5108	PLX	C7-C6	2.17	1.55	1.50
2	A	2806	PLX	C7-C6	2.17	1.55	1.50
2	C	5102	PLX	C7-C6	2.16	1.55	1.50
2	D	5107	PLX	C7-C6	2.16	1.55	1.50
2	B	2801	PLX	C7-C6	2.15	1.55	1.50
2	C	5103	PLX	C7-C6	2.15	1.55	1.50
2	A	2801	PLX	C7-C6	2.15	1.55	1.50
2	A	2805	PLX	C7-C6	2.15	1.55	1.50
2	B	2805	PLX	C7-C6	2.14	1.55	1.50
2	B	2802	PLX	C7-C6	2.14	1.55	1.50
2	D	5106	PLX	C7-C6	2.13	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5106	PLX	C7-C6	2.13	1.55	1.50
2	A	2804	PLX	C7-C6	2.12	1.55	1.50
2	D	5105	PLX	C7-C6	2.11	1.55	1.50
2	D	5108	PLX	C25-C24	2.10	1.55	1.50
2	A	2802	PLX	P1-O4	2.10	1.67	1.59
2	D	5103	PLX	P1-O4	2.10	1.67	1.59
2	C	5107	PLX	P1-O4	2.09	1.67	1.59
2	B	2806	PLX	P1-O4	2.07	1.67	1.59
2	C	5105	PLX	C25-C24	2.07	1.55	1.50
2	A	2805	PLX	P1-O4	2.06	1.67	1.59
2	B	2807	PLX	P1-O4	2.06	1.67	1.59
2	B	2804	PLX	C25-C24	2.06	1.55	1.50
2	A	2803	PLX	P1-O4	2.04	1.67	1.59
2	D	5105	PLX	P1-O4	2.03	1.67	1.59
2	D	5104	PLX	P1-O4	2.03	1.67	1.59
2	C	5108	PLX	P1-O4	2.02	1.67	1.59
2	C	5103	PLX	P1-O4	2.02	1.67	1.59
2	B	2802	PLX	P1-O4	2.02	1.67	1.59
2	B	2804	PLX	P1-O4	2.01	1.67	1.59
2	D	5106	PLX	P1-O4	2.01	1.67	1.59
2	B	2803	PLX	P1-O4	2.00	1.67	1.59

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2807	PLX	C5-O8-C24	4.40	123.25	113.86
2	A	2807	PLX	O7-C6-C7	4.11	120.58	109.37
2	A	2807	PLX	O8-C24-C25	4.08	122.15	109.49
2	B	2803	PLX	O9-C24-C25	4.03	120.37	109.37
2	D	5107	PLX	O9-C24-C25	4.02	120.35	109.37
2	C	5104	PLX	O9-C24-C25	4.02	120.34	109.37
2	B	2806	PLX	O9-C24-C25	4.00	120.28	109.37
2	D	5103	PLX	O9-C24-C25	4.00	120.28	109.37
2	C	5107	PLX	O9-C24-C25	4.00	120.28	109.37
2	C	5108	PLX	C1B-N1-C1C	3.98	119.44	108.98
2	A	2802	PLX	O9-C24-C25	3.97	120.20	109.37
2	D	5104	PLX	C1B-N1-C1C	3.97	119.39	108.98
2	A	2806	PLX	O9-C24-C25	3.94	120.12	109.37
2	D	5105	PLX	O7-C6-C7	3.92	120.07	109.37
2	A	2804	PLX	O7-C6-C7	3.90	120.00	109.37
2	A	2807	PLX	O9-C24-C25	3.89	119.98	109.37
2	A	2805	PLX	O9-C24-C25	3.88	119.96	109.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5104	PLX	C1B-N1-C1C	3.86	119.12	108.98
2	B	2803	PLX	C1B-N1-C1C	3.86	119.12	108.98
2	B	2806	PLX	C1B-N1-C1C	3.86	119.11	108.98
2	C	5107	PLX	C1B-N1-C1C	3.86	119.11	108.98
2	A	2806	PLX	C1B-N1-C1C	3.86	119.11	108.98
2	C	5107	PLX	O7-C6-C7	3.86	119.89	109.37
2	D	5106	PLX	C1B-N1-C1C	3.85	119.10	108.98
2	D	5103	PLX	C1B-N1-C1C	3.85	119.08	108.98
2	A	2802	PLX	C1B-N1-C1C	3.85	119.08	108.98
2	D	5107	PLX	C1B-N1-C1C	3.84	119.07	108.98
2	C	5102	PLX	O7-C6-C7	3.84	119.85	109.37
2	B	2806	PLX	O7-C6-C7	3.84	119.85	109.37
2	C	5103	PLX	O9-C24-C25	3.83	119.83	109.37
2	C	5103	PLX	C1B-N1-C1C	3.83	119.04	108.98
2	A	2802	PLX	O7-C6-C7	3.83	119.82	109.37
2	C	5106	PLX	O7-C6-C7	3.83	119.81	109.37
2	B	2802	PLX	O9-C24-C25	3.83	119.81	109.37
2	B	2802	PLX	C1B-N1-C1C	3.82	119.01	108.98
2	A	2806	PLX	O7-C6-C7	3.82	119.80	109.37
2	D	5107	PLX	O7-C6-C7	3.82	119.80	109.37
2	D	5103	PLX	O7-C6-C7	3.82	119.79	109.37
2	C	5105	PLX	O7-C6-C7	3.82	119.79	109.37
2	A	2805	PLX	O7-C6-C7	3.82	119.79	109.37
2	D	5108	PLX	O7-C6-C7	3.82	119.79	109.37
2	A	2801	PLX	O7-C6-C7	3.82	119.79	109.37
2	D	5106	PLX	O9-C24-C25	3.82	119.78	109.37
2	A	2803	PLX	O9-C24-C25	3.81	119.77	109.37
2	B	2805	PLX	O7-C6-C7	3.81	119.77	109.37
2	B	2803	PLX	O7-C6-C7	3.81	119.76	109.37
2	C	5104	PLX	O7-C6-C7	3.80	119.75	109.37
2	D	5104	PLX	O9-C24-C25	3.80	119.75	109.37
2	D	5102	PLX	O7-C6-C7	3.78	119.70	109.37
2	C	5108	PLX	O9-C24-C25	3.78	119.69	109.37
2	B	2801	PLX	O8-C24-C25	3.78	121.23	109.49
2	B	2807	PLX	O9-C24-C25	3.77	119.65	109.37
2	B	2804	PLX	O7-C6-C7	3.76	119.64	109.37
2	D	5105	PLX	O9-C24-C25	3.76	119.63	109.37
2	B	2802	PLX	O7-C6-C7	3.76	119.63	109.37
2	A	2805	PLX	C1B-N1-C1C	3.75	118.84	108.98
2	C	5102	PLX	O9-C24-C25	3.75	119.60	109.37
2	C	5103	PLX	O7-C6-C7	3.75	119.59	109.37
2	B	2805	PLX	C1B-N1-C1C	3.74	118.80	108.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2801	PLX	C1B-N1-C1C	3.74	118.79	108.98
2	D	5102	PLX	O9-C24-C25	3.73	119.54	109.37
2	B	2805	PLX	O9-C24-C25	3.72	119.53	109.37
2	B	2801	PLX	O7-C6-C7	3.72	119.53	109.37
2	D	5106	PLX	O7-C6-C7	3.72	119.53	109.37
2	D	5102	PLX	C1B-N1-C1C	3.72	118.74	108.98
2	D	5104	PLX	O7-C6-C7	3.72	119.51	109.37
2	A	2804	PLX	O9-C24-C25	3.71	119.50	109.37
2	B	2807	PLX	O7-C6-C7	3.71	119.50	109.37
2	C	5106	PLX	C1B-N1-C1C	3.71	118.72	108.98
2	A	2803	PLX	O7-C6-C7	3.71	119.49	109.37
2	B	2804	PLX	O9-C24-C25	3.70	119.47	109.37
2	C	5108	PLX	O7-C6-C7	3.70	119.47	109.37
2	C	5106	PLX	O9-C24-C25	3.69	119.45	109.37
2	A	2801	PLX	O9-C24-C25	3.68	119.42	109.37
2	D	5108	PLX	O8-C24-C25	3.68	120.90	109.49
2	B	2804	PLX	O8-C24-C25	3.67	120.87	109.49
2	C	5105	PLX	O9-C24-C25	3.66	119.35	109.37
2	A	2803	PLX	C1B-N1-C1C	3.66	118.58	108.98
2	D	5105	PLX	C1B-N1-C1C	3.65	118.57	108.98
2	C	5102	PLX	C1B-N1-C1C	3.64	118.55	108.98
2	A	2804	PLX	C1B-N1-C1C	3.64	118.54	108.98
2	C	5105	PLX	O8-C24-C25	3.63	120.76	109.49
2	D	5108	PLX	O9-C24-C25	3.62	119.25	109.37
2	B	2801	PLX	C1B-N1-C1C	3.57	118.36	108.98
2	B	2807	PLX	C1B-N1-C1C	3.56	118.33	108.98
2	C	5102	PLX	O8-C24-C25	3.49	120.33	109.49
2	A	2804	PLX	O8-C24-C25	3.48	120.29	109.49
2	D	5105	PLX	O8-C24-C25	3.46	120.24	109.49
2	B	2804	PLX	C1B-N1-C1C	3.44	118.02	108.98
2	B	2807	PLX	O8-C24-C25	3.42	120.10	109.49
2	C	5106	PLX	O8-C24-C25	3.39	120.01	109.49
2	D	5102	PLX	O8-C24-C25	3.39	120.01	109.49
2	C	5105	PLX	C1B-N1-C1C	3.38	117.86	108.98
2	C	5108	PLX	O8-C24-C25	3.38	119.99	109.49
2	B	2805	PLX	O8-C24-C25	3.38	119.99	109.49
2	A	2801	PLX	O8-C24-C25	3.38	119.98	109.49
2	A	2806	PLX	O8-C24-C25	3.38	119.98	109.49
2	A	2803	PLX	O8-C24-C25	3.38	119.98	109.49
2	A	2807	PLX	C1B-N1-C1C	3.37	117.83	108.98
2	D	5104	PLX	O8-C24-C25	3.37	119.95	109.49
2	D	5108	PLX	C1B-N1-C1C	3.36	117.79	108.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5106	PLX	O8-C24-C25	3.32	119.80	109.49
2	B	2802	PLX	O8-C24-C25	3.32	119.80	109.49
2	C	5103	PLX	O8-C24-C25	3.31	119.78	109.49
2	A	2805	PLX	O8-C24-C25	3.31	119.77	109.49
2	D	5107	PLX	O8-C24-C25	3.31	119.77	109.49
2	C	5104	PLX	O8-C24-C25	3.30	119.75	109.49
2	A	2802	PLX	O8-C24-C25	3.28	119.67	109.49
2	B	2803	PLX	O8-C24-C25	3.28	119.66	109.49
2	C	5107	PLX	O8-C24-C25	3.27	119.64	109.49
2	D	5103	PLX	O8-C24-C25	3.27	119.63	109.49
2	B	2806	PLX	O8-C24-C25	3.26	119.61	109.49
2	B	2801	PLX	O9-C24-C25	3.15	117.96	109.37
2	B	2801	PLX	O8-C5-C4	-2.33	105.15	110.82
2	A	2802	PLX	O6-C6-C7	2.21	120.32	110.27
2	D	5103	PLX	O6-C6-C7	2.21	120.29	110.27
2	C	5107	PLX	O6-C6-C7	2.20	120.28	110.27
2	B	2806	PLX	O6-C6-C7	2.20	120.27	110.27
2	B	2804	PLX	O6-C6-C7	2.20	120.27	110.27
2	B	2801	PLX	O6-C6-C7	2.19	120.23	110.27
2	B	2802	PLX	O6-C6-C7	2.19	120.23	110.27
2	A	2803	PLX	O6-C6-C7	2.19	120.22	110.27
2	C	5103	PLX	O6-C6-C7	2.19	120.21	110.27
2	A	2805	PLX	O6-C6-C7	2.19	120.21	110.27
2	D	5107	PLX	O6-C6-C7	2.19	120.21	110.27
2	B	2803	PLX	O6-C6-C7	2.19	120.20	110.27
2	D	5106	PLX	O6-C6-C7	2.19	120.20	110.27
2	A	2806	PLX	O6-C6-C7	2.18	120.18	110.27
2	C	5104	PLX	O6-C6-C7	2.18	120.18	110.27
2	C	5105	PLX	O6-C6-C7	2.18	120.17	110.27
2	D	5108	PLX	O6-C6-C7	2.17	120.14	110.27
2	B	2807	PLX	O6-C6-C7	2.16	120.07	110.27
2	D	5104	PLX	O6-C6-C7	2.14	120.00	110.27
2	C	5108	PLX	O6-C6-C7	2.13	119.94	110.27
2	C	5106	PLX	O6-C6-C7	2.11	119.84	110.27
2	D	5102	PLX	O6-C6-C7	2.11	119.84	110.27
2	B	2805	PLX	O6-C6-C7	2.10	119.80	110.27
2	A	2801	PLX	O6-C6-C7	2.10	119.79	110.27
2	C	5102	PLX	O6-C6-C7	2.09	119.75	110.27
2	A	2804	PLX	O6-C6-C7	2.08	119.70	110.27
2	D	5105	PLX	O6-C6-C7	2.07	119.69	110.27
2	A	2807	PLX	C28-C27-C26	2.03	124.64	114.37

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	2805	PLX	C24
2	A	2805	PLX	C6
2	A	2805	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	D	5102	PLX	C24
2	D	5102	PLX	C6
2	D	5102	PLX	C4
2	D	5103	PLX	C24
2	D	5103	PLX	C6
2	D	5103	PLX	C4
2	D	5104	PLX	C24
2	D	5104	PLX	C6
2	D	5104	PLX	C4
2	D	5105	PLX	C24
2	D	5105	PLX	C6
2	D	5105	PLX	C4
2	D	5106	PLX	C24
2	D	5106	PLX	C6
2	D	5106	PLX	C4
2	D	5107	PLX	C24
2	D	5107	PLX	C6
2	D	5107	PLX	C4
2	D	5108	PLX	C24
2	D	5108	PLX	C6
2	D	5108	PLX	C4
2	B	2801	PLX	C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
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
2	B	2806	PLX	C4
2	B	2807	PLX	C24
2	B	2807	PLX	C6
2	B	2807	PLX	C4
2	C	5102	PLX	C24
2	C	5102	PLX	C6
2	C	5102	PLX	C4
2	C	5103	PLX	C24
2	C	5103	PLX	C6
2	C	5103	PLX	C4
2	C	5104	PLX	C24
2	C	5104	PLX	C6
2	C	5104	PLX	C4
2	C	5105	PLX	C24
2	C	5105	PLX	C6
2	C	5105	PLX	C4
2	C	5106	PLX	C24
2	C	5106	PLX	C6
2	C	5106	PLX	C4
2	C	5107	PLX	C24
2	C	5107	PLX	C6
2	C	5107	PLX	C4
2	C	5108	PLX	C24
2	C	5108	PLX	C6
2	C	5108	PLX	C4

All (696) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2807	PLX	O7-C6-O6-C4
2	A	2807	PLX	C3-O4-P1-O1
2	A	2807	PLX	C3-O4-P1-O2
2	A	2807	PLX	C3-O4-P1-O3
2	A	2807	PLX	N1-C1-C2-O1
2	A	2807	PLX	O9-C24-O8-C5
2	A	2807	PLX	C25-C24-O8-C5
2	A	2807	PLX	C24-C25-C26-C27
2	D	5102	PLX	O7-C6-O6-C4
2	D	5102	PLX	O6-C4-C5-O8
2	D	5102	PLX	C3-O4-P1-O1
2	D	5102	PLX	C3-O4-P1-O2
2	D	5102	PLX	C3-O4-P1-O3
2	D	5102	PLX	C25-C24-O8-C5
2	D	5102	PLX	O9-C24-C25-C26
2	D	5103	PLX	O7-C6-O6-C4
2	D	5103	PLX	C3-O4-P1-O1
2	D	5103	PLX	C3-O4-P1-O3
2	D	5104	PLX	O7-C6-O6-C4
2	D	5104	PLX	C3-O4-P1-O1
2	D	5104	PLX	C3-O4-P1-O3
2	D	5104	PLX	N1-C1-C2-O1
2	D	5105	PLX	O6-C4-C5-O8
2	D	5105	PLX	C3-O4-P1-O1
2	D	5105	PLX	C3-O4-P1-O3
2	D	5105	PLX	C2-O1-P1-O4
2	D	5105	PLX	C2-O1-P1-O3
2	D	5105	PLX	C1-C2-O1-P1
2	D	5105	PLX	N1-C1-C2-O1
2	D	5105	PLX	O9-C24-O8-C5
2	D	5105	PLX	O9-C24-C25-C26
2	D	5106	PLX	O7-C6-O6-C4
2	D	5106	PLX	C3-O4-P1-O1
2	D	5106	PLX	C3-O4-P1-O2
2	D	5106	PLX	C2-O1-P1-O4
2	D	5106	PLX	C2-O1-P1-O2
2	D	5106	PLX	N1-C1-C2-O1
2	D	5106	PLX	O9-C24-O8-C5
2	D	5106	PLX	C25-C24-O8-C5
2	D	5107	PLX	O7-C6-O6-C4
2	D	5107	PLX	C3-C4-O6-C6
2	D	5107	PLX	C3-O4-P1-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	5107	PLX	C3-O4-P1-O3
2	D	5107	PLX	C2-O1-P1-O4
2	D	5107	PLX	C2-O1-P1-O3
2	D	5107	PLX	N1-C1-C2-O1
2	D	5108	PLX	O7-C6-O6-C4
2	D	5108	PLX	C3-O4-P1-O1
2	D	5108	PLX	C3-O4-P1-O2
2	D	5108	PLX	C3-O4-P1-O3
2	D	5108	PLX	N1-C1-C2-O1
2	D	5108	PLX	O9-C24-O8-C5
2	B	2801	PLX	C3-O4-P1-O1
2	B	2801	PLX	C2-O1-P1-O4
2	B	2801	PLX	C2-O1-P1-O3
2	B	2801	PLX	N1-C1-C2-O1
2	B	2801	PLX	O9-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	2802	PLX	C2-O1-P1-O4
2	B	2802	PLX	C2-O1-P1-O2
2	B	2802	PLX	N1-C1-C2-O1
2	B	2802	PLX	C25-C24-O8-C5
2	B	2803	PLX	O7-C6-O6-C4
2	B	2803	PLX	C3-C4-O6-C6
2	B	2803	PLX	C3-O4-P1-O1
2	B	2803	PLX	C3-O4-P1-O3
2	B	2803	PLX	C2-O1-P1-O4
2	B	2803	PLX	C2-O1-P1-O3
2	B	2803	PLX	N1-C1-C2-O1
2	B	2804	PLX	O7-C6-O6-C4
2	B	2804	PLX	C3-O4-P1-O1
2	B	2804	PLX	C3-O4-P1-O2
2	B	2804	PLX	C3-O4-P1-O3
2	B	2804	PLX	O9-C24-O8-C5
2	B	2805	PLX	O7-C6-O6-C4
2	B	2805	PLX	O6-C4-C5-O8
2	B	2805	PLX	C3-O4-P1-O1
2	B	2805	PLX	C3-O4-P1-O2
2	B	2805	PLX	C3-O4-P1-O3
2	B	2805	PLX	C25-C24-O8-C5
2	B	2805	PLX	O9-C24-C25-C26
2	B	2806	PLX	O7-C6-O6-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2806	PLX	C3-O4-P1-O1
2	B	2806	PLX	C3-O4-P1-O3
2	B	2807	PLX	O7-C6-O6-C4
2	B	2807	PLX	C3-O4-P1-O1
2	B	2807	PLX	C3-O4-P1-O3
2	B	2807	PLX	C2-O1-P1-O4
2	B	2807	PLX	C2-O1-P1-O2
2	B	2807	PLX	C2-O1-P1-O3
2	B	2807	PLX	N1-C1-C2-O1
2	C	5102	PLX	O6-C4-C5-O8
2	C	5102	PLX	C3-O4-P1-O1
2	C	5102	PLX	C3-O4-P1-O3
2	C	5102	PLX	C2-O1-P1-O4
2	C	5102	PLX	C2-O1-P1-O3
2	C	5102	PLX	C1-C2-O1-P1
2	C	5102	PLX	N1-C1-C2-O1
2	C	5102	PLX	O9-C24-O8-C5
2	C	5102	PLX	O9-C24-C25-C26
2	C	5103	PLX	O7-C6-O6-C4
2	C	5103	PLX	C3-O4-P1-O1
2	C	5103	PLX	C3-O4-P1-O2
2	C	5103	PLX	C2-O1-P1-O4
2	C	5103	PLX	C2-O1-P1-O2
2	C	5103	PLX	N1-C1-C2-O1
2	C	5103	PLX	O9-C24-O8-C5
2	C	5103	PLX	C25-C24-O8-C5
2	C	5104	PLX	O7-C6-O6-C4
2	C	5104	PLX	C3-C4-O6-C6
2	C	5104	PLX	C3-O4-P1-O1
2	C	5104	PLX	C3-O4-P1-O3
2	C	5104	PLX	C2-O1-P1-O4
2	C	5104	PLX	C2-O1-P1-O3
2	C	5104	PLX	N1-C1-C2-O1
2	C	5105	PLX	O7-C6-O6-C4
2	C	5105	PLX	C3-O4-P1-O1
2	C	5105	PLX	C3-O4-P1-O2
2	C	5105	PLX	C3-O4-P1-O3
2	C	5105	PLX	O9-C24-O8-C5
2	C	5106	PLX	O7-C6-O6-C4
2	C	5106	PLX	O6-C4-C5-O8
2	C	5106	PLX	C3-O4-P1-O1
2	C	5106	PLX	C3-O4-P1-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5106	PLX	C3-O4-P1-O3
2	C	5106	PLX	C25-C24-O8-C5
2	C	5106	PLX	O9-C24-C25-C26
2	C	5107	PLX	O7-C6-O6-C4
2	C	5107	PLX	C3-O4-P1-O1
2	C	5107	PLX	C3-O4-P1-O3
2	C	5108	PLX	O7-C6-O6-C4
2	C	5108	PLX	C3-O4-P1-O1
2	C	5108	PLX	C3-O4-P1-O3
2	C	5108	PLX	N1-C1-C2-O1
2	A	2806	PLX	C4-C3-O4-P1
2	D	5107	PLX	C4-C3-O4-P1
2	B	2803	PLX	C4-C3-O4-P1
2	C	5104	PLX	C4-C3-O4-P1
2	B	2801	PLX	O6-C4-C5-O8
2	A	2803	PLX	O6-C6-C7-C8
2	A	2803	PLX	O8-C24-C25-C26
2	A	2804	PLX	O6-C6-C7-C8
2	A	2805	PLX	O8-C24-C25-C26
2	D	5103	PLX	O8-C24-C25-C26
2	D	5104	PLX	O6-C6-C7-C8
2	D	5104	PLX	O8-C24-C25-C26
2	D	5105	PLX	O6-C6-C7-C8
2	D	5106	PLX	O8-C24-C25-C26
2	D	5108	PLX	O8-C24-C25-C26
2	B	2802	PLX	O8-C24-C25-C26
2	B	2804	PLX	O8-C24-C25-C26
2	B	2806	PLX	O8-C24-C25-C26
2	B	2807	PLX	O6-C6-C7-C8
2	B	2807	PLX	O8-C24-C25-C26
2	C	5102	PLX	O6-C6-C7-C8
2	C	5103	PLX	O8-C24-C25-C26
2	C	5105	PLX	O8-C24-C25-C26
2	C	5107	PLX	O8-C24-C25-C26
2	C	5108	PLX	O6-C6-C7-C8
2	C	5108	PLX	O8-C24-C25-C26
2	C	5103	PLX	C26-C27-C28-C29
2	D	5106	PLX	C26-C27-C28-C29
2	B	2802	PLX	C26-C27-C28-C29
2	A	2805	PLX	C26-C27-C28-C29
2	A	2801	PLX	C7-C8-C9-C10
2	A	2804	PLX	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2807	PLX	C9-C10-C11-C12
2	D	5104	PLX	C10-C11-C12-C13
2	D	5105	PLX	C11-C10-C9-C8
2	B	2801	PLX	C11-C10-C9-C8
2	B	2803	PLX	C25-C26-C27-C28
2	B	2805	PLX	C7-C8-C9-C10
2	C	5102	PLX	C11-C10-C9-C8
2	D	5107	PLX	C11-C12-C13-C14
2	A	2803	PLX	O9-C24-C25-C26
2	A	2805	PLX	O9-C24-C25-C26
2	D	5106	PLX	O9-C24-C25-C26
2	C	5103	PLX	O9-C24-C25-C26
2	A	2806	PLX	C11-C12-C13-C14
2	B	2803	PLX	C11-C12-C13-C14
2	C	5104	PLX	C11-C12-C13-C14
2	C	5106	PLX	C7-C8-C9-C10
2	A	2806	PLX	C9-C10-C11-C12
2	D	5105	PLX	C9-C10-C11-C12
2	D	5107	PLX	C9-C10-C11-C12
2	C	5104	PLX	C9-C10-C11-C12
2	C	5108	PLX	C10-C11-C12-C13
2	D	5108	PLX	C26-C27-C28-C29
2	A	2805	PLX	C29-C30-C31-C32
2	D	5106	PLX	C29-C30-C31-C32
2	B	2802	PLX	C29-C30-C31-C32
2	C	5103	PLX	C29-C30-C31-C32
2	B	2807	PLX	C10-C11-C12-C13
2	A	2804	PLX	C9-C10-C11-C12
2	D	5102	PLX	C7-C8-C9-C10
2	C	5102	PLX	C9-C10-C11-C12
2	C	5105	PLX	C9-C10-C11-C12
2	C	5105	PLX	C26-C27-C28-C29
2	A	2803	PLX	C10-C11-C12-C13
2	B	2804	PLX	C35-C36-C37-C38
2	A	2802	PLX	C10-C11-C12-C13
2	D	5108	PLX	C9-C10-C11-C12
2	B	2804	PLX	C11-C10-C9-C8
2	A	2802	PLX	C11-C10-C9-C8
2	D	5107	PLX	C25-C26-C27-C28
2	D	5108	PLX	C11-C10-C9-C8
2	C	5105	PLX	C11-C10-C9-C8
2	D	5108	PLX	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	5103	PLX	C10-C11-C12-C13
2	D	5103	PLX	C11-C10-C9-C8
2	B	2801	PLX	C9-C10-C11-C12
2	B	2803	PLX	C9-C10-C11-C12
2	B	2804	PLX	C9-C10-C11-C12
2	C	5107	PLX	C11-C10-C9-C8
2	B	2806	PLX	C10-C11-C12-C13
2	B	2806	PLX	C11-C10-C9-C8
2	C	5104	PLX	C25-C26-C27-C28
2	C	5107	PLX	C33-C34-C35-C36
2	D	5103	PLX	C33-C34-C35-C36
2	D	5105	PLX	C26-C27-C28-C29
2	B	2806	PLX	C33-C34-C35-C36
2	C	5107	PLX	C10-C11-C12-C13
2	A	2802	PLX	C33-C34-C35-C36
2	A	2804	PLX	C26-C27-C28-C29
2	C	5106	PLX	C27-C28-C29-C30
2	B	2805	PLX	C27-C28-C29-C30
2	C	5105	PLX	C34-C35-C36-C37
2	A	2807	PLX	C33-C34-C35-C36
2	C	5102	PLX	C26-C27-C28-C29
2	A	2807	PLX	C11-C12-C13-C14
2	B	2802	PLX	C11-C10-C9-C8
2	B	2804	PLX	C26-C27-C28-C29
2	A	2806	PLX	C25-C26-C27-C28
2	B	2803	PLX	C10-C11-C12-C13
2	C	5105	PLX	C11-C12-C13-C14
2	C	5105	PLX	C31-C32-C33-C34
2	D	5102	PLX	C27-C28-C29-C30
2	D	5108	PLX	C11-C12-C13-C14
2	A	2801	PLX	C30-C31-C32-C33
2	D	5106	PLX	C11-C10-C9-C8
2	B	2804	PLX	C11-C12-C13-C14
2	A	2807	PLX	C11-C10-C9-C8
2	B	2805	PLX	C35-C36-C37-C38
2	A	2807	PLX	C31-C32-C33-C34
2	C	5103	PLX	C11-C10-C9-C8
2	B	2805	PLX	C30-C31-C32-C33
2	A	2806	PLX	C10-C11-C12-C13
2	D	5104	PLX	C11-C12-C13-C14
2	C	5102	PLX	C27-C28-C29-C30
2	D	5104	PLX	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5108	PLX	C25-C26-C27-C28
2	A	2805	PLX	C11-C10-C9-C8
2	C	5104	PLX	C10-C11-C12-C13
2	A	2803	PLX	C11-C12-C13-C14
2	D	5102	PLX	C35-C36-C37-C38
2	B	2805	PLX	C26-C27-C28-C29
2	D	5105	PLX	C27-C28-C29-C30
2	D	5107	PLX	C10-C11-C12-C13
2	B	2807	PLX	C25-C26-C27-C28
2	A	2801	PLX	C35-C36-C37-C38
2	C	5106	PLX	C26-C27-C28-C29
2	B	2807	PLX	C11-C12-C13-C14
2	C	5106	PLX	C35-C36-C37-C38
2	C	5108	PLX	C29-C30-C31-C32
2	D	5108	PLX	C31-C32-C33-C34
2	D	5104	PLX	C29-C30-C31-C32
2	A	2801	PLX	C27-C28-C29-C30
2	D	5102	PLX	C26-C27-C28-C29
2	C	5108	PLX	C11-C12-C13-C14
2	A	2804	PLX	C27-C28-C29-C30
2	C	5107	PLX	C32-C33-C34-C35
2	D	5103	PLX	C32-C33-C34-C35
2	B	2806	PLX	C32-C33-C34-C35
2	B	2801	PLX	C27-C28-C29-C30
2	A	2801	PLX	C26-C27-C28-C29
2	B	2807	PLX	C29-C30-C31-C32
2	A	2802	PLX	C32-C33-C34-C35
2	A	2804	PLX	O4-C3-C4-C5
2	A	2806	PLX	O4-C3-C4-C5
2	D	5105	PLX	O4-C3-C4-C5
2	D	5107	PLX	O4-C3-C4-C5
2	B	2803	PLX	O4-C3-C4-C5
2	C	5102	PLX	O4-C3-C4-C5
2	C	5104	PLX	O4-C3-C4-C5
2	D	5102	PLX	C30-C31-C32-C33
2	A	2803	PLX	C25-C26-C27-C28
2	B	2806	PLX	C25-C26-C27-C28
2	A	2801	PLX	O6-C6-C7-C8
2	D	5103	PLX	C25-C26-C27-C28
2	C	5107	PLX	C25-C26-C27-C28
2	A	2807	PLX	C35-C36-C37-C38
2	A	2801	PLX	C3-C4-C5-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2805	PLX	C3-C4-C5-O8
2	A	2806	PLX	C3-C4-C5-O8
2	D	5102	PLX	C3-C4-C5-O8
2	D	5103	PLX	C3-C4-C5-O8
2	D	5106	PLX	C3-C4-C5-O8
2	D	5107	PLX	C3-C4-C5-O8
2	B	2801	PLX	C3-C4-C5-O8
2	B	2802	PLX	C3-C4-C5-O8
2	B	2803	PLX	C3-C4-C5-O8
2	B	2805	PLX	C3-C4-C5-O8
2	B	2806	PLX	C3-C4-C5-O8
2	C	5103	PLX	C3-C4-C5-O8
2	C	5104	PLX	C3-C4-C5-O8
2	C	5106	PLX	C3-C4-C5-O8
2	C	5107	PLX	C3-C4-C5-O8
2	C	5106	PLX	C30-C31-C32-C33
2	A	2807	PLX	C27-C28-C29-C30
2	A	2803	PLX	C29-C30-C31-C32
2	D	5103	PLX	C35-C36-C37-C38
2	B	2806	PLX	C35-C36-C37-C38
2	C	5107	PLX	C35-C36-C37-C38
2	A	2802	PLX	C35-C36-C37-C38
2	A	2802	PLX	C27-C28-C29-C30
2	B	2802	PLX	C30-C31-C32-C33
2	D	5108	PLX	C35-C36-C37-C38
2	A	2805	PLX	C30-C31-C32-C33
2	D	5106	PLX	C30-C31-C32-C33
2	A	2807	PLX	C10-C11-C12-C13
2	D	5104	PLX	C9-C10-C11-C12
2	C	5103	PLX	C30-C31-C32-C33
2	B	2804	PLX	C33-C34-C35-C36
2	D	5106	PLX	C9-C10-C11-C12
2	D	5108	PLX	C10-C11-C12-C13
2	B	2802	PLX	C9-C10-C11-C12
2	C	5103	PLX	C9-C10-C11-C12
2	A	2805	PLX	C9-C10-C11-C12
2	B	2801	PLX	C10-C11-C12-C13
2	C	5108	PLX	C9-C10-C11-C12
2	B	2802	PLX	O9-C24-C25-C26
2	C	5108	PLX	C27-C28-C29-C30
2	A	2803	PLX	C27-C28-C29-C30
2	D	5104	PLX	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5105	PLX	C10-C11-C12-C13
2	C	5107	PLX	C27-C28-C29-C30
2	B	2801	PLX	O4-C3-C4-C5
2	B	2807	PLX	C27-C28-C29-C30
2	C	5105	PLX	C27-C28-C29-C30
2	C	5105	PLX	C35-C36-C37-C38
2	B	2801	PLX	C25-C26-C27-C28
2	D	5103	PLX	C27-C28-C29-C30
2	B	2805	PLX	C34-C35-C36-C37
2	D	5108	PLX	C27-C28-C29-C30
2	A	2807	PLX	C30-C31-C32-C33
2	C	5106	PLX	C34-C35-C36-C37
2	A	2806	PLX	C13-C14-C15-C16
2	D	5107	PLX	C13-C14-C15-C16
2	C	5104	PLX	C13-C14-C15-C16
2	A	2802	PLX	C3-C4-C5-O8
2	A	2804	PLX	C3-C4-C5-O8
2	D	5105	PLX	C3-C4-C5-O8
2	B	2807	PLX	C3-C4-C5-O8
2	C	5102	PLX	C3-C4-C5-O8
2	D	5102	PLX	C34-C35-C36-C37
2	B	2804	PLX	C10-C11-C12-C13
2	B	2807	PLX	C9-C10-C11-C12
2	A	2804	PLX	O4-C3-C4-O6
2	A	2806	PLX	O4-C3-C4-O6
2	D	5105	PLX	O4-C3-C4-O6
2	D	5107	PLX	O4-C3-C4-O6
2	B	2803	PLX	O4-C3-C4-O6
2	C	5102	PLX	O4-C3-C4-O6
2	C	5104	PLX	O4-C3-C4-O6
2	A	2807	PLX	C34-C35-C36-C37
2	C	5102	PLX	C25-C26-C27-C28
2	A	2804	PLX	C25-C26-C27-C28
2	B	2803	PLX	C13-C14-C15-C16
2	D	5106	PLX	C28-C29-C30-C31
2	A	2802	PLX	O6-C4-C5-O8
2	A	2806	PLX	O6-C4-C5-O8
2	D	5107	PLX	O6-C4-C5-O8
2	B	2803	PLX	O6-C4-C5-O8
2	B	2807	PLX	O6-C4-C5-O8
2	C	5104	PLX	O6-C4-C5-O8
2	A	2802	PLX	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	5103	PLX	C26-C27-C28-C29
2	C	5107	PLX	C26-C27-C28-C29
2	D	5105	PLX	C25-C26-C27-C28
2	A	2805	PLX	C28-C29-C30-C31
2	B	2806	PLX	C26-C27-C28-C29
2	B	2806	PLX	C27-C28-C29-C30
2	C	5103	PLX	C28-C29-C30-C31
2	A	2806	PLX	O6-C6-C7-C8
2	A	2806	PLX	O8-C24-C25-C26
2	D	5107	PLX	O8-C24-C25-C26
2	B	2801	PLX	O6-C6-C7-C8
2	B	2803	PLX	O8-C24-C25-C26
2	C	5104	PLX	O8-C24-C25-C26
2	A	2801	PLX	C34-C35-C36-C37
2	C	5108	PLX	C24-C25-C26-C27
2	B	2807	PLX	C13-C14-C15-C16
2	A	2802	PLX	C26-C27-C28-C29
2	C	5108	PLX	C13-C14-C15-C16
2	A	2803	PLX	C13-C14-C15-C16
2	A	2805	PLX	C4-C5-O8-C24
2	D	5106	PLX	C4-C5-O8-C24
2	B	2802	PLX	C4-C5-O8-C24
2	C	5103	PLX	C4-C5-O8-C24
2	B	2807	PLX	C24-C25-C26-C27
2	D	5104	PLX	C13-C14-C15-C16
2	B	2802	PLX	C28-C29-C30-C31
2	D	5104	PLX	C24-C25-C26-C27
2	A	2802	PLX	O4-C3-C4-O6
2	D	5103	PLX	O4-C3-C4-O6
2	B	2806	PLX	O4-C3-C4-O6
2	C	5107	PLX	O4-C3-C4-O6
2	D	5104	PLX	C3-C4-C5-O8
2	C	5108	PLX	C3-C4-C5-O8
2	B	2802	PLX	C27-C28-C29-C30
2	A	2805	PLX	C1-C2-O1-P1
2	A	2806	PLX	C1-C2-O1-P1
2	D	5106	PLX	C1-C2-O1-P1
2	D	5107	PLX	C1-C2-O1-P1
2	B	2801	PLX	C1-C2-O1-P1
2	B	2802	PLX	C1-C2-O1-P1
2	B	2803	PLX	C1-C2-O1-P1
2	C	5103	PLX	C1-C2-O1-P1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5104	PLX	C1-C2-O1-P1
2	A	2803	PLX	C26-C27-C28-C29
2	D	5103	PLX	O6-C4-C5-O8
2	D	5106	PLX	O6-C4-C5-O8
2	B	2806	PLX	O6-C4-C5-O8
2	C	5103	PLX	O6-C4-C5-O8
2	C	5107	PLX	O6-C4-C5-O8
2	B	2804	PLX	C36-C37-C38-C39
2	A	2805	PLX	C27-C28-C29-C30
2	D	5106	PLX	C27-C28-C29-C30
2	B	2801	PLX	C24-C25-C26-C27
2	C	5103	PLX	C27-C28-C29-C30
2	D	5104	PLX	C26-C27-C28-C29
2	A	2801	PLX	N1-C1-C2-O1
2	A	2802	PLX	N1-C1-C2-O1
2	D	5102	PLX	N1-C1-C2-O1
2	D	5103	PLX	N1-C1-C2-O1
2	B	2804	PLX	N1-C1-C2-O1
2	B	2805	PLX	N1-C1-C2-O1
2	B	2806	PLX	N1-C1-C2-O1
2	C	5105	PLX	N1-C1-C2-O1
2	C	5106	PLX	N1-C1-C2-O1
2	C	5107	PLX	N1-C1-C2-O1
2	B	2807	PLX	C26-C27-C28-C29
2	C	5108	PLX	C26-C27-C28-C29
2	B	2801	PLX	C28-C29-C30-C31
2	D	5104	PLX	O9-C24-C25-C26
2	B	2807	PLX	O9-C24-C25-C26
2	C	5108	PLX	O9-C24-C25-C26
2	A	2802	PLX	C25-C24-O8-C5
2	A	2804	PLX	C25-C24-O8-C5
2	A	2806	PLX	C25-C24-O8-C5
2	D	5103	PLX	C25-C24-O8-C5
2	D	5105	PLX	C25-C24-O8-C5
2	D	5107	PLX	C25-C24-O8-C5
2	D	5108	PLX	C25-C24-O8-C5
2	B	2803	PLX	C25-C24-O8-C5
2	B	2804	PLX	C25-C24-O8-C5
2	B	2806	PLX	C25-C24-O8-C5
2	C	5102	PLX	C25-C24-O8-C5
2	C	5104	PLX	C25-C24-O8-C5
2	C	5105	PLX	C25-C24-O8-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5107	PLX	C25-C24-O8-C5
2	D	5104	PLX	C11-C10-C9-C8
2	A	2802	PLX	O4-C3-C4-C5
2	D	5103	PLX	O4-C3-C4-C5
2	B	2806	PLX	O4-C3-C4-C5
2	C	5107	PLX	O4-C3-C4-C5
2	C	5106	PLX	C11-C12-C13-C14
2	B	2805	PLX	C11-C12-C13-C14
2	A	2802	PLX	O6-C6-C7-C8
2	A	2805	PLX	O6-C6-C7-C8
2	D	5102	PLX	O6-C6-C7-C8
2	D	5103	PLX	O6-C6-C7-C8
2	D	5106	PLX	O6-C6-C7-C8
2	D	5107	PLX	O6-C6-C7-C8
2	D	5108	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	2805	PLX	O6-C6-C7-C8
2	B	2806	PLX	O6-C6-C7-C8
2	C	5103	PLX	O6-C6-C7-C8
2	C	5104	PLX	O6-C6-C7-C8
2	C	5105	PLX	O6-C6-C7-C8
2	C	5106	PLX	O6-C6-C7-C8
2	C	5107	PLX	O6-C6-C7-C8
2	B	2801	PLX	O4-C3-C4-O6
2	D	5102	PLX	C28-C29-C30-C31
2	A	2801	PLX	C11-C12-C13-C14
2	D	5102	PLX	C11-C12-C13-C14
2	B	2807	PLX	C11-C10-C9-C8
2	A	2803	PLX	O6-C4-C5-O8
2	A	2805	PLX	O6-C4-C5-O8
2	D	5104	PLX	O6-C4-C5-O8
2	B	2802	PLX	O6-C4-C5-O8
2	C	5108	PLX	O6-C4-C5-O8
2	C	5108	PLX	C11-C10-C9-C8
2	B	2801	PLX	C30-C31-C32-C33
2	A	2803	PLX	C3-C4-C5-O8
2	A	2802	PLX	C9-C10-C11-C12
2	A	2801	PLX	C28-C29-C30-C31
2	A	2802	PLX	C3-O4-P1-O2
2	A	2803	PLX	C3-C4-O6-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	2803	PLX	C5-C4-O6-C6
2	A	2804	PLX	C3-O4-P1-O2
2	A	2806	PLX	C3-O4-P1-O2
2	D	5103	PLX	C3-O4-P1-O2
2	D	5103	PLX	C2-O1-P1-O2
2	D	5104	PLX	C3-C4-O6-C6
2	D	5104	PLX	C5-C4-O6-C6
2	D	5104	PLX	C3-O4-P1-O2
2	D	5105	PLX	C3-O4-P1-O2
2	D	5106	PLX	C3-O4-P1-O3
2	D	5107	PLX	C3-O4-P1-O2
2	B	2801	PLX	C3-O4-P1-O2
2	B	2802	PLX	C3-O4-P1-O3
2	B	2803	PLX	C3-O4-P1-O2
2	B	2806	PLX	C3-O4-P1-O2
2	B	2806	PLX	C2-O1-P1-O2
2	B	2807	PLX	C3-C4-O6-C6
2	B	2807	PLX	C5-C4-O6-C6
2	B	2807	PLX	C3-O4-P1-O2
2	C	5102	PLX	C3-O4-P1-O2
2	C	5103	PLX	C3-O4-P1-O3
2	C	5104	PLX	C3-O4-P1-O2
2	C	5107	PLX	C3-O4-P1-O2
2	C	5107	PLX	C2-O1-P1-O2
2	C	5108	PLX	C3-C4-O6-C6
2	C	5108	PLX	C5-C4-O6-C6
2	C	5108	PLX	C3-O4-P1-O2
2	C	5106	PLX	C28-C29-C30-C31
2	D	5102	PLX	C9-C10-C11-C12
2	D	5107	PLX	C28-C29-C30-C31
2	A	2807	PLX	C4-C3-O4-P1
2	D	5102	PLX	C4-C3-O4-P1
2	B	2805	PLX	C4-C3-O4-P1
2	C	5106	PLX	C4-C3-O4-P1
2	C	5104	PLX	C12-C13-C14-C15
2	A	2806	PLX	C12-C13-C14-C15
2	D	5107	PLX	C12-C13-C14-C15
2	C	5104	PLX	C28-C29-C30-C31
2	A	2803	PLX	C9-C10-C11-C12
2	D	5103	PLX	C9-C10-C11-C12
2	A	2807	PLX	C32-C33-C34-C35
2	D	5105	PLX	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	2806	PLX	C9-C10-C11-C12
2	C	5107	PLX	C9-C10-C11-C12
2	B	2803	PLX	C11-C10-C9-C8
2	C	5105	PLX	C28-C29-C30-C31
2	A	2801	PLX	C9-C10-C11-C12
2	B	2803	PLX	C12-C13-C14-C15
2	B	2804	PLX	C31-C32-C33-C34
2	A	2802	PLX	C24-C25-C26-C27
2	A	2803	PLX	C24-C25-C26-C27
2	D	5103	PLX	C24-C25-C26-C27
2	D	5105	PLX	C10-C11-C12-C13
2	A	2801	PLX	C24-C25-C26-C27
2	B	2806	PLX	C24-C25-C26-C27
2	C	5106	PLX	C24-C25-C26-C27
2	C	5107	PLX	C24-C25-C26-C27
2	A	2804	PLX	C28-C29-C30-C31
2	A	2807	PLX	C28-C29-C30-C31
2	A	2807	PLX	O8-C24-C25-C26
2	D	5102	PLX	C24-C25-C26-C27
2	B	2805	PLX	C24-C25-C26-C27
2	A	2804	PLX	C10-C11-C12-C13
2	C	5106	PLX	C9-C10-C11-C12
2	B	2805	PLX	C9-C10-C11-C12
2	D	5107	PLX	C11-C10-C9-C8
2	C	5104	PLX	C11-C10-C9-C8
2	C	5105	PLX	C33-C34-C35-C36
2	A	2806	PLX	C11-C10-C9-C8
2	C	5102	PLX	C28-C29-C30-C31
2	A	2802	PLX	C11-C12-C13-C14
2	D	5102	PLX	C6-C7-C8-C9
2	C	5108	PLX	C30-C31-C32-C33
2	D	5103	PLX	C11-C12-C13-C14
2	A	2803	PLX	C11-C10-C9-C8
2	A	2801	PLX	C4-C3-O4-P1
2	B	2806	PLX	C11-C12-C13-C14
2	C	5107	PLX	C11-C12-C13-C14
2	D	5103	PLX	C6-C7-C8-C9
2	C	5107	PLX	C6-C7-C8-C9
2	B	2802	PLX	C31-C32-C33-C34
2	D	5108	PLX	C28-C29-C30-C31
2	A	2804	PLX	O8-C24-C25-C26
2	D	5105	PLX	O8-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5102	PLX	O8-C24-C25-C26
2	B	2806	PLX	C6-C7-C8-C9
2	D	5104	PLX	C30-C31-C32-C33
2	A	2806	PLX	C14-C15-C16-C17
2	B	2803	PLX	C14-C15-C16-C17
2	C	5104	PLX	C14-C15-C16-C17
2	D	5107	PLX	C14-C15-C16-C17
2	A	2802	PLX	O9-C24-C25-C26
2	D	5103	PLX	O9-C24-C25-C26
2	B	2806	PLX	O9-C24-C25-C26
2	C	5107	PLX	O9-C24-C25-C26
2	B	2805	PLX	C28-C29-C30-C31
2	A	2804	PLX	C24-C25-C26-C27
2	B	2805	PLX	C6-C7-C8-C9
2	A	2806	PLX	C28-C29-C30-C31
2	B	2807	PLX	C30-C31-C32-C33
2	A	2805	PLX	C31-C32-C33-C34
2	D	5106	PLX	C31-C32-C33-C34
2	C	5103	PLX	C31-C32-C33-C34
2	B	2806	PLX	C7-C8-C9-C10
2	D	5105	PLX	C24-C25-C26-C27
2	C	5106	PLX	C6-C7-C8-C9
2	C	5107	PLX	C7-C8-C9-C10
2	C	5106	PLX	C32-C33-C34-C35
2	D	5103	PLX	C7-C8-C9-C10
2	A	2801	PLX	C31-C32-C33-C34
2	A	2807	PLX	C2-C1-N1-C1B
2	D	5105	PLX	C4-C3-O4-P1
2	C	5102	PLX	C4-C3-O4-P1
2	A	2806	PLX	C7-C8-C9-C10
2	A	2801	PLX	C6-C7-C8-C9
2	C	5106	PLX	C10-C11-C12-C13
2	C	5106	PLX	C31-C32-C33-C34
2	D	5107	PLX	C7-C8-C9-C10
2	C	5102	PLX	C10-C11-C12-C13
2	B	2804	PLX	C6-C7-C8-C9
2	C	5104	PLX	C7-C8-C9-C10
2	A	2804	PLX	C4-C3-O4-P1
2	D	5102	PLX	C31-C32-C33-C34
2	C	5102	PLX	C24-C25-C26-C27
2	B	2805	PLX	C10-C11-C12-C13
2	C	5108	PLX	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	5105	PLX	C6-C7-C8-C9
2	D	5108	PLX	C24-C25-C26-C27
2	A	2802	PLX	C6-C7-C8-C9
2	C	5105	PLX	C24-C25-C26-C27
2	D	5104	PLX	C28-C29-C30-C31
2	A	2802	PLX	C4-C3-O4-P1
2	C	5103	PLX	C24-C25-C26-C27
2	D	5102	PLX	O8-C24-C25-C26
2	A	2805	PLX	C24-C25-C26-C27
2	D	5108	PLX	C6-C7-C8-C9
2	B	2802	PLX	C24-C25-C26-C27
2	A	2803	PLX	O9-C24-O8-C5
2	D	5102	PLX	O9-C24-O8-C5
2	B	2801	PLX	O9-C24-O8-C5
2	B	2802	PLX	O9-C24-O8-C5
2	B	2805	PLX	O9-C24-O8-C5
2	C	5106	PLX	O9-C24-O8-C5
2	B	2804	PLX	C34-C35-C36-C37
2	D	5106	PLX	C24-C25-C26-C27
2	D	5102	PLX	C13-C14-C15-C16
2	B	2804	PLX	C4-C3-O4-P1
2	B	2806	PLX	C4-C3-O4-P1
2	B	2807	PLX	C28-C29-C30-C31

There are no ring outliers.

25 monomers are involved in 39 short contacts:

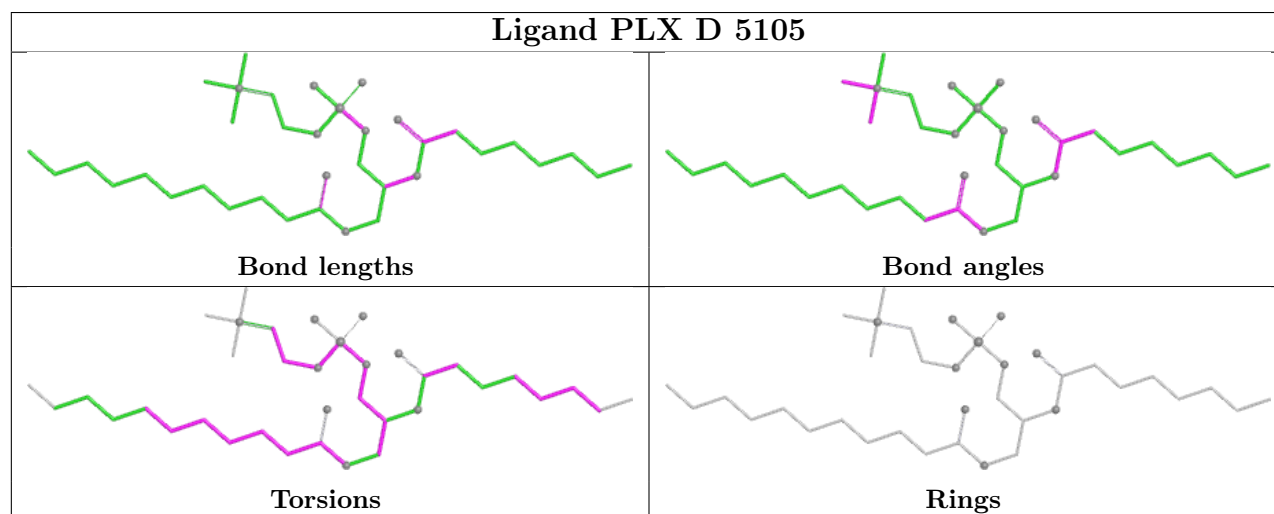
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5105	PLX	1	0
2	A	2807	PLX	3	0
2	C	5105	PLX	1	0
2	A	2806	PLX	1	0
2	C	5107	PLX	3	0
2	C	5102	PLX	1	0
2	D	5103	PLX	3	0
2	B	2805	PLX	3	0
2	D	5107	PLX	2	0
2	D	5108	PLX	1	0
2	B	2802	PLX	1	0
2	B	2807	PLX	1	0
2	C	5103	PLX	1	0
2	D	5102	PLX	1	0

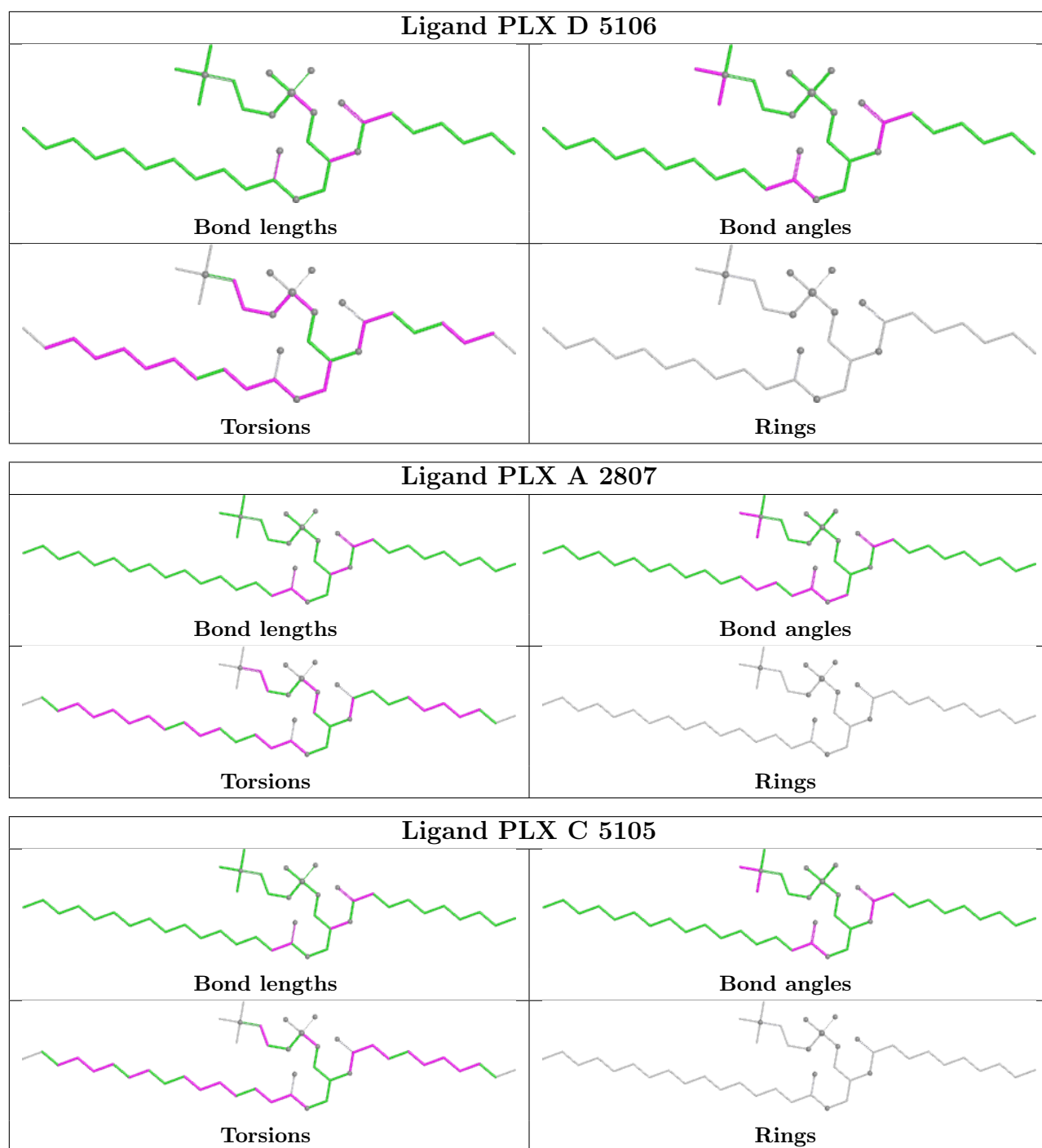
Continued on next page...

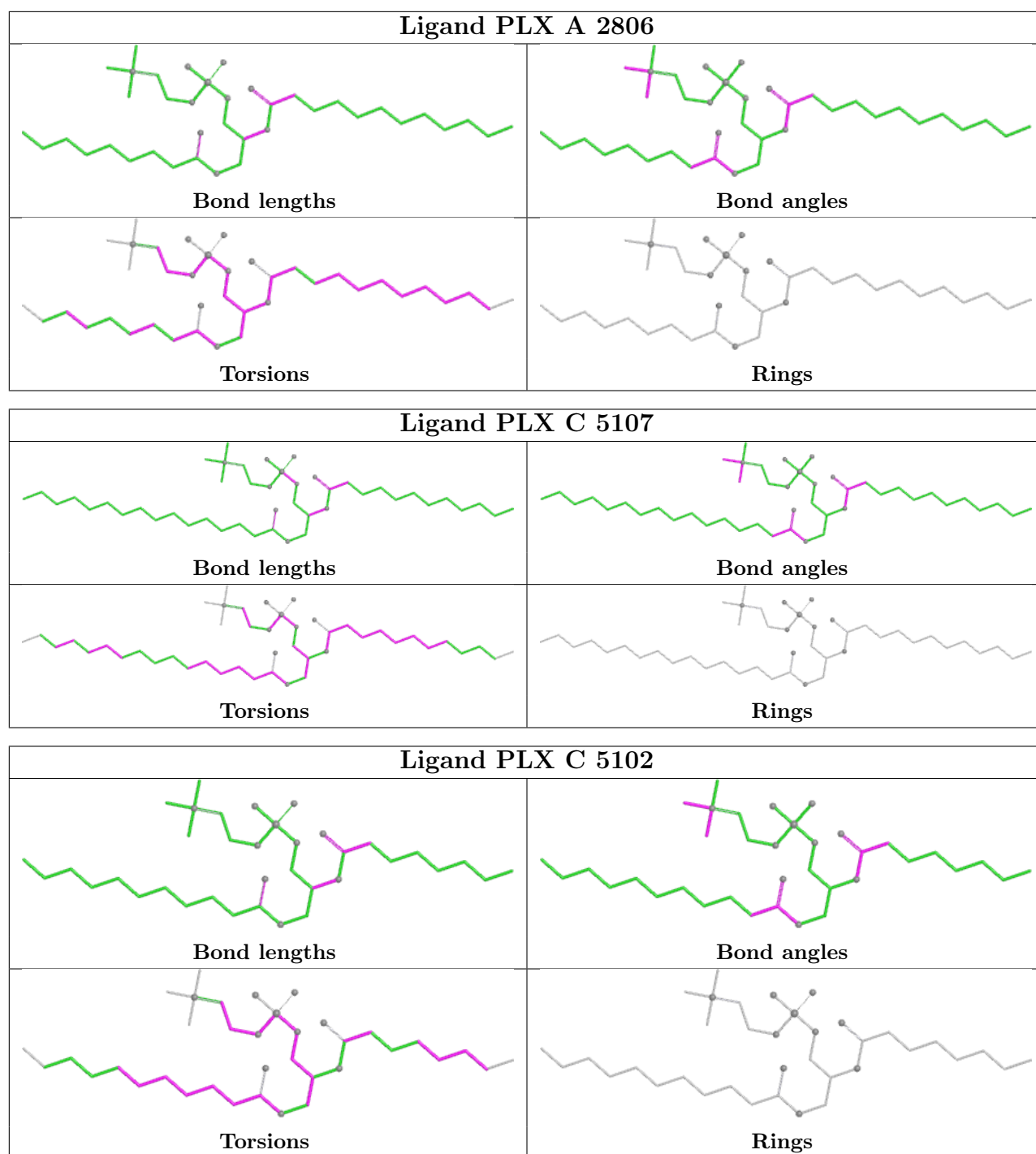
Continued from previous page...

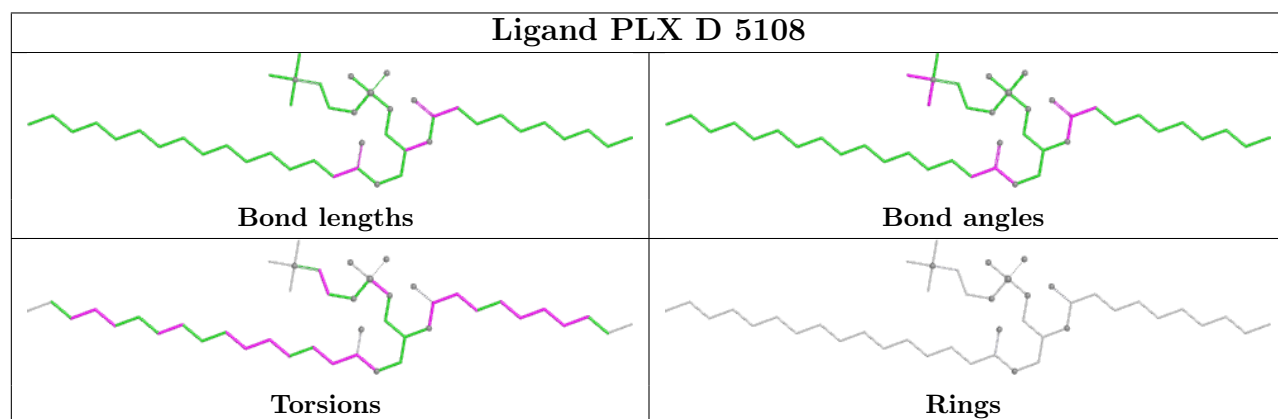
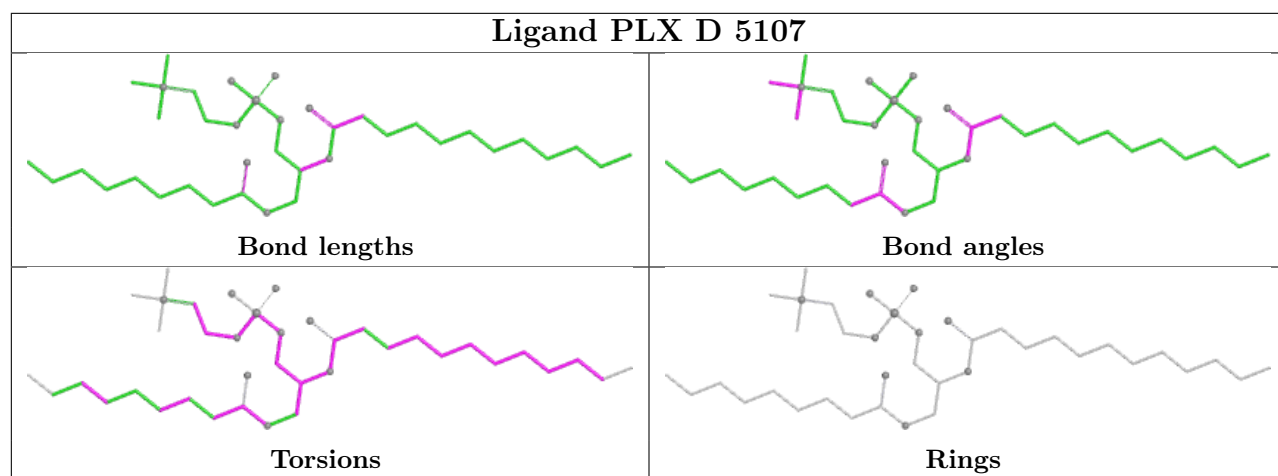
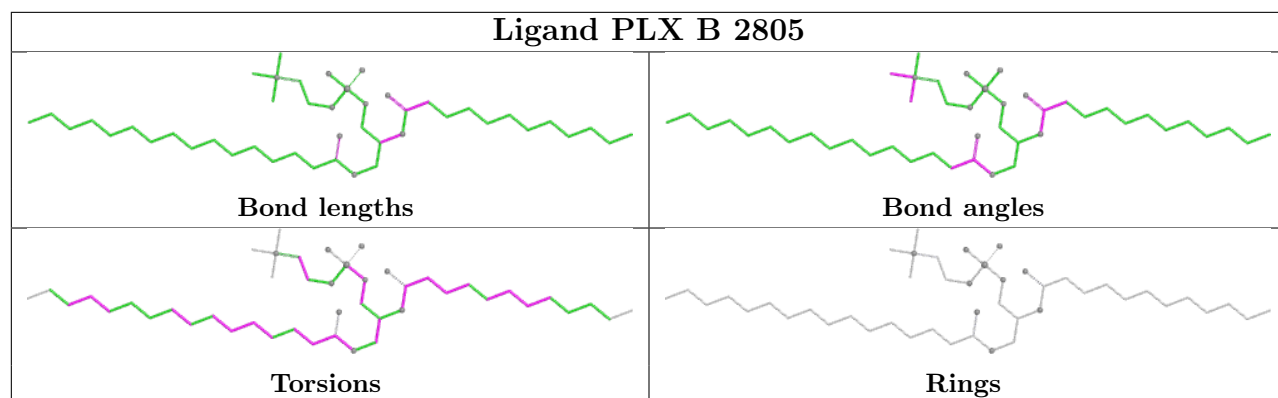
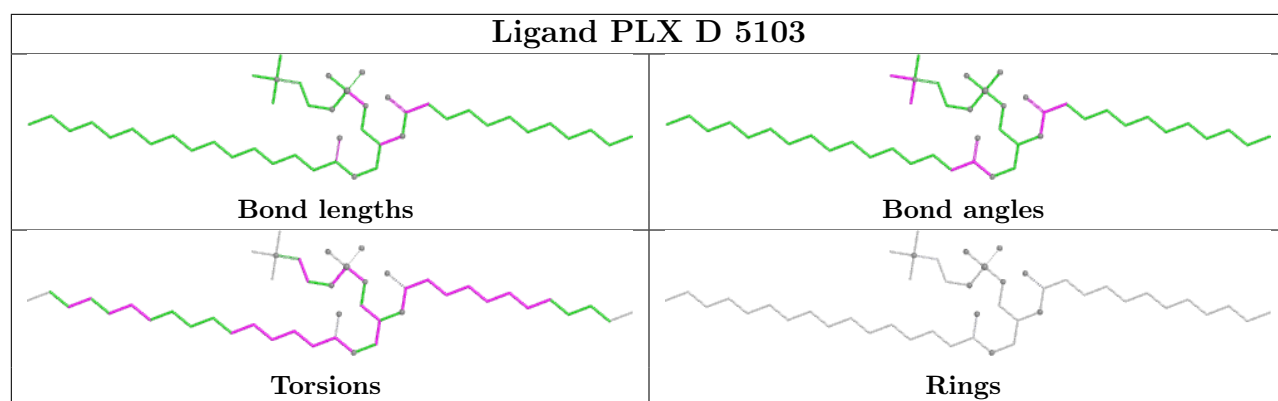
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2802	PLX	3	0
2	B	2803	PLX	1	0
2	A	2805	PLX	2	0
2	D	5104	PLX	1	0
2	A	2803	PLX	1	0
2	A	2801	PLX	1	0
2	A	2804	PLX	1	0
2	C	5106	PLX	1	0
2	C	5104	PLX	1	0
2	B	2801	PLX	2	0
2	B	2806	PLX	3	0

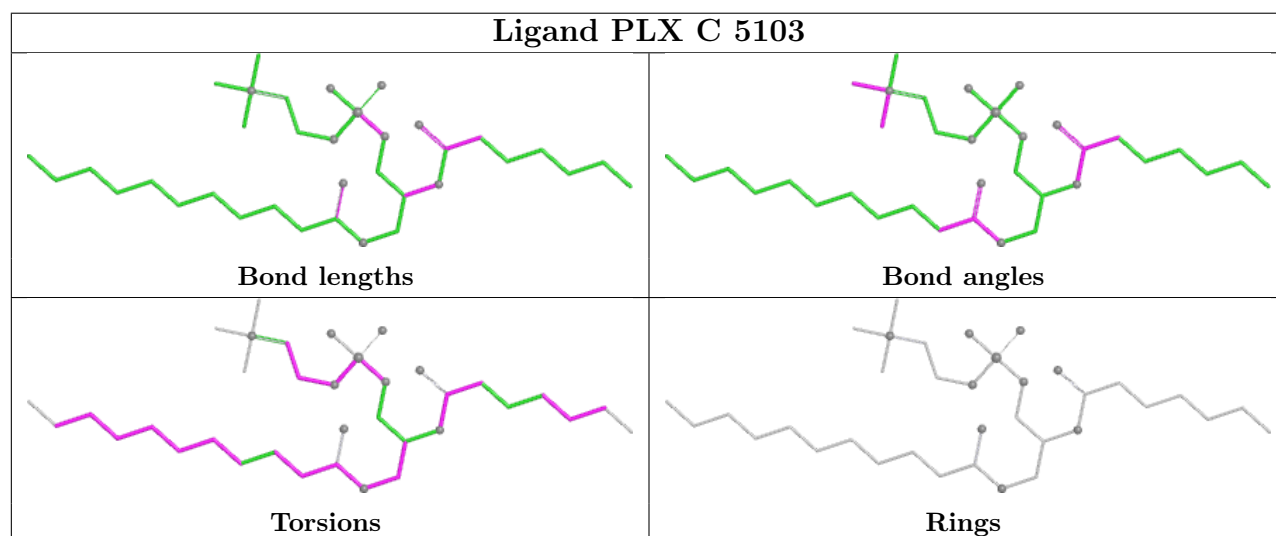
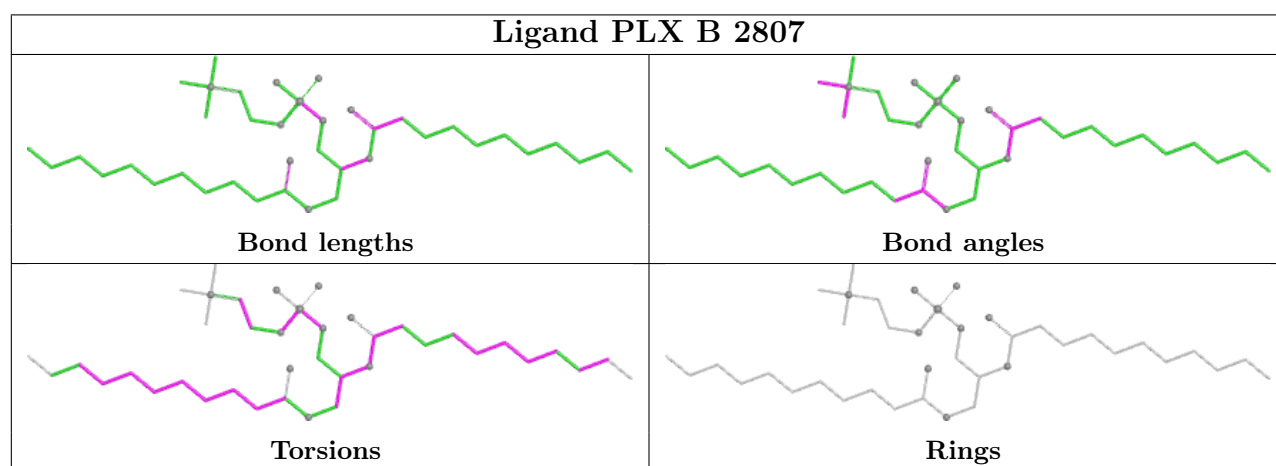
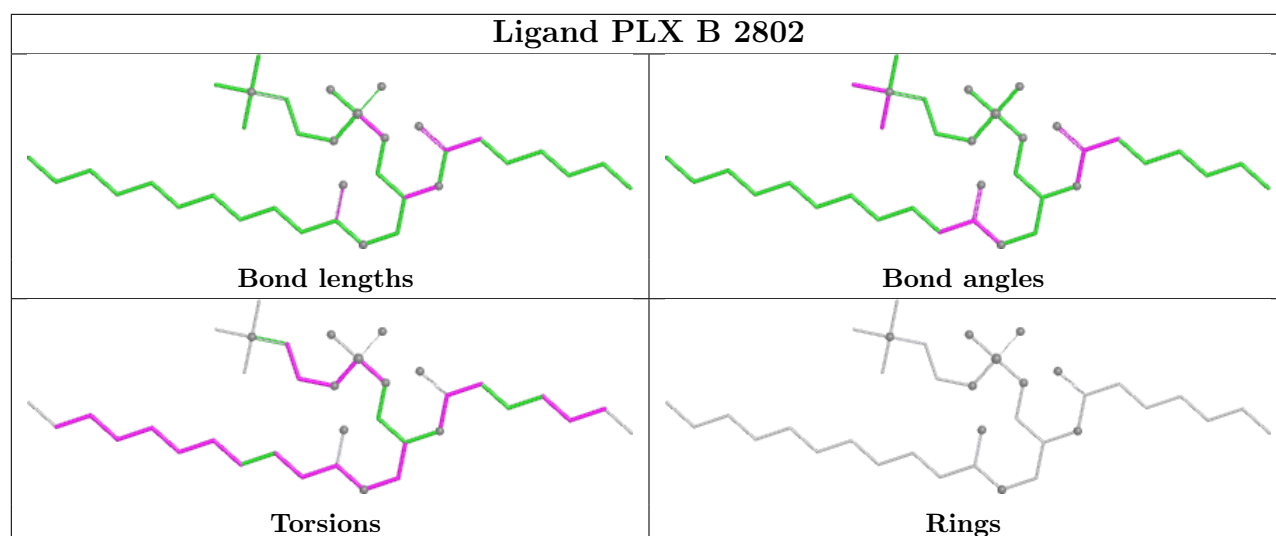
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

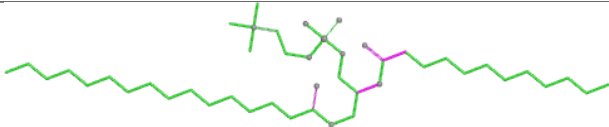
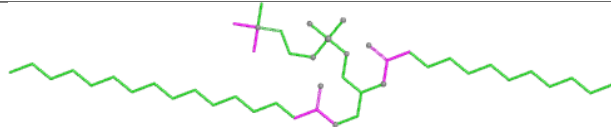
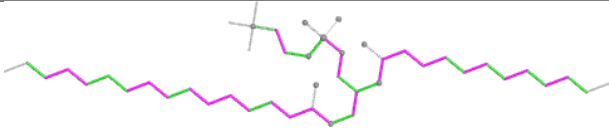
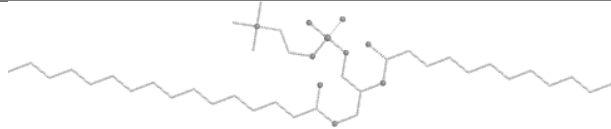
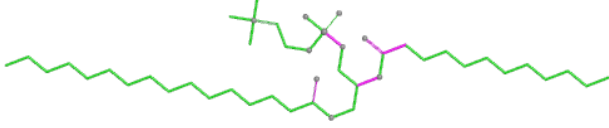
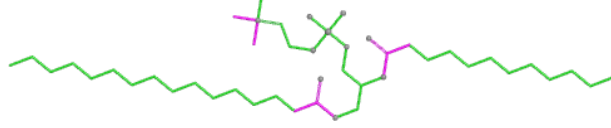
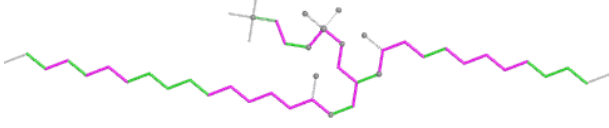
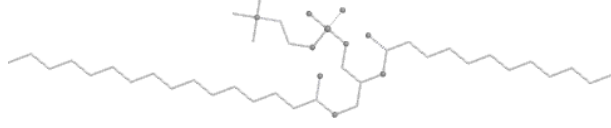
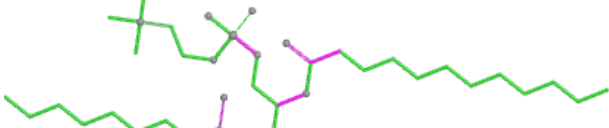
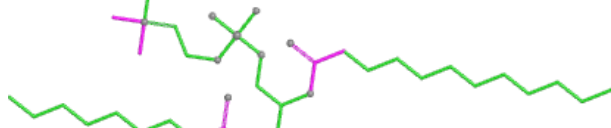
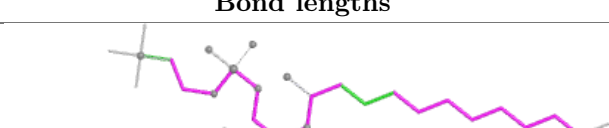
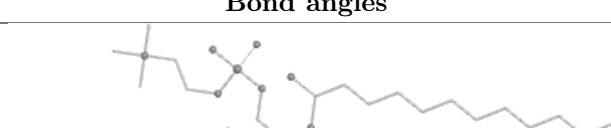


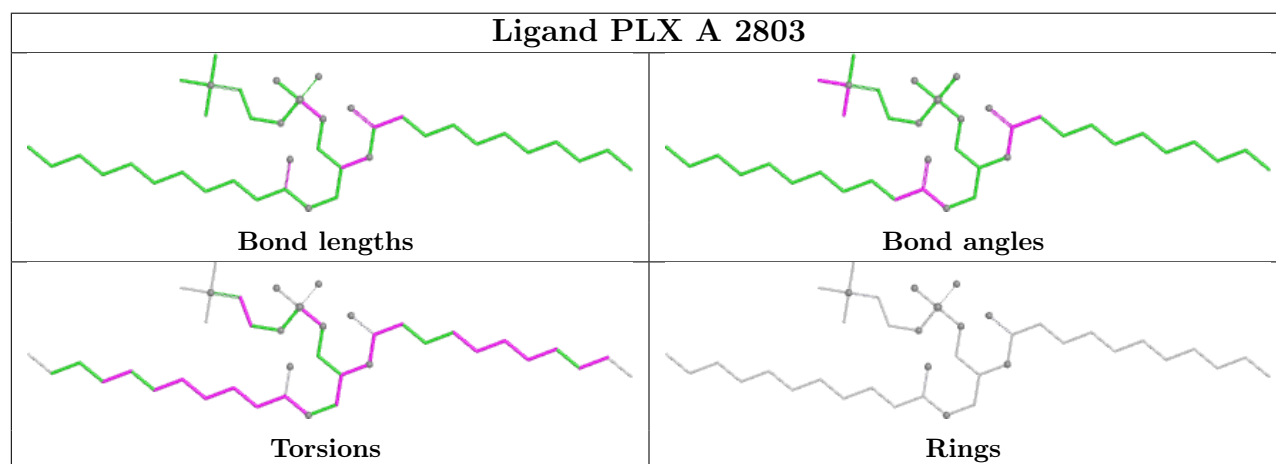
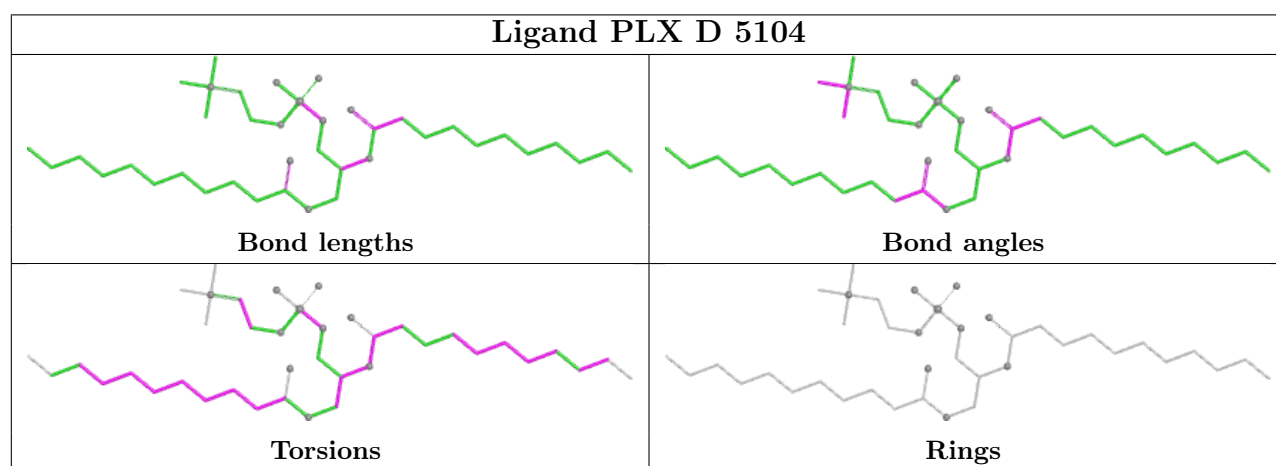
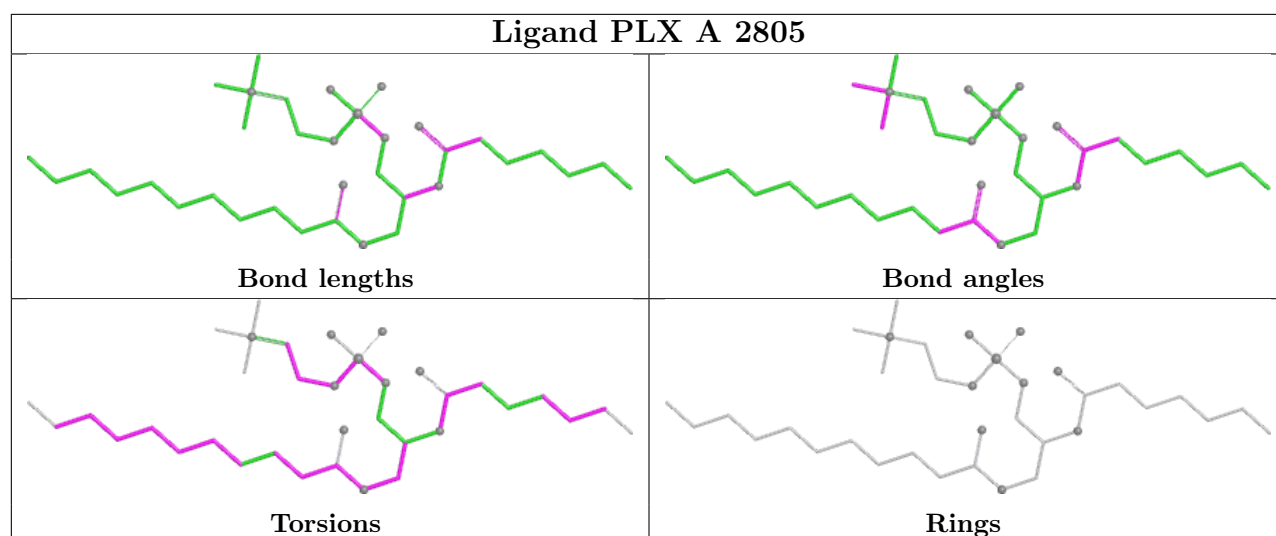


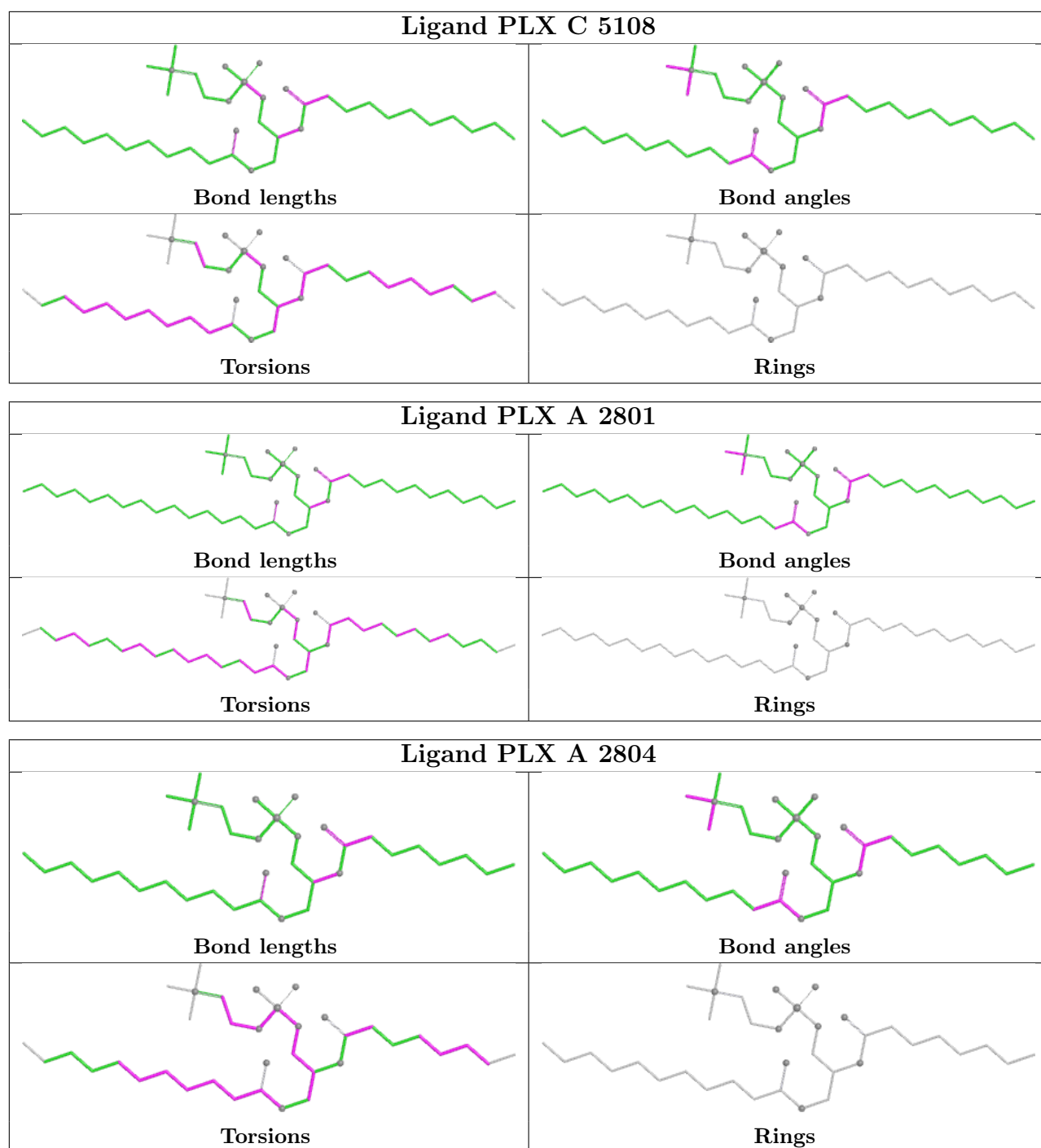


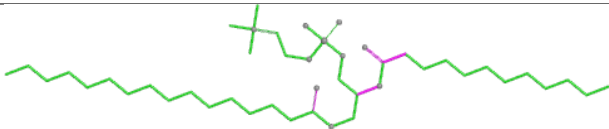
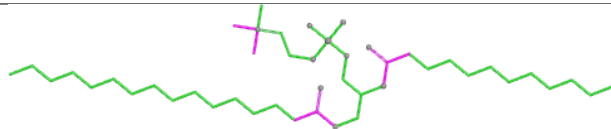
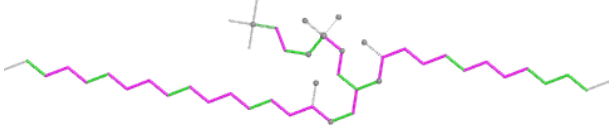
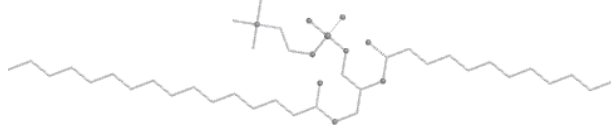


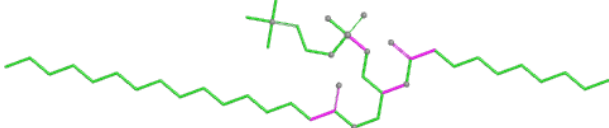
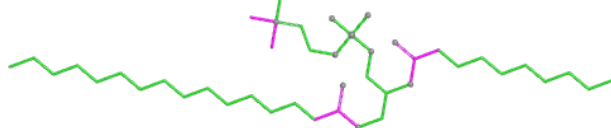
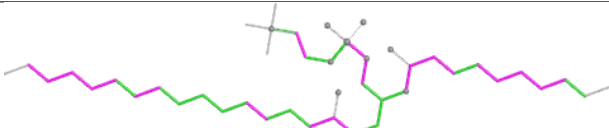
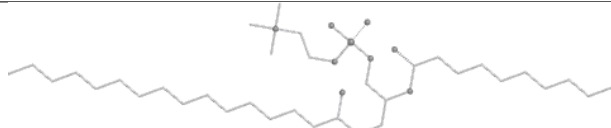


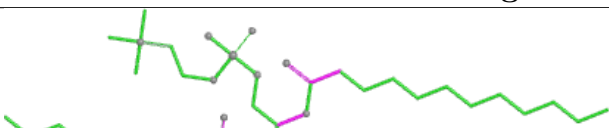
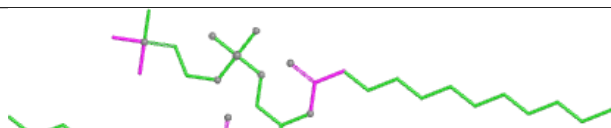
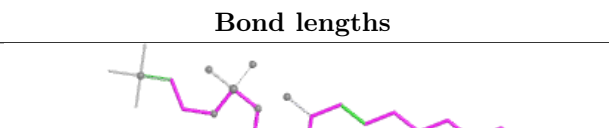
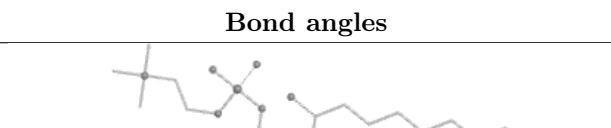
Ligand PLX D 5102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX A 2802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX B 2803	
 Bond lengths	 Bond angles
 Torsions	 Rings

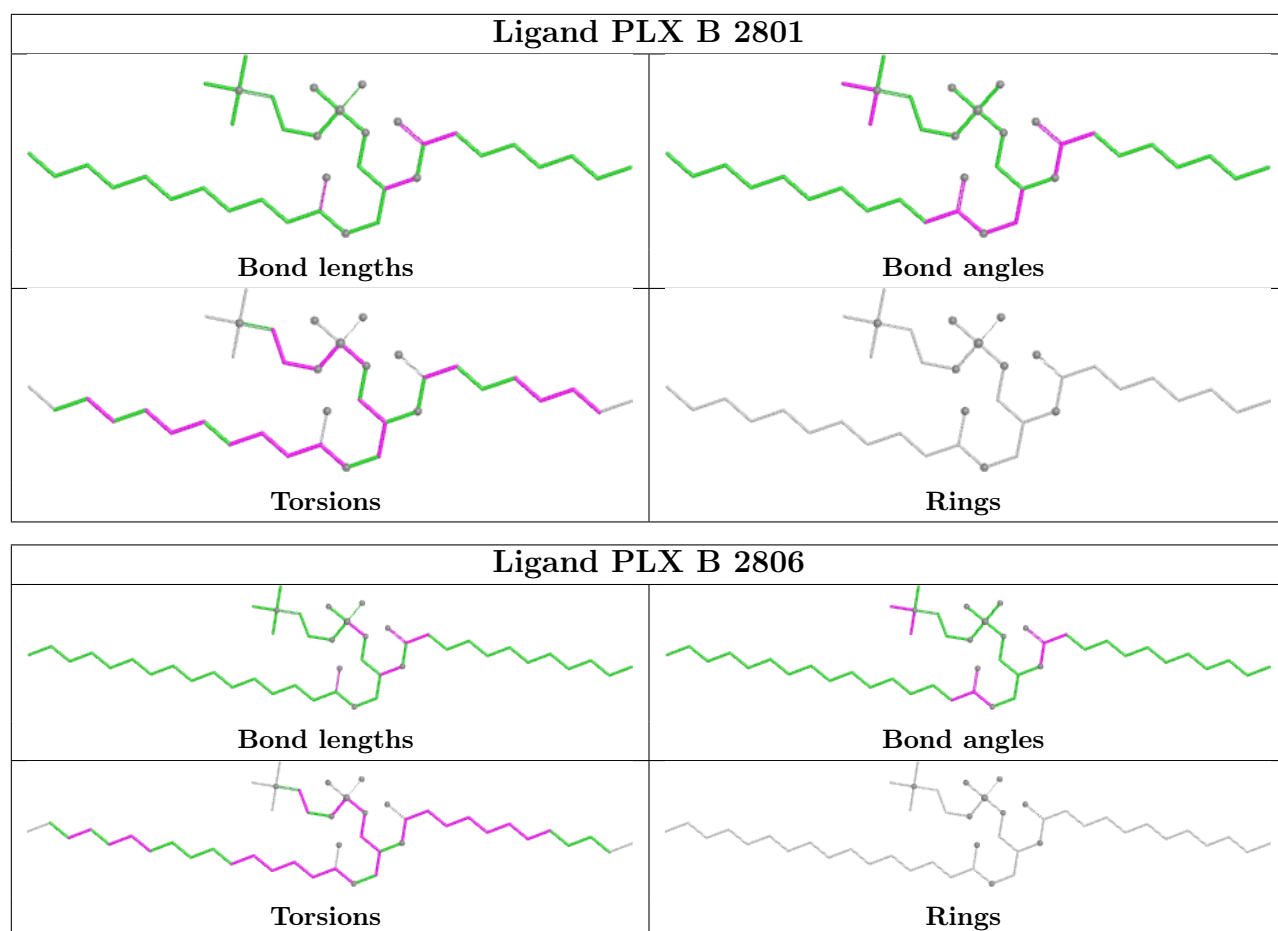




Ligand PLX C 5106	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX B 2804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX C 5104	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

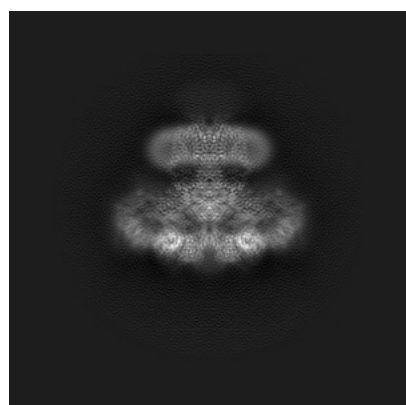
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23338. These allow visual inspection of the internal detail of the map and identification of artifacts.

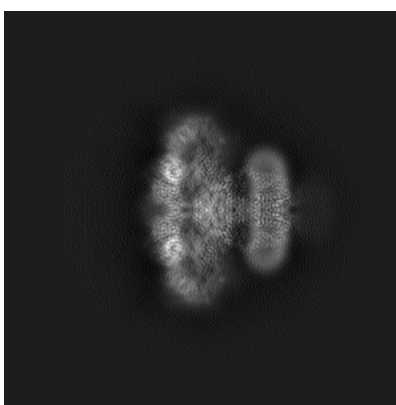
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

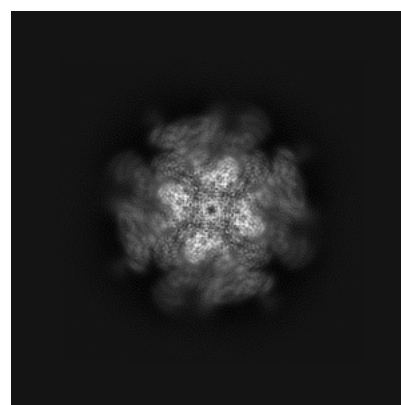
6.1.1 Primary map



X



Y

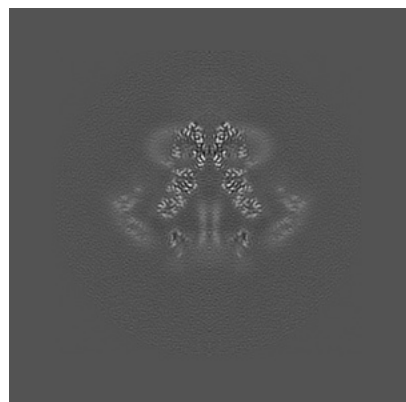


Z

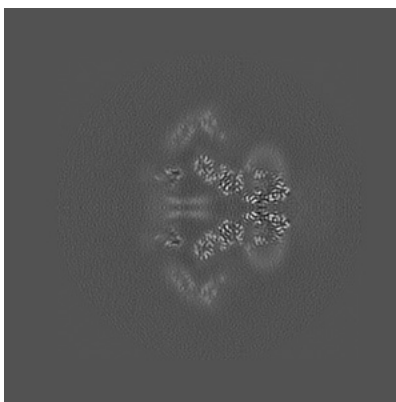
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

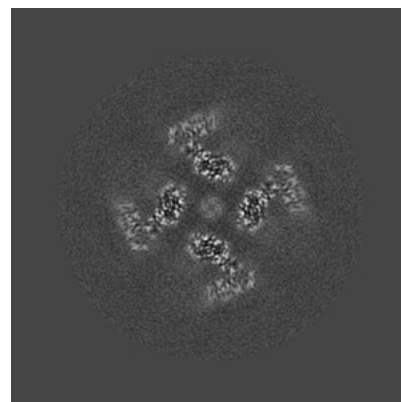
6.2.1 Primary map



X Index: 220



Y Index: 220

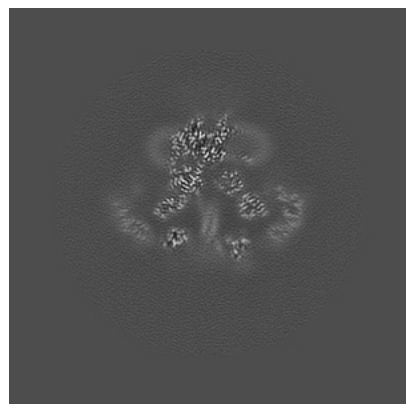


Z Index: 220

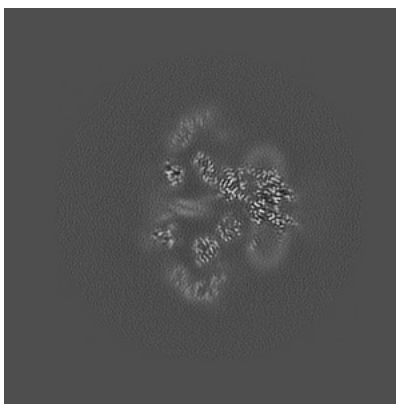
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

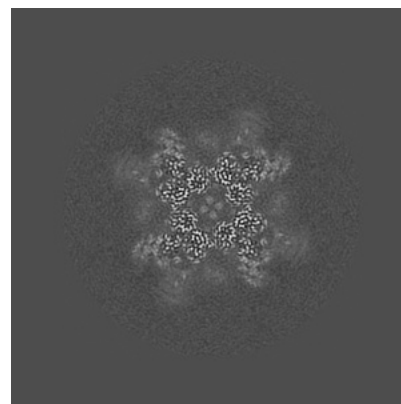
6.3.1 Primary map



X Index: 215



Y Index: 215

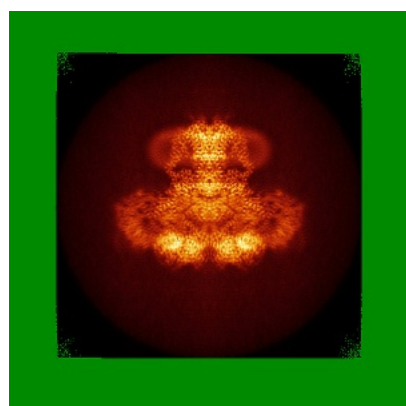


Z Index: 182

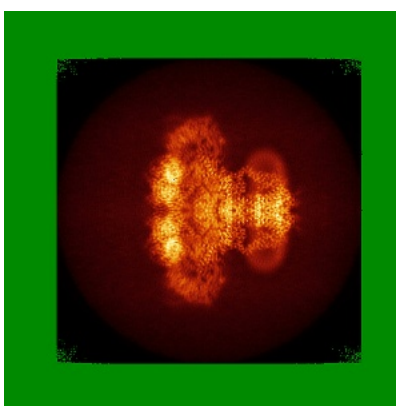
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

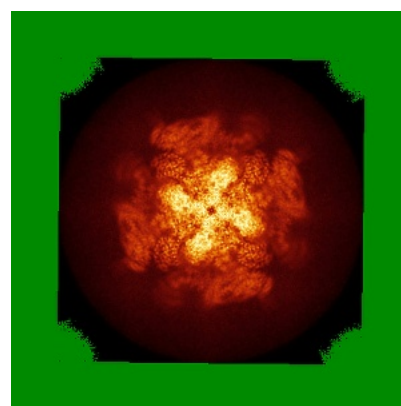
6.4.1 Primary map



X



Y

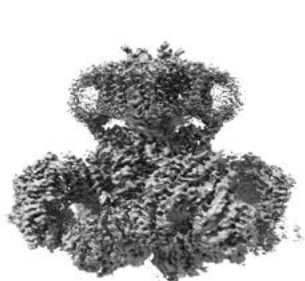


Z

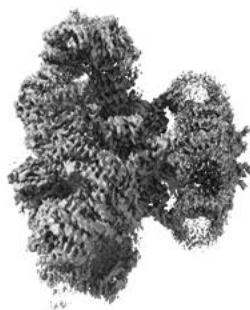
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

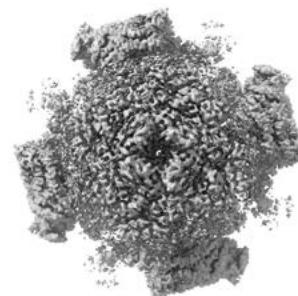
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

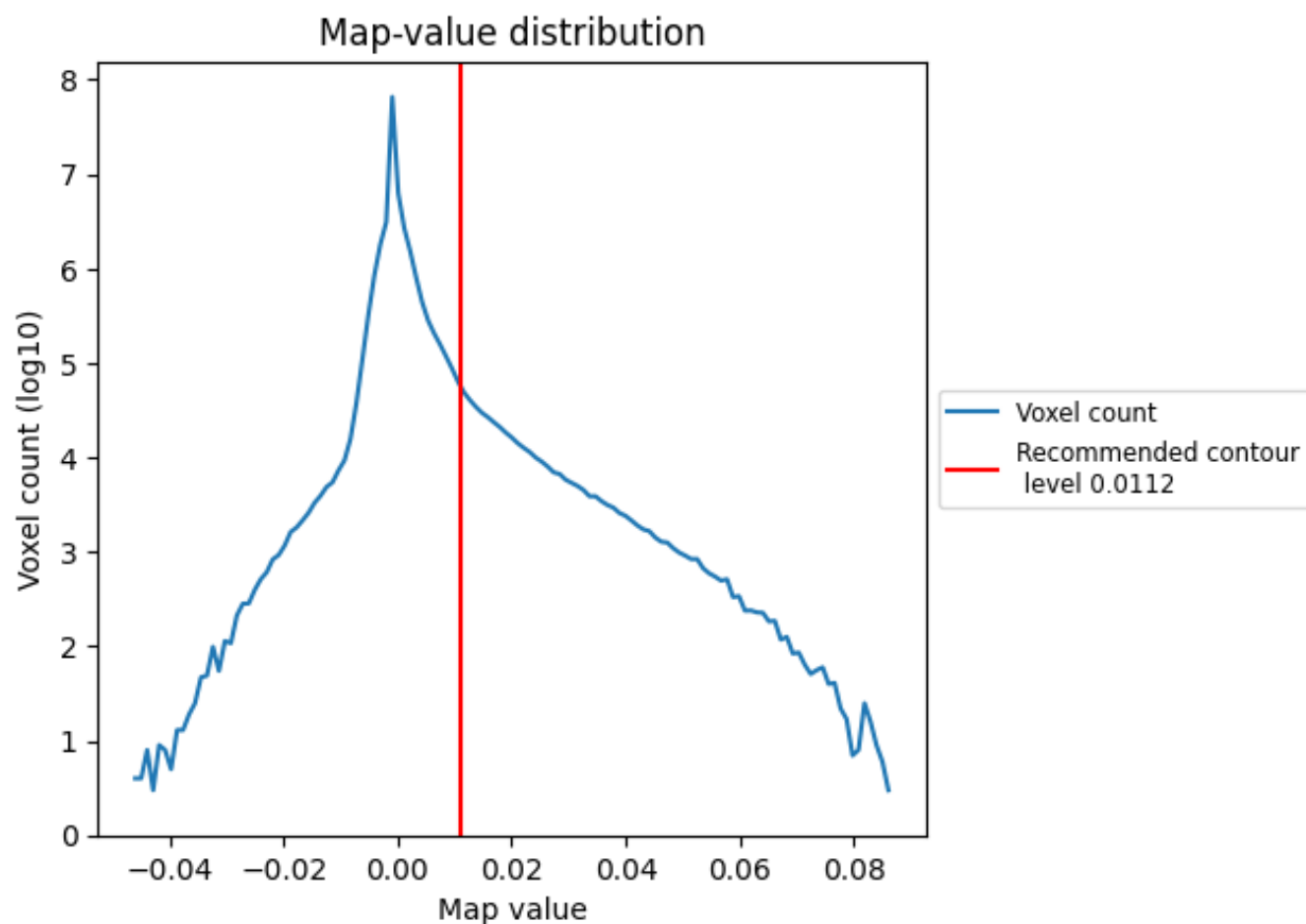
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

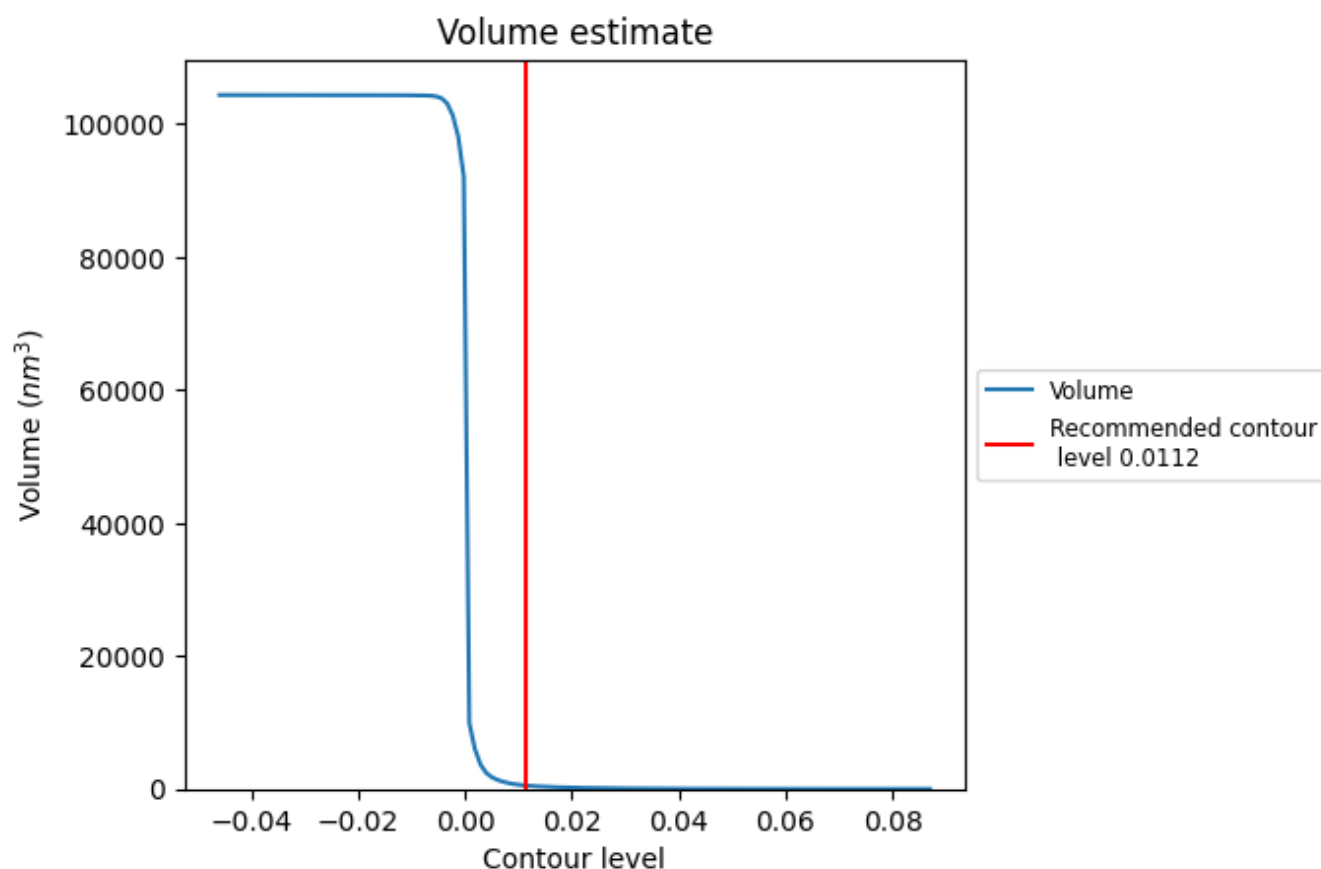
This section contains the results of statistical analysis of the map.

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.

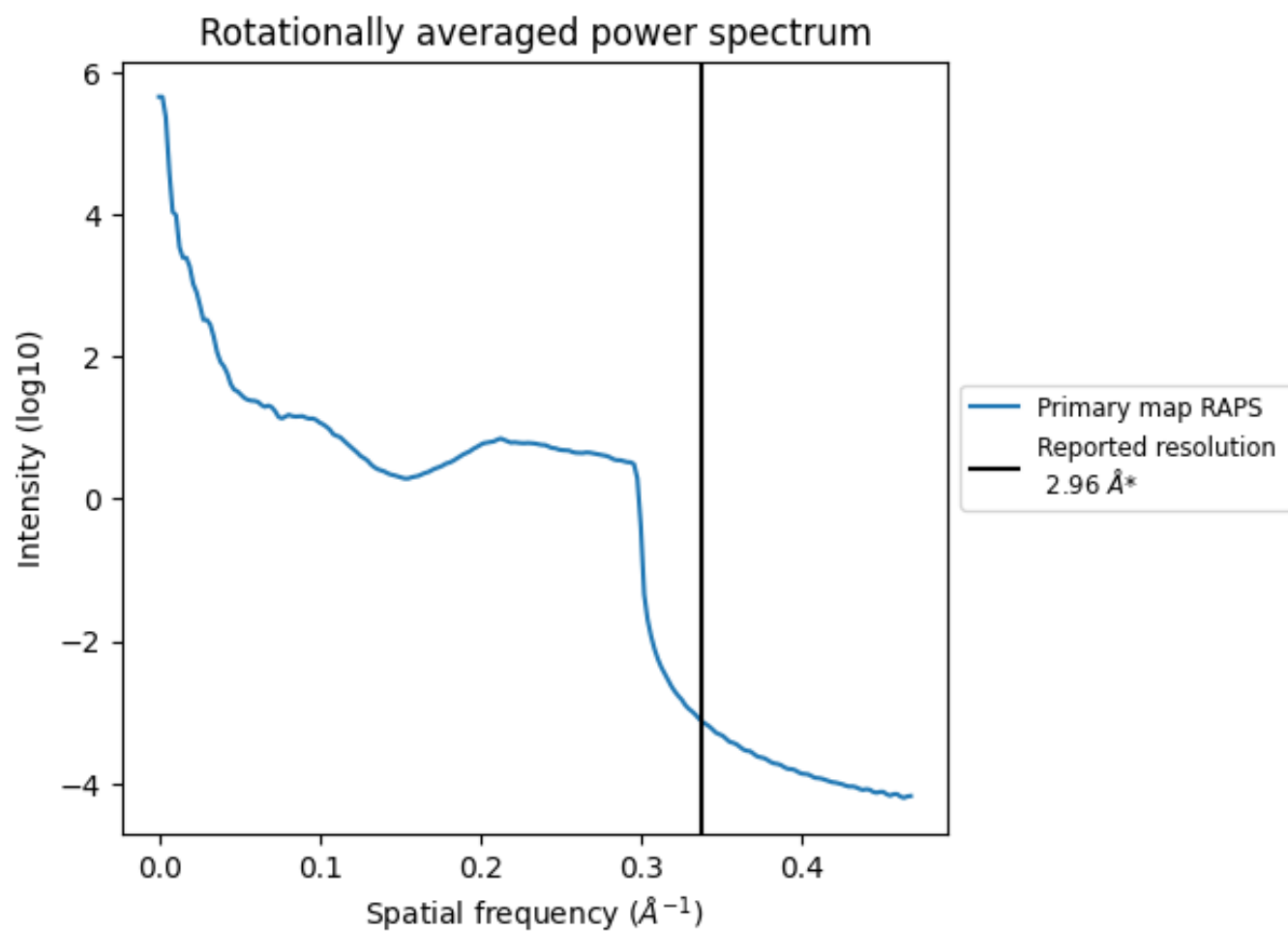
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 524 nm^3 ; this corresponds to an approximate mass of 474 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 0.338 Å⁻¹

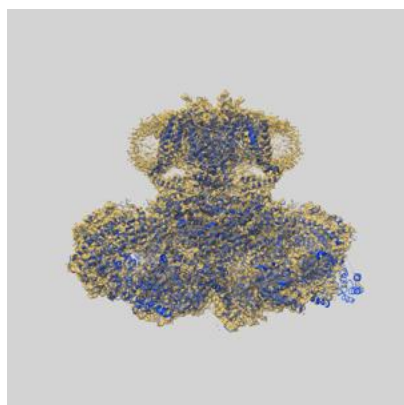
8 Fourier-Shell correlation ⓘ

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

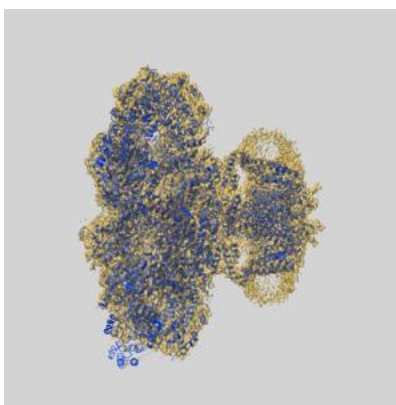
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23338 and PDB model 7LHF. Per-residue inclusion information can be found in section 3 on page 7.

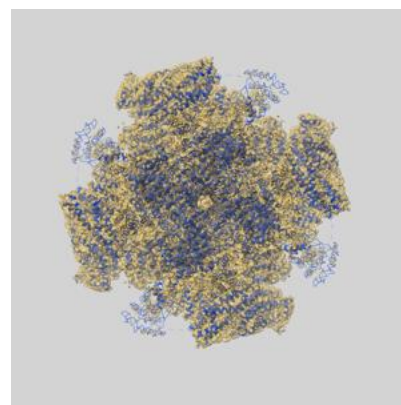
9.1 Map-model overlay [i](#)



X



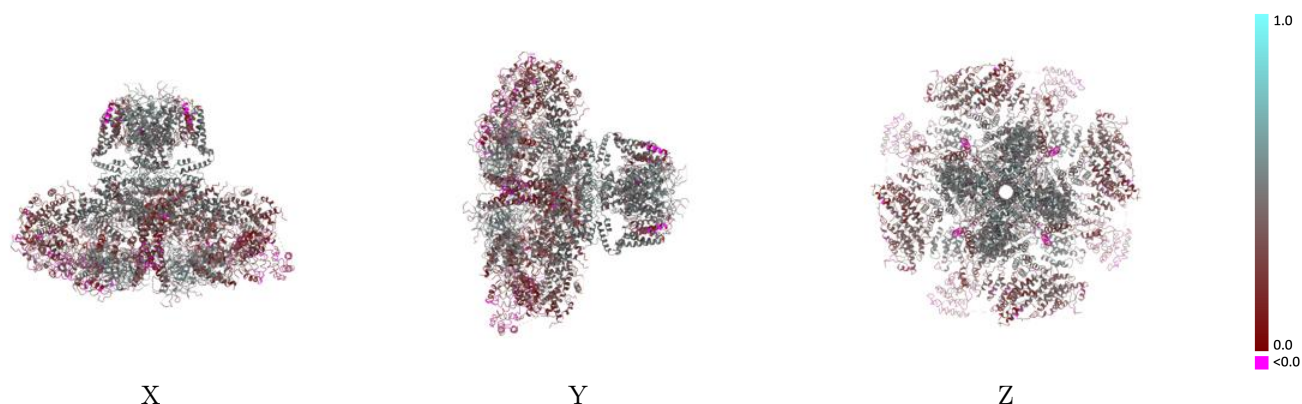
Y



Z

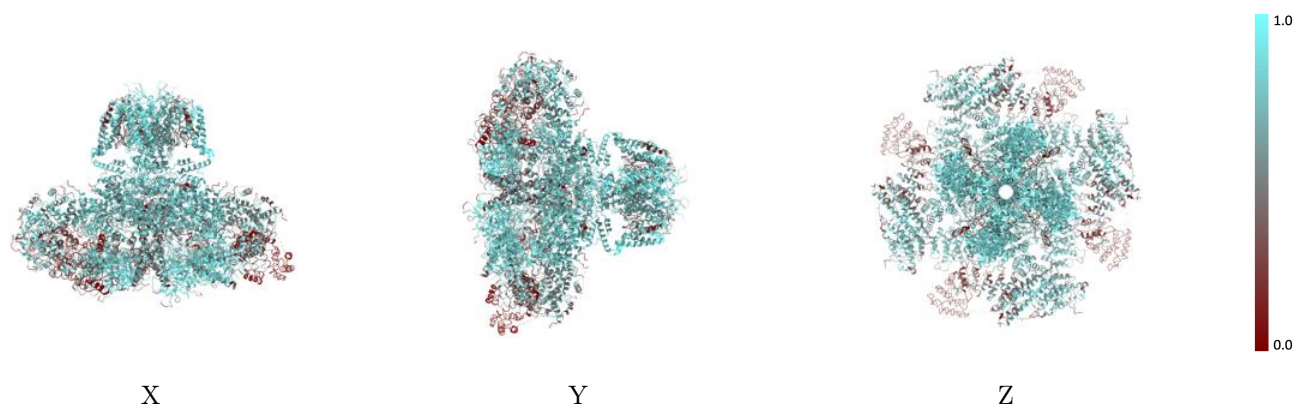
The images above show the 3D surface view of the map at the recommended contour level 0.0112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



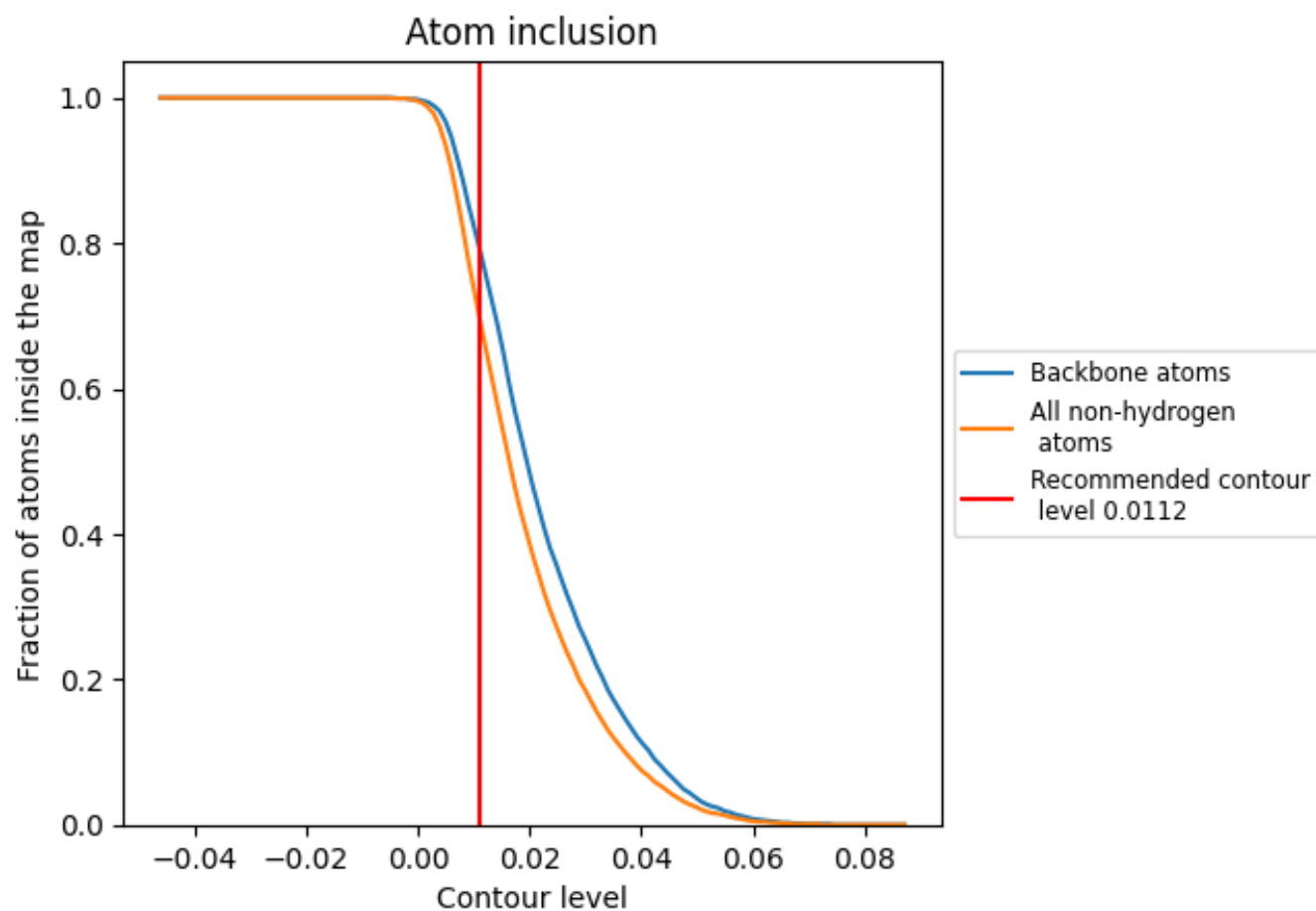
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 69% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6920	0.3760
A	0.6930	0.3760
B	0.6910	0.3750
C	0.6920	0.3760
D	0.6920	0.3760

