



Full wwPDB EM Validation Report ⓘ

Apr 26, 2026 – 04:58 PM JST

PDB ID : 9W7X / pdb_00009w7x
EMDB ID : EMD-65735
Title : Cryo-EM structure of dPIEZO channel
Authors : Liu, S.; Li, X.; Xiao, B.
Deposited on : 2025-08-07
Resolution : 3.95 Å(reported)

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 : 1.8.5 (274361), CSD as541be (2020)
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

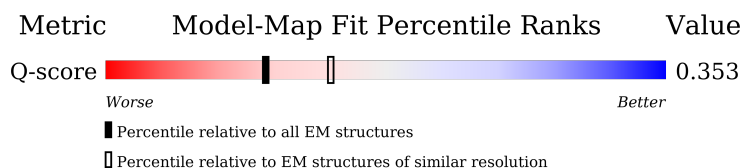
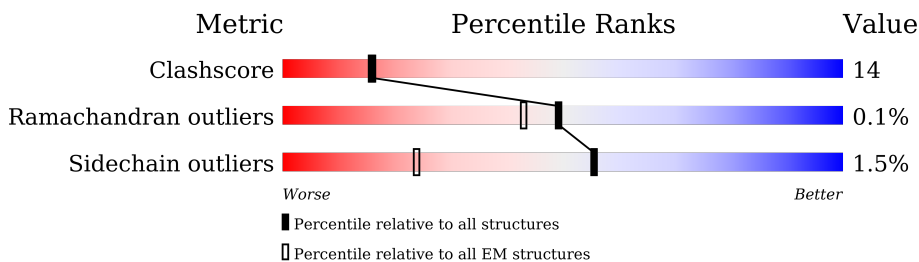
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.95 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	7707 (3.45 - 4.45)

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	2551	
1	B	2551	
1	C	2551	

2 Entry composition (i)

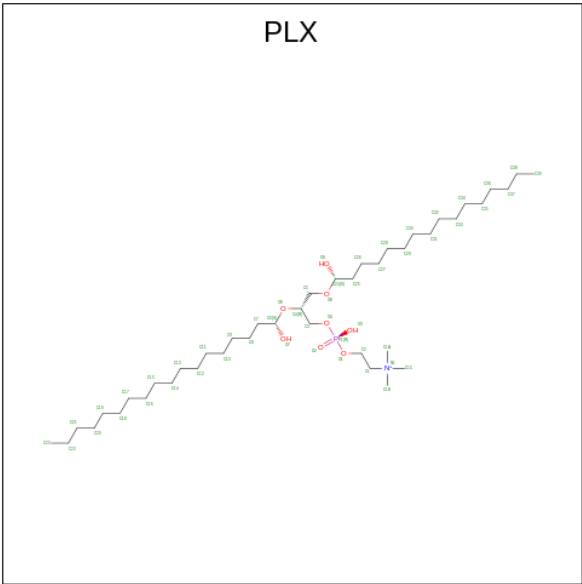
There are 4 unique types of molecules in this entry. The entry contains 31971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Piezo-type mechanosensitive ion channel component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1305	Total	C	N	O	S	0	0
			10344	6816	1704	1765	59		
1	A	1305	Total	C	N	O	S	0	0
			10344	6816	1704	1765	59		
1	C	1305	Total	C	N	O	S	0	0
			10344	6816	1704	1765	59		

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



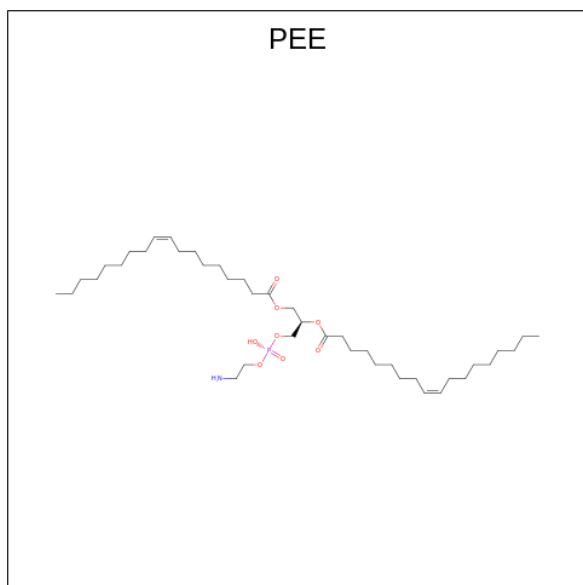
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 3 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



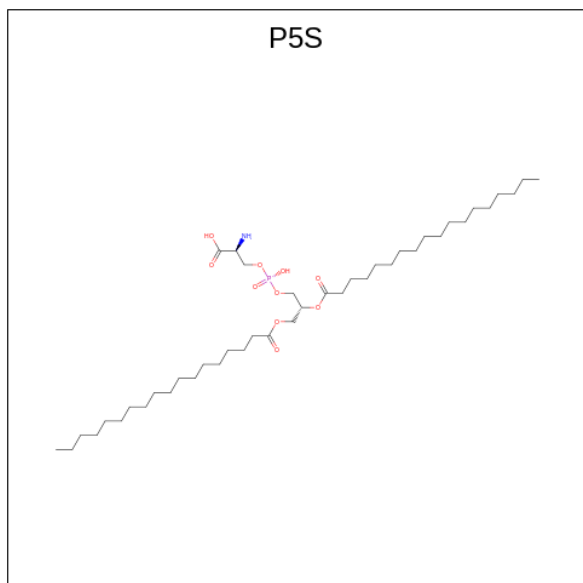
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P) (labeled as "Ligand of Interest" by depositor).

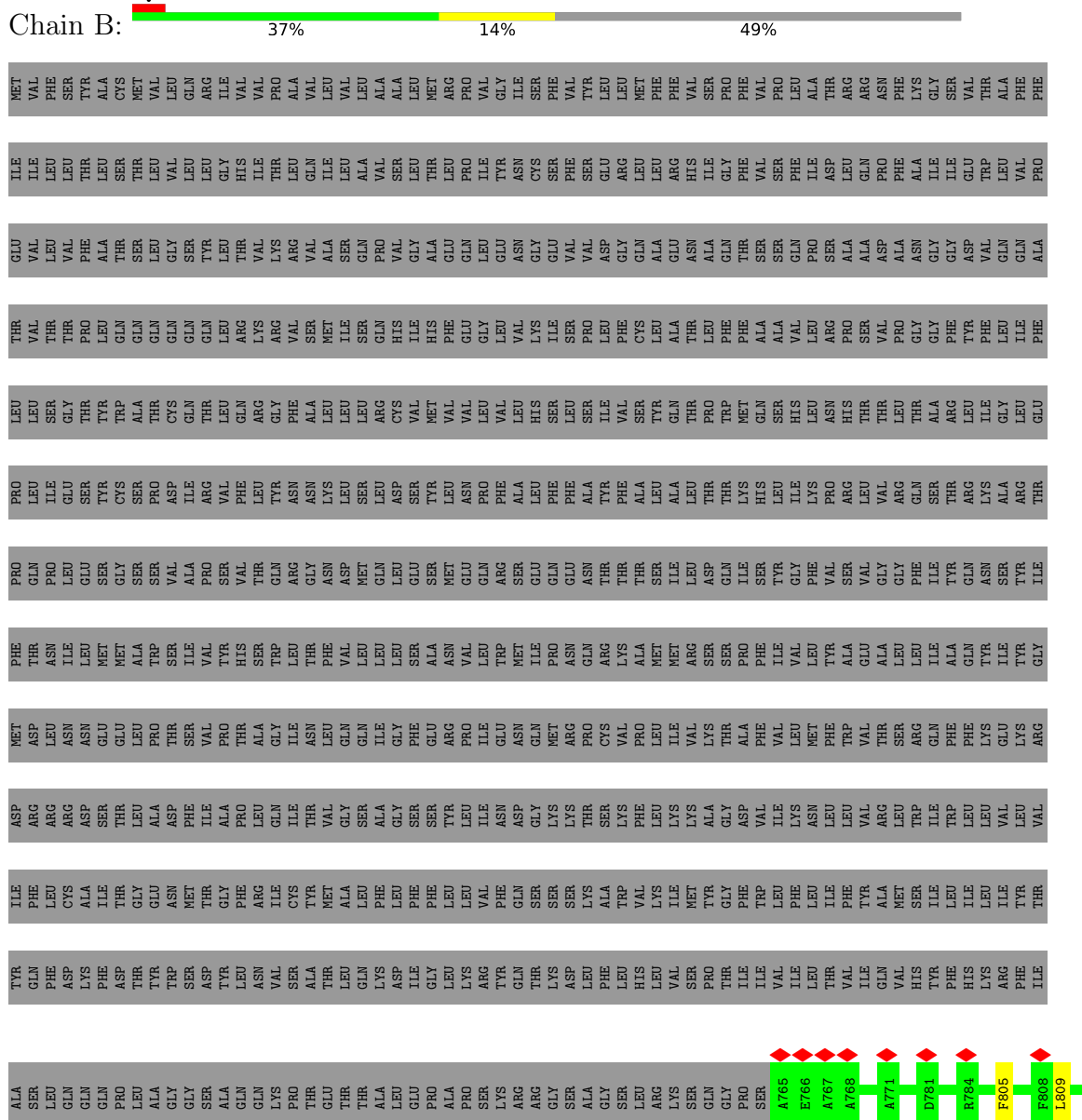


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
4	C	1	Total	C	N	O	P	0
			54	42	1	10	1	

3 Residue-property plots

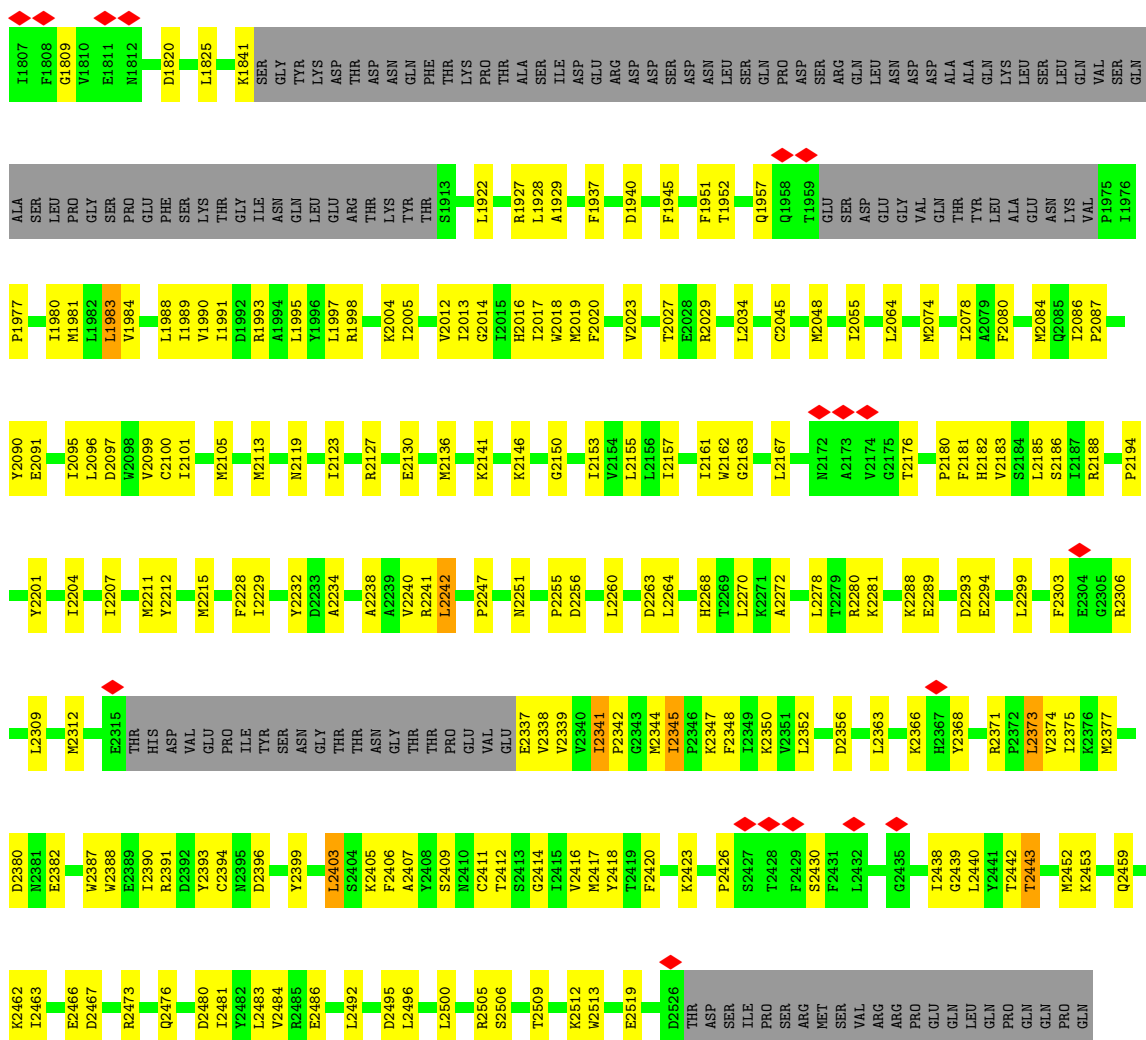
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Piezo-type mechanosensitive ion channel component



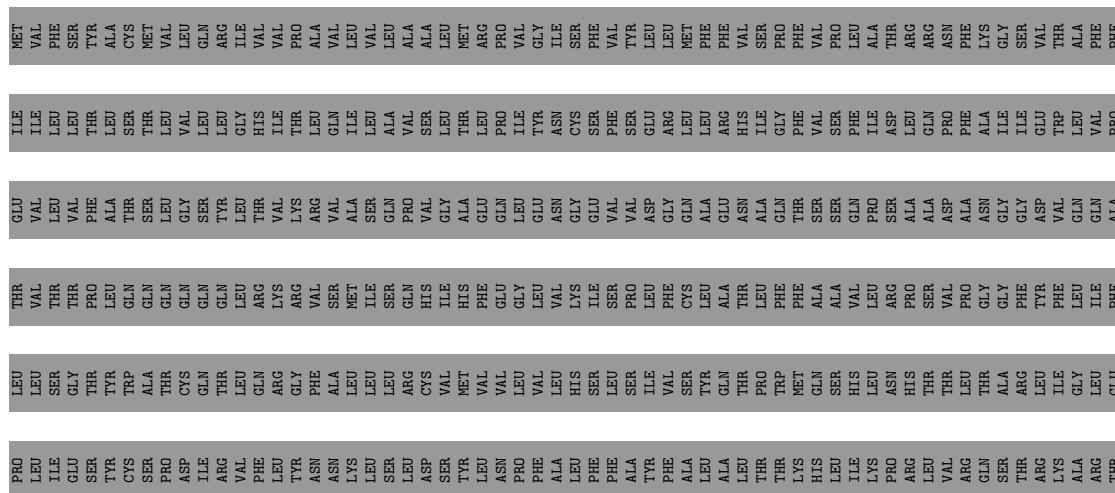






● Molecule 1: Piezo-type mechanosensitive ion channel component

Chain C: 36% 15% 49%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	678118	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.018	Depositor
Minimum map value	-1.462	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	399.0, 399.0, 399.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, PLX, P5S

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	0.15	0/10590	0.34	1/14368 (0.0%)
1	B	0.16	0/10590	0.35	2/14368 (0.0%)
1	C	0.15	0/10590	0.32	0/14368
All	All	0.15	0/31770	0.34	3/43104 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2394	CYS	CA-CB-SG	8.91	134.90	114.40
1	B	1788	LYS	CA-CB-CG	5.50	125.10	114.10
1	B	2211	MET	CB-CG-SD	-5.38	96.55	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10344	0	10361	307	0
1	B	10344	0	10361	302	0
1	C	10344	0	10361	322	0
2	A	260	0	440	24	0
2	B	156	0	264	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	208	0	352	21	0
3	A	51	0	78	12	0
3	B	51	0	76	8	0
3	C	51	0	82	15	0
4	A	54	0	80	9	0
4	B	54	0	80	3	0
4	C	54	0	80	11	0
All	All	31971	0	32615	927	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 14.

All (927) 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:1991:ILE:HD11	2:A:2603:PLX:H142	1.32	1.09
1:B:2211:MET:HE2	1:B:2407:ALA:HA	1.35	1.05
1:B:1780:LEU:HD12	2:B:2602:PLX:H331	1.39	1.04
1:C:1149:LYS:HZ1	1:C:1302:TYR:HE2	1.15	0.94
1:A:1991:ILE:HD11	2:A:2603:PLX:C14	1.99	0.91
1:C:2399:TYR:HA	1:C:2403:LEU:HD23	1.49	0.91
1:B:2270:LEU:HB2	1:B:2299:LEU:HD13	1.54	0.89
1:C:2399:TYR:OH	1:C:2409:SER:O	1.89	0.89
1:A:1149:LYS:HZ1	1:A:1302:TYR:HE2	1.17	0.88
1:B:1149:LYS:HZ1	1:B:1302:TYR:HE2	1.16	0.88
1:A:2399:TYR:HA	1:A:2403:LEU:HD23	1.56	0.88
1:B:2261:LEU:HB3	1:B:2265:ARG:HH21	1.39	0.87
1:A:1945:PHE:HE2	3:A:2606:PEE:H38	1.40	0.87
1:A:2242:LEU:HD11	1:A:2417:MET:HE1	1.56	0.86
1:B:2345:ILE:HG23	1:B:2371:ARG:HB2	1.58	0.86
1:B:2399:TYR:HA	1:B:2403:LEU:HD23	1.58	0.86
1:B:2399:TYR:OH	1:B:2409:SER:O	1.93	0.86
1:C:1991:ILE:HD11	2:C:2602:PLX:H141	1.56	0.85
1:A:1991:ILE:CD1	2:A:2603:PLX:H131	2.07	0.83
1:A:2399:TYR:OH	1:A:2409:SER:O	1.97	0.83
1:B:2180:PRO:HA	1:B:2280:ARG:HB3	1.60	0.82
1:C:2228:PHE:HD2	1:C:2362:VAL:HG11	1.43	0.82
1:A:2345:ILE:HG23	1:A:2371:ARG:HB2	1.61	0.82
1:A:2113:MET:HE1	1:A:2500:LEU:HD23	1.61	0.82
1:C:2349:ILE:HD11	1:C:2357:ALA:HB1	1.62	0.81
1:C:2270:LEU:HB2	1:C:2299:LEU:HD13	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1034:ILE:HD11	1:C:1084:ASP:HB3	1.63	0.81
1:B:2232:TYR:CE2	1:B:2420:PHE:HB3	2.15	0.81
4:A:2607:P5S:O18	4:A:2607:P5S:O15	1.98	0.81
1:B:1034:ILE:HD11	1:B:1084:ASP:HB3	1.63	0.80
1:B:805:PHE:O	1:B:809:LEU:HB2	1.82	0.80
1:C:2345:ILE:HG23	1:C:2371:ARG:HB2	1.61	0.80
1:B:2204:ILE:HD11	1:B:2238:ALA:HB1	1.62	0.80
1:A:2204:ILE:HD11	1:A:2238:ALA:HB1	1.62	0.79
1:C:2180:PRO:HA	1:C:2280:ARG:HB3	1.62	0.79
1:A:805:PHE:O	1:A:809:LEU:HB2	1.82	0.79
1:A:2337:GLU:HG2	1:A:2338:VAL:HG23	1.65	0.79
1:A:2506:SER:HG	1:A:2509:THR:HG1	1.29	0.79
1:C:805:PHE:O	1:C:809:LEU:HB2	1.82	0.79
1:A:1034:ILE:HD11	1:A:1084:ASP:HB3	1.63	0.79
1:A:2161:ILE:HG23	1:A:2162:TRP:CD1	2.18	0.78
1:C:2215:MET:HE1	1:C:2406:PHE:HA	1.65	0.78
1:B:1352:ARG:NH2	1:B:2480:ASP:OD2	2.17	0.78
1:B:2345:ILE:HD11	1:B:2417:MET:HG3	1.65	0.78
1:B:2467:ASP:HB3	1:C:2505:ARG:HD2	1.64	0.78
1:C:2204:ILE:HD11	1:C:2238:ALA:HB1	1.64	0.77
1:B:1780:LEU:HD12	2:B:2602:PLX:C33	2.13	0.77
1:C:1122:ILE:HD13	4:C:2606:P5S:N	2.00	0.77
1:A:2180:PRO:HA	1:A:2280:ARG:HB3	1.65	0.76
1:C:968:LEU:HD11	4:C:2606:P5S:H39A	1.67	0.76
1:B:2161:ILE:HG23	1:B:2162:TRP:CD1	2.20	0.76
1:C:1352:ARG:NH2	1:C:2480:ASP:OD2	2.18	0.76
1:B:2349:ILE:HD11	1:B:2357:ALA:HB1	1.66	0.76
2:C:2602:PLX:H342	2:C:2602:PLX:H171	1.67	0.76
1:A:1957:GLN:HG3	1:A:2029:ARG:HH21	1.52	0.75
1:C:2211:MET:HE2	1:C:2407:ALA:HA	1.69	0.74
1:C:2242:LEU:HD11	1:C:2417:MET:HE1	1.69	0.74
1:A:2306:ARG:HA	1:A:2309:LEU:HD12	1.69	0.74
1:C:1957:GLN:HG3	1:C:2029:ARG:HH21	1.51	0.74
1:B:1780:LEU:CD1	2:B:2602:PLX:H331	2.16	0.73
1:A:1991:ILE:HD11	2:A:2603:PLX:C13	2.19	0.72
1:B:2506:SER:HG	1:B:2509:THR:HG1	1.34	0.72
1:B:1222:PHE:HE2	1:B:1244:LEU:HD13	1.54	0.72
1:B:1989:ILE:HG21	3:B:2604:PEE:H61	1.73	0.71
1:C:2344:MET:HA	1:C:2344:MET:HE2	1.72	0.70
1:A:2348:PHE:HE1	1:A:2418:TYR:HD2	1.39	0.70
1:A:2270:LEU:HB2	1:A:2299:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1991:ILE:CD1	2:A:2603:PLX:C13	2.70	0.69
1:C:2309:LEU:HD13	1:C:2339:VAL:HG21	1.75	0.69
1:C:2228:PHE:CD2	1:C:2362:VAL:HG11	2.25	0.69
1:B:2505:ARG:HD2	1:A:2467:ASP:HB3	1.75	0.69
1:B:1060:GLY:O	1:B:1064:GLN:HG3	1.92	0.69
1:A:2338:VAL:HG13	1:A:2374:VAL:HG13	1.72	0.69
1:A:2215:MET:HE1	1:A:2405:LYS:O	1.93	0.69
1:A:2303:PHE:HE2	1:A:2309:LEU:HD11	1.58	0.69
1:B:2087:PRO:HG2	3:B:2604:PEE:H75	1.74	0.68
1:B:2232:TYR:HE2	1:B:2420:PHE:HB3	1.57	0.68
1:B:2183:VAL:HG22	1:B:2278:LEU:HD22	1.74	0.68
1:B:2403:LEU:HA	1:B:2406:PHE:CD2	2.28	0.68
1:A:2505:ARG:HD2	1:C:2467:ASP:HB3	1.74	0.68
1:C:1222:PHE:HD2	1:C:1246:ILE:HG12	1.59	0.68
1:B:926:MET:SD	1:B:927:HIS:ND1	2.67	0.67
1:C:958:ARG:HH21	4:C:2606:P5S:HB	1.59	0.67
1:C:2345:ILE:HD11	1:C:2417:MET:HG3	1.76	0.67
1:C:1747:PRO:HB2	1:C:1774:TYR:HE2	1.59	0.67
1:A:1010:VAL:O	1:A:1014:LEU:HG	1.93	0.67
2:C:2602:PLX:H292	2:C:2602:PLX:H132	1.76	0.67
1:A:2087:PRO:HG2	3:A:2606:PEE:H75	1.77	0.66
1:B:1010:VAL:O	1:B:1014:LEU:HG	1.96	0.66
1:A:2312:MET:HE1	1:A:2377:MET:H	1.59	0.66
1:B:1769:VAL:HG11	2:B:2602:PLX:H6	1.77	0.66
1:B:2242:LEU:HD11	1:B:2417:MET:HE1	1.77	0.66
1:B:1747:PRO:HB3	2:B:2603:PLX:H161	1.78	0.66
1:B:1957:GLN:HE21	1:B:2029:ARG:HG3	1.60	0.66
1:A:996:ARG:HD3	1:A:1080:LYS:HB3	1.78	0.66
1:A:822:PHE:HE2	1:A:1078:VAL:HG13	1.62	0.65
1:B:2345:ILE:CG2	1:B:2371:ARG:HB2	2.26	0.65
1:C:958:ARG:NH2	4:C:2606:P5S:HB	2.11	0.65
1:A:1005:ALA:O	1:A:1009:VAL:HG13	1.97	0.65
1:C:1980:ILE:O	1:C:1984:VAL:HG23	1.97	0.65
1:A:1243:MET:SD	1:A:1244:LEU:HG	2.37	0.65
1:B:1755:TRP:CZ3	1:B:1770:THR:HG21	2.32	0.65
1:C:2506:SER:OG	1:C:2509:THR:OG1	2.14	0.65
1:A:1774:TYR:CE1	2:A:2604:PLX:H211	2.32	0.65
1:C:1034:ILE:HD12	1:C:1088:LEU:HD11	1.79	0.65
1:B:2506:SER:OG	1:B:2509:THR:OG1	2.15	0.64
2:A:2602:PLX:H271	2:A:2602:PLX:H121	1.79	0.64
1:C:2373:LEU:HD21	1:C:2390:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2084:MET:O	1:A:2453:LYS:NZ	2.23	0.64
1:A:2161:ILE:HG23	1:A:2162:TRP:HD1	1.62	0.64
1:C:2377:MET:HE1	1:C:2386:LEU:HD23	1.79	0.64
1:B:2519:GLU:O	1:C:1386:LYS:NZ	2.30	0.64
1:A:1034:ILE:HD12	1:A:1088:LEU:HD11	1.79	0.64
4:A:2607:P5S:H31	4:A:2607:P5S:H52A	1.79	0.64
1:A:981:GLY:HA3	1:A:1094:GLN:HE22	1.63	0.64
1:C:996:ARG:HD3	1:C:1080:LYS:HB3	1.80	0.64
1:B:822:PHE:HE2	1:B:1078:VAL:HG13	1.61	0.64
1:C:1346:ILE:HD12	1:C:2483:LEU:HD11	1.80	0.64
1:B:1991:ILE:HD11	2:A:2601:PLX:H141	1.80	0.64
1:B:1034:ILE:HD12	1:B:1088:LEU:HD11	1.80	0.64
1:C:1063:ILE:HG22	1:C:1069:LEU:HD12	1.80	0.64
1:B:2215:MET:HE1	1:B:2407:ALA:N	2.13	0.64
1:C:822:PHE:HE2	1:C:1078:VAL:HG13	1.62	0.64
1:C:1993:ARG:HD3	3:C:2605:PEE:H50	1.81	0.63
1:B:2204:ILE:HD13	1:B:2240:VAL:HG22	1.80	0.63
1:B:2252:ILE:HD13	1:B:2257:ARG:HG2	1.81	0.63
1:B:1754:LEU:HD21	1:B:2012:VAL:HG11	1.81	0.63
1:A:980:PHE:CE1	4:A:2607:P5S:O15	2.52	0.63
1:A:1754:LEU:HD21	1:A:2012:VAL:HG11	1.80	0.63
1:C:1282:LEU:O	1:C:1286:ILE:HG13	1.99	0.63
1:A:1980:ILE:O	1:A:1984:VAL:HG23	1.98	0.63
1:A:2345:ILE:HD11	1:A:2417:MET:HG3	1.81	0.63
1:C:1094:GLN:HG3	1:C:1098:PHE:CE2	2.33	0.63
1:B:1063:ILE:HG22	1:B:1069:LEU:HD12	1.81	0.63
1:B:1954:PHE:CD2	1:B:1981:MET:HE1	2.34	0.63
1:A:2403:LEU:HA	1:A:2406:PHE:CD2	2.34	0.63
1:C:1754:LEU:HD12	2:C:2604:PLX:H301	1.81	0.63
1:A:2084:MET:HE1	1:A:2090:TYR:CD2	2.34	0.62
1:C:2029:ARG:NH1	1:C:2034:LEU:HD11	2.14	0.62
1:C:2252:ILE:HD13	1:C:2257:ARG:HG2	1.80	0.62
1:B:1386:LYS:NZ	1:A:2519:GLU:O	2.31	0.62
1:C:980:PHE:HZ	4:C:2606:P5S:H2	1.62	0.62
1:A:2348:PHE:CE1	1:A:2418:TYR:HD2	2.16	0.62
1:A:1222:PHE:HD2	1:A:1246:ILE:HG12	1.65	0.62
1:A:1007:TRP:O	1:A:1011:LEU:HG	2.00	0.62
1:A:2232:TYR:CE2	1:A:2420:PHE:HB3	2.35	0.62
1:A:2029:ARG:NH1	1:A:2034:LEU:HD11	2.14	0.62
1:A:2373:LEU:HD22	1:A:2375:ILE:HD13	1.80	0.62
1:B:1082:ILE:O	1:B:1086:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1937:PHE:CE1	3:C:2605:PEE:H51	2.35	0.61
1:C:2362:VAL:HG13	1:C:2363:LEU:HD12	1.82	0.61
1:A:1386:LYS:NZ	1:C:2519:GLU:O	2.31	0.61
1:C:2027:THR:OG1	1:C:2029:ARG:NH1	2.33	0.61
1:B:2241:ARG:NH2	1:B:2408:TYR:HB3	2.14	0.61
1:A:1346:ILE:HD12	1:A:2483:LEU:HD11	1.81	0.61
1:C:2348:PHE:HE1	1:C:2418:TYR:HD2	1.46	0.61
1:C:2403:LEU:HA	1:C:2406:PHE:CD2	2.36	0.61
1:B:1403:PHE:O	1:B:2512:LYS:NZ	2.33	0.61
1:A:1063:ILE:HG22	1:A:1069:LEU:HD12	1.81	0.61
1:B:2347:LYS:HE2	1:B:2371:ARG:HG3	1.83	0.61
1:A:1015:ARG:H	1:A:1018:GLN:HE22	1.49	0.61
1:A:1149:LYS:NZ	1:A:1302:TYR:HE2	1.97	0.61
1:A:1403:PHE:O	1:A:2512:LYS:NZ	2.33	0.61
1:C:1754:LEU:HD21	1:C:2012:VAL:HG11	1.82	0.60
1:A:980:PHE:CZ	4:A:2607:P5S:O15	2.54	0.60
1:A:2027:THR:OG1	1:A:2029:ARG:NH1	2.33	0.60
1:A:2074:MET:O	1:A:2078:ILE:HG12	2.01	0.60
1:B:2237:VAL:HG22	1:B:2420:PHE:HD1	1.65	0.60
1:A:1008:LEU:HA	1:A:1011:LEU:HD12	1.82	0.60
1:A:2004:LYS:HG3	1:A:2055:ILE:HD11	1.83	0.60
1:B:2348:PHE:HE1	1:B:2418:TYR:CD2	2.19	0.60
1:C:1237:CYS:HB3	1:C:1240:LEU:HB3	1.83	0.60
1:C:1403:PHE:O	1:C:2512:LYS:NZ	2.34	0.60
2:C:2604:PLX:H292	2:C:2604:PLX:H122	1.84	0.60
1:B:2453:LYS:NZ	1:C:2084:MET:O	2.27	0.60
1:B:923:ILE:HG23	1:B:927:HIS:CE1	2.37	0.59
1:A:1237:CYS:HB3	1:A:1240:LEU:HB3	1.83	0.59
1:C:2004:LYS:HG3	1:C:2055:ILE:HD11	1.83	0.59
1:B:1345:LYS:NZ	1:B:1414:LEU:O	2.32	0.59
1:A:1977:PRO:O	1:A:1981:MET:HG3	2.03	0.59
2:A:2601:PLX:H272	2:A:2601:PLX:H132	1.83	0.59
1:C:1549:SER:HB3	1:C:1720:ALA:HA	1.83	0.59
1:B:2004:LYS:HG3	1:B:2055:ILE:HD11	1.84	0.59
1:C:1142:ARG:NE	1:C:1146:ASP:OD2	2.35	0.59
1:B:1179:TYR:HD1	1:B:1211:PHE:HE2	1.50	0.59
1:C:2272:ALA:HB2	1:C:2299:LEU:HD11	1.84	0.59
1:A:1396:ARG:NH2	1:C:2130:GLU:OE2	2.29	0.59
1:C:923:ILE:HG23	1:C:927:HIS:CE1	2.38	0.59
1:C:2161:ILE:HG23	1:C:2162:TRP:CD1	2.38	0.59
1:B:1085:PHE:HA	1:B:1088:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2176:THR:O	1:C:2423:LYS:NZ	2.32	0.59
1:B:1237:CYS:HB3	1:B:1240:LEU:HB3	1.84	0.59
1:B:2161:ILE:HG23	1:B:2162:TRP:HD1	1.67	0.59
1:C:1085:PHE:HA	1:C:1088:LEU:HD12	1.85	0.59
1:A:1937:PHE:CE1	3:A:2606:PEE:H51	2.37	0.59
1:C:1937:PHE:CD2	3:C:2605:PEE:H8	2.37	0.59
1:A:2368:TYR:HE1	1:A:2371:ARG:NE	2.01	0.58
1:A:2476:GLN:NE2	1:A:2480:ASP:OD2	2.36	0.58
1:C:1082:ILE:O	1:C:1086:ILE:HG13	2.02	0.58
1:C:1769:VAL:HG11	2:C:2603:PLX:H6	1.84	0.58
1:C:2312:MET:SD	1:C:2312:MET:N	2.75	0.58
1:A:2462:LYS:HG3	1:A:2466:GLU:OE1	2.04	0.58
1:C:2261:LEU:HD21	1:C:2313:LEU:HB3	1.85	0.58
1:B:1755:TRP:HZ3	1:B:1770:THR:HG21	1.68	0.58
1:B:2462:LYS:HG3	1:B:2466:GLU:OE1	2.04	0.58
1:C:2240:VAL:HB	1:C:2417:MET:HE2	1.85	0.58
1:B:1346:ILE:HD12	1:B:2483:LEU:HD11	1.85	0.58
1:A:2157:ILE:O	1:A:2161:ILE:HG22	2.04	0.58
1:A:2215:MET:HE1	1:A:2406:PHE:HA	1.85	0.58
1:B:2130:GLU:OE2	1:C:1396:ARG:NH2	2.29	0.58
1:C:1981:MET:HG2	1:C:2018:TRP:CZ2	2.39	0.58
1:C:2492:LEU:HA	1:C:2495:ASP:OD2	2.04	0.58
1:B:1957:GLN:NE2	1:B:2027:THR:O	2.37	0.58
1:B:2084:MET:HE1	1:B:2090:TYR:CZ	2.38	0.58
1:A:1549:SER:HB3	1:A:1720:ALA:HA	1.83	0.58
1:A:2176:THR:O	1:A:2423:LYS:NZ	2.32	0.58
1:B:1549:SER:HB3	1:B:1720:ALA:HA	1.84	0.58
1:B:1818:ILE:HD12	1:B:1821:LEU:HD23	1.86	0.58
1:B:2005:ILE:HG12	1:B:2055:ILE:HD12	1.86	0.58
1:C:2352:LEU:HB2	1:C:2356:ASP:OD1	2.03	0.58
1:C:1937:PHE:CZ	3:C:2605:PEE:H48	2.39	0.57
1:C:2005:ILE:HG12	1:C:2055:ILE:HD12	1.86	0.57
1:C:2136:MET:HE3	1:C:2136:MET:HA	1.85	0.57
1:B:2309:LEU:HG	1:B:2339:VAL:HG11	1.84	0.57
1:A:1085:PHE:HA	1:A:1088:LEU:HD12	1.85	0.57
1:A:1188:TRP:NE1	2:A:2604:PLX:O9	2.37	0.57
1:A:2215:MET:N	1:A:2215:MET:HE2	2.19	0.57
1:C:1546:ASN:HA	1:C:1553:ARG:HH22	1.69	0.57
1:B:981:GLY:HA3	1:B:1094:GLN:OE1	2.03	0.57
2:A:2604:PLX:H221	2:A:2604:PLX:H393	1.84	0.57
2:C:2602:PLX:H321	2:C:2602:PLX:H151	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2091:GLU:HG2	1:A:2452:MET:HG2	1.85	0.57
1:B:2299:LEU:HD12	1:B:2299:LEU:H	1.70	0.57
1:A:1560:ALA:O	1:A:1564:LYS:HG2	2.05	0.57
1:A:1937:PHE:CD2	3:A:2606:PEE:H8	2.39	0.57
1:C:1241:VAL:HG23	1:C:1246:ILE:HD12	1.86	0.57
1:B:1243:MET:SD	1:B:1244:LEU:HG	2.44	0.57
1:B:2452:MET:HG2	1:C:2091:GLU:HG2	1.86	0.57
1:A:2345:ILE:CG2	1:A:2371:ARG:HB2	2.34	0.57
4:A:2607:P5S:H33	4:A:2607:P5S:H54A	1.86	0.57
1:B:1396:ARG:NH2	1:A:2130:GLU:OE2	2.29	0.57
1:C:1345:LYS:NZ	1:C:1414:LEU:O	2.35	0.57
1:B:1560:ALA:O	1:B:1564:LYS:HG2	2.05	0.57
1:B:1937:PHE:CE1	3:B:2604:PEE:H53	2.40	0.57
1:A:2492:LEU:HA	1:A:2495:ASP:OD2	2.05	0.57
1:B:2176:THR:O	1:B:2423:LYS:NZ	2.32	0.56
1:C:975:PHE:HB3	1:C:978:TYR:HD2	1.70	0.56
1:A:915:ARG:O	1:A:919:ILE:HG13	2.06	0.56
1:A:1240:LEU:O	1:A:1243:MET:HE3	2.05	0.56
1:A:2005:ILE:HG12	1:A:2055:ILE:HD12	1.87	0.56
1:C:915:ARG:O	1:C:919:ILE:HG13	2.06	0.56
1:C:1243:MET:SD	1:C:1244:LEU:HG	2.46	0.56
1:C:981:GLY:HA3	1:C:1094:GLN:OE1	2.06	0.56
1:C:1094:GLN:HG3	1:C:1098:PHE:HE2	1.71	0.56
1:C:2036:PRO:HA	1:C:2039:ILE:HD12	1.87	0.56
1:A:2350:LYS:HE3	1:A:2352:LEU:HD21	1.87	0.56
1:B:1149:LYS:NZ	1:B:1302:TYR:HE2	1.96	0.56
1:B:1977:PRO:O	1:B:1981:MET:HG3	2.06	0.56
1:B:915:ARG:O	1:B:919:ILE:HG13	2.06	0.56
1:C:815:LYS:HA	1:C:1085:PHE:HE2	1.70	0.56
1:B:1987:LEU:HD11	2:A:2601:PLX:H172	1.86	0.56
1:B:2017:ILE:HG13	1:B:2018:TRP:N	2.20	0.56
1:A:1222:PHE:CE2	1:A:1244:LEU:HD13	2.40	0.56
1:A:2091:GLU:HG2	1:C:2452:MET:HG2	1.87	0.56
1:C:1135:HIS:CE1	1:C:1142:ARG:HH21	2.24	0.56
1:A:2299:LEU:H	1:A:2299:LEU:HD12	1.70	0.56
1:B:815:LYS:HA	1:B:1085:PHE:HE2	1.70	0.55
1:A:815:LYS:HA	1:A:1085:PHE:HE2	1.70	0.55
1:A:1082:ILE:O	1:A:1086:ILE:HG13	2.06	0.55
1:C:1560:ALA:O	1:C:1564:LYS:HG2	2.05	0.55
1:C:2348:PHE:HB2	1:C:2360:VAL:HB	1.89	0.55
1:C:2207:ILE:HG23	1:C:2211:MET:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2045:CYS:HA	1:A:2048:MET:HE3	1.89	0.55
1:C:1780:LEU:HD12	2:C:2603:PLX:H332	1.87	0.55
1:B:2092:LEU:HD13	3:B:2604:PEE:H58	1.88	0.55
1:B:2228:PHE:HE1	1:B:2232:TYR:OH	1.89	0.55
1:B:1079:PRO:HA	1:B:1082:ILE:HG12	1.88	0.55
1:A:2017:ILE:HG13	1:A:2018:TRP:N	2.21	0.55
1:A:2280:ARG:O	1:A:2289:GLU:HG2	2.06	0.55
1:C:2158:VAL:HA	1:C:2161:ILE:HG22	1.89	0.55
1:B:957:ILE:HG12	1:B:958:ARG:H	1.71	0.55
1:A:1079:PRO:HA	1:A:1082:ILE:HG12	1.88	0.55
1:C:1079:PRO:HA	1:C:1082:ILE:HG12	1.88	0.55
1:C:2017:ILE:HG13	1:C:2018:TRP:N	2.21	0.55
1:C:1149:LYS:NZ	1:C:1302:TYR:HE2	1.96	0.54
1:C:2204:ILE:HD13	1:C:2240:VAL:HG22	1.89	0.54
1:C:2462:LYS:HG3	1:C:2466:GLU:OE1	2.06	0.54
1:B:2237:VAL:HG22	1:B:2420:PHE:CD1	2.42	0.54
1:A:981:GLY:HA3	1:A:1094:GLN:NE2	2.22	0.54
1:B:1280:VAL:HG23	1:B:1281:LEU:HD12	1.90	0.54
1:C:1774:TYR:CE1	2:C:2603:PLX:H211	2.43	0.54
1:C:2341:ILE:HD12	1:C:2342:PRO:HD2	1.89	0.54
1:B:1061:GLU:HA	1:B:1064:GLN:OE1	2.07	0.54
1:B:1240:LEU:O	1:B:1243:MET:HE3	2.07	0.54
1:A:1774:TYR:HE1	2:A:2604:PLX:H211	1.71	0.54
1:A:1280:VAL:HG23	1:A:1281:LEU:HD12	1.90	0.54
1:C:2399:TYR:HA	1:C:2403:LEU:CD2	2.31	0.54
1:B:2064:LEU:HB3	1:B:2486:GLU:HG3	1.90	0.54
1:B:2348:PHE:HE1	1:B:2418:TYR:HD2	1.56	0.54
1:A:1158:TRP:HH2	1:A:1190:GLY:HA2	1.72	0.54
1:A:1742:SER:HB2	1:A:1809:GLY:HA3	1.90	0.54
1:A:2136:MET:HA	1:A:2136:MET:HE3	1.90	0.54
1:C:1303:PHE:O	1:C:1307:ILE:HG23	2.08	0.54
1:A:2309:LEU:HD21	1:A:2339:VAL:HG11	1.89	0.53
1:C:1747:PRO:HB3	2:C:2604:PLX:H162	1.89	0.53
2:A:2602:PLX:H32	2:A:2602:PLX:H22	1.90	0.53
1:C:1307:ILE:O	1:C:1311:LYS:HG3	2.09	0.53
1:B:1937:PHE:CZ	3:B:2604:PEE:H48	2.43	0.53
1:B:1158:TRP:HH2	1:B:1190:GLY:HA2	1.73	0.53
1:B:1303:PHE:O	1:B:1307:ILE:HG23	2.09	0.53
1:B:1922:LEU:O	1:B:1927:ARG:NH1	2.42	0.53
1:C:2064:LEU:HB3	1:C:2486:GLU:HG3	1.89	0.53
1:A:1096:SER:O	1:A:1100:ILE:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2215:MET:HE1	1:C:2406:PHE:CA	2.38	0.53
1:B:1222:PHE:CE2	1:B:1244:LEU:HD13	2.41	0.53
1:A:1222:PHE:HE2	1:A:1244:LEU:HD13	1.74	0.53
1:C:1754:LEU:HB2	2:C:2604:PLX:H281	1.90	0.53
2:C:2601:PLX:H121	2:C:2601:PLX:H271	1.90	0.53
1:B:1096:SER:O	1:B:1100:ILE:HG23	2.09	0.53
1:A:1303:PHE:O	1:A:1307:ILE:HG23	2.08	0.53
1:C:844:ALA:O	1:C:1092:ASN:ND2	2.42	0.53
1:B:2123:ILE:O	1:B:2127:ARG:HG2	2.09	0.53
1:B:2014:GLY:O	1:B:2018:TRP:HB3	2.10	0.52
1:A:1009:VAL:HG11	1:A:1217:LEU:HD22	1.91	0.52
1:A:1209:LEU:HD21	1:A:1292:ILE:HD13	1.91	0.52
1:A:2064:LEU:HB3	1:A:2486:GLU:HG3	1.90	0.52
1:C:1096:SER:O	1:C:1100:ILE:HG23	2.10	0.52
1:C:1945:PHE:HE2	3:C:2605:PEE:H37	1.74	0.52
1:C:2158:VAL:HG13	1:C:2159:ILE:HD13	1.90	0.52
1:C:1922:LEU:O	1:C:1927:ARG:NH1	2.42	0.52
2:C:2604:PLX:H122	2:C:2604:PLX:C29	2.39	0.52
1:B:1766:THR:O	1:B:1770:THR:HG22	2.10	0.52
1:B:1957:GLN:HE21	1:B:2029:ARG:CG	2.23	0.52
1:A:2123:ILE:O	1:A:2127:ARG:HG2	2.09	0.52
1:C:1280:VAL:HG23	1:C:1281:LEU:HD12	1.92	0.52
1:C:2192:TYR:HD2	1:C:2256:ASP:HB3	1.74	0.52
1:B:1152:VAL:HG11	4:B:2605:P5S:H40A	1.92	0.52
1:B:2368:TYR:CE2	1:B:2398:PHE:CD1	2.97	0.52
3:A:2606:PEE:H20	3:A:2606:PEE:H28	1.91	0.52
1:B:1539:VAL:O	1:B:1543:ILE:HG12	2.10	0.52
1:B:2344:MET:N	1:B:2371:ARG:O	2.34	0.52
1:C:2123:ILE:O	1:C:2127:ARG:HG2	2.09	0.52
1:B:1027:GLN:NE2	1:B:1092:ASN:OD1	2.43	0.52
1:C:1337:ASP:HA	1:C:1340:LYS:HE2	1.91	0.52
1:C:2192:TYR:OH	1:C:2259:ARG:HG2	2.09	0.52
1:C:2399:TYR:C	1:C:2399:TYR:CD1	2.88	0.52
1:B:2368:TYR:HE2	1:B:2398:PHE:CD1	2.28	0.52
1:C:2403:LEU:HA	1:C:2406:PHE:CG	2.44	0.52
1:A:2180:PRO:HG3	1:A:2278:LEU:HD23	1.91	0.52
1:C:2311:HIS:ND1	1:C:2312:MET:SD	2.72	0.52
1:B:2157:ILE:O	1:B:2161:ILE:HG22	2.09	0.52
1:A:1015:ARG:NH2	1:A:1017:SER:OG	2.43	0.52
1:A:1539:VAL:O	1:A:1543:ILE:HG12	2.10	0.52
1:A:1922:LEU:O	1:A:1927:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2606:P5S:H1A	4:C:2606:P5S:P12	2.50	0.52
1:B:1774:TYR:CE1	2:B:2602:PLX:H211	2.44	0.51
1:C:1742:SER:HB2	1:C:1809:GLY:HA3	1.91	0.51
1:B:1015:ARG:NH2	1:B:1017:SER:OG	2.44	0.51
1:B:2185:LEU:HD12	1:B:2186:SER:N	2.25	0.51
1:A:1712:GLU:O	1:A:1715:ILE:HG22	2.09	0.51
1:A:1841:LYS:C	1:A:1841:LYS:HD2	2.35	0.51
1:A:1007:TRP:O	1:A:1010:VAL:HG12	2.10	0.51
1:C:1015:ARG:NH2	1:C:1017:SER:OG	2.44	0.51
1:C:2338:VAL:HG13	1:C:2374:VAL:HG13	1.92	0.51
1:C:2399:TYR:C	1:C:2399:TYR:HD1	2.19	0.51
1:B:1712:GLU:O	1:B:1715:ILE:HG22	2.10	0.51
1:B:1742:SER:HB2	1:B:1809:GLY:HA3	1.91	0.51
1:A:1769:VAL:HG11	2:A:2604:PLX:H6	1.92	0.51
1:A:2272:ALA:HB2	1:A:2299:LEU:HD11	1.92	0.51
1:B:2368:TYR:OH	1:B:2371:ARG:CZ	2.59	0.51
4:A:2607:P5S:H1A	4:A:2607:P5S:P12	2.50	0.51
1:C:2345:ILE:HD12	1:C:2415:ILE:HD11	1.93	0.51
1:B:2476:GLN:NE2	1:B:2480:ASP:OD1	2.44	0.51
1:A:1937:PHE:CZ	3:A:2606:PEE:H48	2.45	0.51
1:A:1993:ARG:HD3	3:A:2606:PEE:H50	1.93	0.51
1:A:2185:LEU:HD12	1:A:2186:SER:N	2.25	0.51
1:C:1539:VAL:O	1:C:1543:ILE:HG12	2.10	0.51
1:C:2371:ARG:NH2	1:C:2393:TYR:O	2.40	0.51
1:B:2084:MET:HE1	1:B:2090:TYR:CE1	2.46	0.51
1:B:2211:MET:CE	1:B:2407:ALA:HA	2.25	0.51
1:B:2208:ASN:HB2	1:B:2210:GLU:OE1	2.10	0.51
1:B:2044:LYS:O	1:B:2048:MET:HE2	2.11	0.50
1:A:2228:PHE:HE1	1:A:2232:TYR:OH	1.93	0.50
1:B:923:ILE:O	1:B:927:HIS:ND1	2.44	0.50
1:B:1159:PHE:HE2	1:B:1290:PHE:CZ	2.29	0.50
1:B:2255:PRO:HG3	1:C:2387:TRP:CE2	2.47	0.50
1:A:2241:ARG:HG2	1:A:2416:VAL:HG12	1.93	0.50
1:B:1179:TYR:CD1	1:B:1211:PHE:HE2	2.29	0.50
1:A:2373:LEU:HD21	1:A:2390:ILE:HB	1.93	0.50
1:A:2382:GLU:N	1:A:2382:GLU:OE1	2.45	0.50
1:A:2399:TYR:CD1	1:A:2403:LEU:HB2	2.46	0.50
4:A:2607:P5S:H1	4:A:2607:P5S:H40A	1.94	0.50
1:C:1180:LEU:HD21	1:C:1779:VAL:HG12	1.94	0.50
1:A:2344:MET:N	1:A:2371:ARG:O	2.40	0.50
1:B:1037:GLN:HG2	1:B:1068:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:ALA:HB2	1:A:1299:LYS:HB3	1.94	0.50
1:A:2352:LEU:HB2	1:A:2356:ASP:OD1	2.11	0.50
1:A:2484:VAL:HG21	1:A:2492:LEU:HD11	1.93	0.50
1:B:2399:TYR:CD1	1:B:2399:TYR:C	2.89	0.50
1:C:1739:VAL:HG21	1:C:1819:TYR:CE2	2.47	0.50
1:C:1014:LEU:HD21	1:C:1018:GLN:HB2	1.94	0.50
1:B:1007:TRP:O	1:B:1011:LEU:HG	2.12	0.50
1:B:1011:LEU:HA	1:B:1014:LEU:HD12	1.94	0.50
1:B:2015:ILE:HG21	1:B:2048:MET:SD	2.52	0.50
1:B:2192:TYR:HD2	1:B:2256:ASP:HB3	1.77	0.50
1:B:2272:ALA:HB2	1:B:2299:LEU:HD11	1.94	0.50
1:A:914:LEU:O	1:A:917:TYR:HB2	2.12	0.50
1:C:1336:HIS:HB3	1:C:1340:LYS:NZ	2.27	0.50
1:B:914:LEU:O	1:B:917:TYR:HB2	2.12	0.49
4:C:2606:P5S:H1A	4:C:2606:P5S:O13	2.12	0.49
1:A:2084:MET:O	1:C:2453:LYS:NZ	2.29	0.49
1:A:2399:TYR:CD1	1:A:2399:TYR:C	2.90	0.49
1:B:2481:ILE:HG12	1:B:2496:LEU:HB3	1.93	0.49
1:C:2382:GLU:N	1:C:2382:GLU:OE1	2.45	0.49
1:C:2210:GLU:O	1:C:2214:GLN:HG2	2.12	0.49
1:A:1335:ARG:HH12	1:A:1928:LEU:HB3	1.77	0.49
1:C:2210:GLU:OE2	1:C:2210:GLU:N	2.37	0.49
1:B:1179:TYR:OH	1:B:1212:ASN:ND2	2.29	0.49
1:B:1209:LEU:HD21	1:B:1292:ILE:HD13	1.94	0.49
1:B:1335:ARG:HG3	1:B:1928:LEU:HD13	1.95	0.49
1:B:1700:GLU:HB2	1:B:1707:HIS:HB3	1.95	0.49
1:B:2045:CYS:HA	1:B:2048:MET:CE	2.43	0.49
1:B:2095:ILE:HG13	1:A:2153:ILE:HG21	1.94	0.49
1:B:2338:VAL:HG13	1:B:2374:VAL:HG13	1.95	0.49
1:B:2371:ARG:NH2	1:B:2393:TYR:HB3	2.28	0.49
1:C:914:LEU:O	1:C:917:TYR:HB2	2.12	0.49
1:C:1059:PHE:O	1:C:1063:ILE:HG13	2.13	0.49
1:B:1020:ALA:HA	1:B:1098:PHE:CD2	2.48	0.49
1:C:1192:ASP:HA	1:C:1195:LEU:HD23	1.95	0.49
1:C:2312:MET:HE2	1:C:2337:GLU:N	2.27	0.49
1:C:957:ILE:HG23	1:C:959:ALA:H	1.77	0.49
1:B:2210:GLU:O	1:B:2213:SER:OG	2.28	0.49
1:C:1192:ASP:OD2	1:C:1835:LYS:NZ	2.46	0.49
1:C:2348:PHE:CE1	1:C:2418:TYR:HD2	2.29	0.49
1:B:2387:TRP:CE2	1:A:2255:PRO:HG3	2.48	0.48
1:A:2481:ILE:HG12	1:A:2496:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1192:ASP:OD2	1:B:1835:LYS:NZ	2.46	0.48
1:A:1700:GLU:HB2	1:A:1707:HIS:HB3	1.95	0.48
1:C:2155:LEU:O	1:C:2159:ILE:HG12	2.13	0.48
1:B:1059:PHE:O	1:B:1063:ILE:HG13	2.13	0.48
1:B:2153:ILE:HG21	1:C:2095:ILE:HG13	1.94	0.48
1:B:2163:GLY:O	1:B:2167:LEU:HG	2.13	0.48
1:B:2215:MET:HE1	1:B:2407:ALA:H	1.77	0.48
1:B:2426:PRO:O	1:B:2430:SER:OG	2.29	0.48
1:A:2403:LEU:HA	1:A:2406:PHE:CG	2.48	0.48
1:C:1007:TRP:O	1:C:1011:LEU:HG	2.13	0.48
1:C:1360:MET:HE2	1:C:1402:MET:HA	1.95	0.48
1:A:1297:ILE:HD11	4:A:2607:P5S:H20A	1.96	0.48
1:A:1345:LYS:NZ	1:A:1414:LEU:O	2.34	0.48
1:A:2095:ILE:HG13	1:C:2153:ILE:HG21	1.94	0.48
1:B:1788:LYS:HD3	1:B:1791:TRP:HB2	1.96	0.48
1:B:2280:ARG:O	1:B:2289:GLU:HG2	2.13	0.48
1:C:1755:TRP:CZ3	2:C:2604:PLX:H91	2.48	0.48
1:C:2087:PRO:HG2	3:C:2605:PEE:H75	1.96	0.48
1:C:2180:PRO:HG3	1:C:2278:LEU:HD23	1.94	0.48
1:B:2492:LEU:HA	1:B:2495:ASP:OD2	2.13	0.48
1:A:2204:ILE:HD13	1:A:2240:VAL:HG22	1.96	0.48
1:C:1392:PRO:HA	1:C:1395:THR:HG22	1.96	0.48
1:C:2399:TYR:CA	1:C:2403:LEU:HD23	2.34	0.48
1:B:2241:ARG:HH21	1:B:2408:TYR:HB3	1.79	0.48
1:A:957:ILE:HG23	1:A:959:ALA:H	1.78	0.48
1:A:1005:ALA:HB1	1:A:1217:LEU:HD13	1.95	0.48
1:C:923:ILE:O	1:C:927:HIS:ND1	2.47	0.48
1:C:1336:HIS:HB3	1:C:1340:LYS:HZ1	1.78	0.48
1:C:1726:ASP:N	1:C:1726:ASP:OD1	2.47	0.48
1:B:1028:ALA:O	1:B:1032:ILE:HG23	2.14	0.48
1:B:1388:ILE:O	1:B:1388:ILE:HG22	2.14	0.48
1:B:2356:ASP:OD1	1:B:2356:ASP:N	2.47	0.48
1:A:1059:PHE:O	1:A:1063:ILE:HG13	2.13	0.48
1:A:2387:TRP:CE2	1:C:2255:PRO:HG3	2.48	0.48
1:B:830:CYS:HB2	1:B:833:HIS:HB3	1.96	0.47
1:B:2180:PRO:HD3	1:B:2421:ASN:OD1	2.13	0.47
1:A:923:ILE:O	1:A:926:MET:HG3	2.13	0.47
1:C:1086:ILE:HA	1:C:1089:VAL:HG12	1.96	0.47
1:B:1726:ASP:OD1	1:B:1726:ASP:N	2.45	0.47
1:C:1028:ALA:O	1:C:1032:ILE:HG23	2.14	0.47
1:B:2074:MET:O	1:B:2078:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2012:VAL:HG23	1:A:2048:MET:SD	2.55	0.47
1:C:2377:MET:CE	1:C:2386:LEU:HD23	2.43	0.47
1:B:1957:GLN:HG3	1:B:2029:ARG:CZ	2.44	0.47
1:B:2399:TYR:C	1:B:2399:TYR:HD1	2.21	0.47
1:A:830:CYS:HB2	1:A:833:HIS:HB3	1.96	0.47
1:A:844:ALA:O	1:A:1092:ASN:ND2	2.48	0.47
1:A:1995:LEU:HD13	1:A:2004:LYS:HA	1.97	0.47
1:A:2347:LYS:HE2	1:A:2371:ARG:HG3	1.95	0.47
1:A:1940:ASP:HB3	1:A:1989:ILE:HG12	1.96	0.47
1:A:1991:ILE:CD1	2:A:2603:PLX:C14	2.83	0.47
1:C:2014:GLY:O	1:C:2018:TRP:HB3	2.14	0.47
1:B:2391:ARG:NH2	1:B:2412:THR:O	2.47	0.47
1:A:1945:PHE:CE2	3:A:2606:PEE:H38	2.32	0.47
1:C:2391:ARG:HH12	1:C:2414:GLY:HA2	1.80	0.47
1:B:2023:VAL:O	1:B:2027:THR:HG22	2.15	0.47
1:B:2182:HIS:HB3	1:B:2279:THR:OG1	2.15	0.47
1:B:2473:ARG:NH1	1:B:2513:TRP:O	2.47	0.47
1:A:1294:GLN:HG3	1:A:1298:PHE:CE2	2.50	0.47
1:A:2014:GLY:O	1:A:2018:TRP:HB3	2.15	0.47
1:A:2127:ARG:O	1:A:2130:GLU:HG2	2.14	0.47
1:A:2303:PHE:CE2	1:A:2309:LEU:HD11	2.44	0.47
1:A:2371:ARG:NH2	1:A:2393:TYR:O	2.45	0.47
1:C:1700:GLU:HB2	1:C:1707:HIS:HB3	1.95	0.47
1:C:1937:PHE:CG	3:C:2605:PEE:H8	2.50	0.47
1:B:1294:GLN:HG3	1:B:1298:PHE:CE2	2.49	0.47
2:B:2601:PLX:H282	2:B:2601:PLX:H121	1.97	0.47
1:A:1937:PHE:CG	3:A:2606:PEE:H8	2.50	0.47
1:A:1983:LEU:HD13	1:C:2162:TRP:CZ3	2.50	0.47
1:A:2023:VAL:O	1:A:2027:THR:HG22	2.15	0.47
1:A:2459:GLN:O	1:A:2463:ILE:HG13	2.14	0.47
1:C:2280:ARG:O	1:C:2289:GLU:HG2	2.15	0.47
1:C:2459:GLN:O	1:C:2463:ILE:HG13	2.15	0.47
1:B:1995:LEU:HD13	1:B:2004:LYS:HA	1.97	0.47
1:A:1983:LEU:HA	1:C:2162:TRP:HH2	1.79	0.47
1:C:1240:LEU:O	1:C:1243:MET:HE3	2.15	0.47
1:C:1995:LEU:HD13	1:C:2004:LYS:HA	1.96	0.47
1:B:2127:ARG:O	1:B:2130:GLU:HG2	2.15	0.47
1:A:1028:ALA:O	1:A:1032:ILE:HG23	2.14	0.47
1:B:1764:THR:HG22	1:B:1766:THR:H	1.80	0.46
1:B:2027:THR:OG1	1:B:2029:ARG:NH2	2.45	0.46
1:A:1993:ARG:NE	3:A:2606:PEE:O5	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1294:GLN:HG3	1:C:1298:PHE:CE2	2.50	0.46
1:B:825:SER:O	1:B:825:SER:OG	2.31	0.46
1:A:1081:LEU:HD23	1:A:1081:LEU:HA	1.77	0.46
1:A:2019:MET:HE2	1:A:2019:MET:HB2	1.71	0.46
1:A:2185:LEU:HD12	1:A:2186:SER:H	1.80	0.46
1:C:2023:VAL:O	1:C:2027:THR:HG22	2.14	0.46
1:B:1337:ASP:O	1:B:1341:GLN:HG2	2.16	0.46
1:A:2113:MET:HE2	1:A:2113:MET:HA	1.96	0.46
1:A:2391:ARG:HH12	1:A:2414:GLY:HA2	1.80	0.46
1:C:830:CYS:HB2	1:C:833:HIS:HB3	1.96	0.46
1:C:2426:PRO:O	1:C:2430:SER:OG	2.29	0.46
1:B:1182:GLY:HA2	1:B:1185:ILE:HD12	1.97	0.46
1:A:1182:GLY:HA2	1:A:1185:ILE:HD12	1.98	0.46
2:A:2602:PLX:H52	2:A:2602:PLX:H251	1.48	0.46
1:C:983:GLU:HG3	1:C:1292:ILE:HG13	1.97	0.46
1:B:1086:ILE:HA	1:B:1089:VAL:HG12	1.97	0.46
1:B:2185:LEU:HD23	1:B:2242:LEU:HD22	1.98	0.46
1:B:2459:GLN:O	1:B:2463:ILE:HG13	2.14	0.46
1:A:1075:PHE:HB3	1:A:1077:HIS:CE1	2.50	0.46
1:A:1335:ARG:NH1	1:A:1928:LEU:HB3	2.31	0.46
1:A:2288:LYS:HB3	1:A:2288:LYS:HE2	1.74	0.46
1:C:1075:PHE:HB3	1:C:1077:HIS:CE1	2.51	0.46
1:C:2481:ILE:HG12	1:C:2496:LEU:HB3	1.96	0.46
1:B:970:LYS:HD2	1:B:970:LYS:HA	1.72	0.46
1:A:1388:ILE:HG22	1:A:1388:ILE:O	2.14	0.46
1:C:2344:MET:N	1:C:2371:ARG:O	2.40	0.46
1:A:977:PHE:HE2	1:A:1093:ARG:HB3	1.80	0.46
1:A:1392:PRO:HA	1:A:1395:THR:HG22	1.98	0.46
1:C:2127:ARG:O	1:C:2130:GLU:HG2	2.15	0.46
1:C:2366:LYS:HB2	1:C:2366:LYS:HE2	1.78	0.46
1:C:2377:MET:HG3	1:C:2388:TRP:CZ2	2.51	0.46
1:B:1139:SER:C	1:B:1140:TYR:HD1	2.24	0.46
1:A:1305:HIS:CD2	1:A:1305:HIS:N	2.84	0.46
1:A:1764:THR:HG22	1:A:1766:THR:H	1.81	0.46
1:A:1983:LEU:HD22	1:C:2162:TRP:HZ3	1.81	0.46
1:B:1127:ARG:HD2	1:B:1127:ARG:HA	1.78	0.46
1:A:1726:ASP:N	1:A:1726:ASP:OD1	2.46	0.46
1:A:2391:ARG:NH2	1:A:2412:THR:O	2.49	0.46
1:C:1209:LEU:HD21	1:C:1292:ILE:HD13	1.97	0.46
1:C:2391:ARG:NH2	1:C:2412:THR:O	2.49	0.46
1:B:815:LYS:HA	1:B:1085:PHE:CE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1063:ILE:CG2	1:B:1069:LEU:HD12	2.46	0.45
1:B:1075:PHE:HB3	1:B:1077:HIS:CE1	2.50	0.45
1:B:1392:PRO:HA	1:B:1395:THR:HG22	1.97	0.45
1:B:2247:PRO:HA	1:A:2256:ASP:OD2	2.17	0.45
1:B:2403:LEU:HD13	1:B:2406:PHE:CD2	2.51	0.45
1:C:809:LEU:HA	1:C:812:HIS:HB3	1.98	0.45
1:C:1388:ILE:HG22	1:C:1388:ILE:O	2.15	0.45
1:C:1986:PHE:HE1	3:C:2605:PEE:H60	1.81	0.45
1:B:2162:TRP:HH2	1:C:1983:LEU:N	2.14	0.45
1:A:1086:ILE:HA	1:A:1089:VAL:HG12	1.97	0.45
1:C:1945:PHE:CZ	3:C:2605:PEE:H44	2.51	0.45
1:B:982:ILE:HG23	1:B:983:GLU:OE1	2.16	0.45
1:B:1018:GLN:O	1:B:1022:ILE:HG13	2.17	0.45
1:A:2013:ILE:O	1:A:2017:ILE:HG23	2.16	0.45
1:A:2380:ASP:OD2	1:A:2382:GLU:HG2	2.17	0.45
1:C:965:LEU:HA	1:C:1145:SER:HB2	1.98	0.45
1:C:1764:THR:HG22	1:C:1766:THR:H	1.81	0.45
1:B:1824:LEU:HD23	1:B:1824:LEU:HA	1.81	0.45
1:C:818:TYR:CZ	1:C:840:CYS:HB3	2.52	0.45
1:C:2084:MET:HE1	1:C:2090:TYR:CZ	2.52	0.45
1:B:2265:ARG:HD3	1:B:2265:ARG:N	2.30	0.45
1:B:2399:TYR:CD1	1:B:2403:LEU:HB2	2.51	0.45
1:C:1182:GLY:HA2	1:C:1185:ILE:HD12	1.97	0.45
1:B:965:LEU:HA	1:B:1145:SER:HB2	1.99	0.45
1:B:2185:LEU:HD12	1:B:2186:SER:H	1.80	0.45
1:B:2281:LYS:HZ3	1:B:2282:ALA:HB3	1.81	0.45
1:A:1337:ASP:O	1:A:1341:GLN:HG2	2.16	0.45
1:A:2341:ILE:HD12	1:A:2342:PRO:HD2	1.98	0.45
1:A:2440:LEU:O	1:A:2443:THR:HG22	2.16	0.45
1:C:923:ILE:O	1:C:926:MET:HG3	2.16	0.45
1:C:1337:ASP:O	1:C:1341:GLN:HG2	2.17	0.45
1:C:2013:ILE:O	1:C:2017:ILE:HG23	2.16	0.45
1:C:2141:LYS:HB2	1:C:2146:LYS:HE3	1.98	0.45
1:B:818:TYR:CZ	1:B:840:CYS:HB3	2.51	0.45
1:A:1360:MET:SD	1:A:1402:MET:HA	2.57	0.45
1:C:815:LYS:HA	1:C:1085:PHE:CE2	2.50	0.45
1:C:825:SER:O	1:C:825:SER:OG	2.31	0.45
1:C:1301:HIS:HD2	4:C:2606:P5S:OXT	2.00	0.45
1:C:1940:ASP:HB3	1:C:1989:ILE:HG12	1.99	0.45
1:C:2030:THR:O	1:C:2033:SER:OG	2.32	0.45
1:C:2114:GLU:OE1	1:C:2482:TYR:OH	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2049:LEU:HD23	1:B:2049:LEU:HA	1.86	0.45
1:B:2240:VAL:HB	1:B:2417:MET:HE2	1.98	0.45
1:B:2440:LEU:O	1:B:2443:THR:HG22	2.16	0.45
1:A:965:LEU:HA	1:A:1145:SER:HB2	1.99	0.45
1:C:1945:PHE:HE2	3:C:2605:PEE:C23	2.30	0.45
1:C:2228:PHE:HE1	1:C:2232:TYR:OH	2.00	0.45
1:B:2439:GLY:O	1:B:2442:THR:HG22	2.17	0.45
1:A:972:LEU:HD23	1:A:972:LEU:HA	1.85	0.45
1:A:2374:VAL:HB	1:A:2391:ARG:HB2	1.99	0.45
1:A:2473:ARG:NH1	1:A:2513:TRP:O	2.47	0.45
1:C:1302:TYR:N	1:C:1302:TYR:CD1	2.85	0.45
1:C:2374:VAL:HB	1:C:2391:ARG:HB2	1.98	0.45
1:B:926:MET:SD	1:B:927:HIS:N	2.90	0.45
1:B:1940:ASP:HB3	1:B:1989:ILE:HG12	1.99	0.45
1:B:2018:TRP:CD1	1:B:2018:TRP:C	2.95	0.45
1:B:2251:ASN:OD1	1:B:2251:ASN:N	2.50	0.45
1:A:1139:SER:C	1:A:1140:TYR:HD1	2.24	0.45
1:A:1216:ILE:HD11	1:A:1284:ASP:HB3	1.99	0.45
1:A:1998:ARG:HA	1:A:1998:ARG:HD2	1.78	0.45
1:C:1188:TRP:CZ2	2:C:2603:PLX:H271	2.52	0.45
1:C:2345:ILE:CG2	1:C:2371:ARG:HB2	2.40	0.45
1:C:2347:LYS:HA	1:C:2347:LYS:HD3	1.68	0.45
1:B:957:ILE:HG12	1:B:958:ARG:N	2.31	0.44
1:A:2100:CYS:SG	2:A:2603:PLX:H72	2.57	0.44
1:B:2013:ILE:O	1:B:2017:ILE:HG23	2.17	0.44
1:A:1061:GLU:HA	1:A:1064:GLN:OE1	2.18	0.44
1:A:2399:TYR:C	1:A:2399:TYR:HD1	2.26	0.44
1:C:970:LYS:HD2	1:C:970:LYS:HA	1.73	0.44
1:C:980:PHE:CZ	4:C:2606:P5S:H2	2.49	0.44
1:C:1990:VAL:HG13	1:C:2096:LEU:HD11	1.99	0.44
1:C:2473:ARG:NH1	1:C:2513:TRP:O	2.46	0.44
1:A:1006:LEU:O	1:A:1009:VAL:HG22	2.16	0.44
1:A:2251:ASN:OD1	1:A:2251:ASN:N	2.49	0.44
1:C:1305:HIS:CD2	1:C:1305:HIS:N	2.84	0.44
1:C:2232:TYR:CE2	1:C:2420:PHE:HB3	2.52	0.44
1:C:2380:ASP:OD2	1:C:2382:GLU:HG2	2.17	0.44
1:B:1983:LEU:N	1:A:2162:TRP:HH2	2.15	0.44
1:B:1993:ARG:NE	3:B:2604:PEE:H51	2.33	0.44
1:B:2141:LYS:HB2	1:B:2146:LYS:HE3	1.98	0.44
1:B:2347:LYS:HA	1:B:2347:LYS:HD3	1.68	0.44
1:B:2374:VAL:HB	1:B:2391:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:ILE:HD12	1:A:1292:ILE:HA	1.88	0.44
1:A:1302:TYR:N	1:A:1302:TYR:CD1	2.85	0.44
1:B:2293:ASP:OD1	1:B:2294:GLU:N	2.50	0.44
1:A:923:ILE:HG23	1:A:927:HIS:CE1	2.52	0.44
1:A:1736:ASN:ND2	1:A:1820:ASP:OD1	2.50	0.44
1:A:2029:ARG:HH11	1:A:2034:LEU:HD11	1.82	0.44
1:B:2155:LEU:O	1:B:2159:ILE:HG12	2.17	0.44
1:B:2288:LYS:HE2	1:B:2288:LYS:HB3	1.73	0.44
1:B:2371:ARG:HH21	1:B:2393:TYR:HB3	1.81	0.44
1:A:815:LYS:HA	1:A:1085:PHE:CE2	2.50	0.44
1:A:1023:TRP:NE1	1:A:1094:GLN:HB3	2.32	0.44
1:C:2340:VAL:HG22	1:C:2374:VAL:HG22	2.00	0.44
1:C:2390:ILE:HD11	1:C:2415:ILE:HG21	1.99	0.44
1:C:2440:LEU:O	1:C:2443:THR:HG22	2.16	0.44
1:B:1986:PHE:CE1	3:B:2604:PEE:H60	2.52	0.44
1:A:957:ILE:HG12	1:A:958:ARG:H	1.82	0.44
1:A:1181:ILE:O	1:A:1185:ILE:HG13	2.18	0.44
1:C:1139:SER:C	1:C:1140:TYR:HD1	2.25	0.44
1:C:1981:MET:HG2	1:C:2018:TRP:CE2	2.53	0.44
1:A:2309:LEU:O	1:A:2312:MET:HG3	2.18	0.44
1:C:2373:LEU:HD22	1:C:2375:ILE:HD13	2.00	0.44
1:A:1094:GLN:HG3	1:A:1098:PHE:CE1	2.53	0.44
1:A:2141:LYS:HB2	1:A:2146:LYS:HE3	1.98	0.44
2:A:2603:PLX:H281	1:C:2147:LEU:HD21	2.00	0.44
1:C:1302:TYR:N	1:C:1302:TYR:HD1	2.16	0.44
1:C:2207:ILE:HB	1:C:2237:VAL:HG13	2.00	0.44
1:C:2489:GLU:HG2	1:C:2492:LEU:HD22	1.98	0.44
1:B:1020:ALA:HA	1:B:1098:PHE:CE2	2.53	0.43
1:B:2207:ILE:HG22	1:B:2237:VAL:O	2.18	0.43
1:A:1209:LEU:HD13	1:A:1291:ILE:CG2	2.47	0.43
1:A:1302:TYR:N	1:A:1302:TYR:HD1	2.16	0.43
1:A:2181:PHE:HD1	1:A:2280:ARG:HA	1.82	0.43
1:A:2366:LYS:HB2	1:A:2366:LYS:HE2	1.78	0.43
1:C:1166:LEU:HD23	1:C:1166:LEU:HA	1.82	0.43
1:C:2019:MET:HE2	1:C:2019:MET:HB2	1.52	0.43
2:C:2601:PLX:H52	2:C:2601:PLX:H251	1.44	0.43
1:B:2192:TYR:N	1:B:2192:TYR:CD1	2.85	0.43
1:B:2229:ILE:HD11	1:B:2363:LEU:HD21	2.00	0.43
1:B:2340:VAL:HG22	1:B:2374:VAL:HG22	2.00	0.43
1:A:1166:LEU:HD23	1:A:1166:LEU:HA	1.82	0.43
1:A:1746:LEU:HD13	1:A:2020:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:GLN:HA	1:B:1068:MET:HE1	1.99	0.43
1:B:1181:ILE:O	1:B:1185:ILE:HG13	2.18	0.43
1:B:1319:ARG:O	1:B:1323:ILE:HG13	2.19	0.43
2:B:2601:PLX:H282	2:B:2601:PLX:C12	2.48	0.43
2:B:2601:PLX:H32	2:B:2601:PLX:H22	1.99	0.43
1:A:1984:VAL:O	1:A:1988:LEU:HG	2.18	0.43
1:A:2188:ARG:HH11	1:A:2194:PRO:HD3	1.83	0.43
1:C:1216:ILE:HD11	1:C:1284:ASP:HB3	1.99	0.43
1:C:2032:ASN:OD1	1:C:2032:ASN:N	2.50	0.43
1:C:2262:ASN:O	1:C:2265:ARG:HG3	2.18	0.43
1:B:1158:TRP:CH2	1:B:1190:GLY:HA2	2.52	0.43
1:B:2211:MET:HE2	1:B:2407:ALA:CA	2.26	0.43
1:B:2272:ALA:N	1:B:2299:LEU:HD11	2.33	0.43
1:B:2377:MET:HG3	1:B:2388:TRP:CZ2	2.54	0.43
1:C:1063:ILE:CG2	1:C:1069:LEU:HD12	2.47	0.43
1:C:1171:ILE:HG13	1:C:1176:ALA:HB2	2.00	0.43
1:C:1746:LEU:HD13	1:C:2020:PHE:CD2	2.53	0.43
1:C:1984:VAL:O	1:C:1988:LEU:HG	2.19	0.43
1:B:1388:ILE:HG21	1:B:1394:ALA:HA	2.00	0.43
1:B:2188:ARG:HH11	1:B:2194:PRO:HD3	1.84	0.43
1:A:970:LYS:HD2	1:A:970:LYS:HA	1.73	0.43
1:A:1241:VAL:HG23	1:A:1246:ILE:HB	2.00	0.43
1:C:1319:ARG:O	1:C:1323:ILE:HG13	2.19	0.43
1:C:2029:ARG:HH11	1:C:2034:LEU:HD11	1.82	0.43
1:C:1935:LEU:HD13	2:C:2601:PLX:H102	2.00	0.43
1:C:2182:HIS:HB2	1:C:2201:TYR:CD2	2.53	0.43
1:A:1747:PRO:HB3	2:A:2605:PLX:H152	2.00	0.43
1:A:2163:GLY:O	1:A:2167:LEU:HG	2.18	0.43
1:A:2309:LEU:CD2	1:A:2339:VAL:HG11	2.49	0.43
1:C:963:LYS:HD2	1:C:964:ASP:HB2	2.00	0.43
1:C:2293:ASP:OD1	1:C:2294:GLU:N	2.50	0.43
1:B:958:ARG:HA	1:B:971:TYR:CE2	2.53	0.43
1:B:1957:GLN:HE21	1:B:2029:ARG:CD	2.32	0.43
1:A:963:LYS:HD2	1:A:964:ASP:HB2	2.01	0.43
1:A:2407:ALA:HB3	1:A:2418:TYR:CE1	2.54	0.43
1:C:1023:TRP:HB3	1:C:1095:LYS:HE2	2.01	0.43
1:B:1171:ILE:HG13	1:B:1176:ALA:HB2	2.01	0.43
1:A:1171:ILE:HG13	1:A:1176:ALA:HB2	2.00	0.43
1:C:1192:ASP:HA	1:C:1195:LEU:CD2	2.49	0.43
1:C:2288:LYS:HE2	1:C:2288:LYS:HB3	1.74	0.43
1:B:1990:VAL:HG13	1:B:2096:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2445:VAL:HG21	3:C:2605:PEE:H81	2.01	0.43
1:A:813:ILE:HD12	1:A:813:ILE:HA	1.88	0.43
1:A:2229:ILE:HD11	1:A:2363:LEU:HD21	2.00	0.43
1:A:2247:PRO:HA	1:C:2256:ASP:OD2	2.18	0.43
1:C:975:PHE:HB3	1:C:978:TYR:CD2	2.52	0.43
1:C:1774:TYR:HE1	2:C:2603:PLX:H211	1.82	0.43
1:B:975:PHE:HB3	1:B:978:TYR:HD2	1.83	0.42
1:B:1148:LEU:HD23	4:B:2605:P5S:H41A	2.00	0.42
1:A:1005:ALA:CB	1:A:1217:LEU:HD13	2.49	0.42
1:C:978:TYR:HA	1:C:1097:ILE:HD13	2.01	0.42
1:C:2188:ARG:HH11	1:C:2194:PRO:HD3	1.83	0.42
1:B:1554:PHE:O	1:B:1558:ILE:HG12	2.19	0.42
1:B:1710:ILE:O	1:B:1713:VAL:HG12	2.19	0.42
1:B:2104:THR:HG21	1:B:2490:PHE:HB3	2.02	0.42
1:B:2369:ASP:OD1	1:B:2369:ASP:N	2.51	0.42
1:A:1388:ILE:HG21	1:A:1394:ALA:HA	2.01	0.42
1:A:2426:PRO:O	1:A:2430:SER:OG	2.29	0.42
1:B:2182:HIS:HB2	1:B:2201:TYR:CD2	2.53	0.42
1:B:2215:MET:HE1	1:B:2406:PHE:HA	2.01	0.42
1:A:1319:ARG:O	1:A:1323:ILE:HG13	2.19	0.42
1:C:982:ILE:HG23	1:C:983:GLU:OE1	2.19	0.42
1:B:2013:ILE:CD1	2:B:2603:PLX:H342	2.49	0.42
1:B:2256:ASP:OD2	1:C:2247:PRO:HA	2.20	0.42
1:A:2293:ASP:OD1	1:A:2294:GLU:N	2.49	0.42
1:C:1027:GLN:HE22	1:C:1092:ASN:CG	2.28	0.42
1:C:1296:ARG:HA	1:C:1296:ARG:HD2	1.85	0.42
1:C:2018:TRP:CD1	1:C:2018:TRP:C	2.98	0.42
1:B:1037:GLN:CG	1:B:1068:MET:HE1	2.49	0.42
1:A:1027:GLN:HE22	1:A:1092:ASN:CG	2.28	0.42
1:A:1305:HIS:CD2	1:A:1305:HIS:H	2.37	0.42
1:A:1951:PHE:CE1	1:A:1952:THR:HG23	2.55	0.42
1:A:2099:VAL:HG21	1:C:2150:GLY:HA3	2.00	0.42
1:A:2207:ILE:HG23	1:A:2211:MET:HB3	2.02	0.42
2:A:2603:PLX:H233	2:A:2603:PLX:H382	2.01	0.42
1:C:916:THR:HA	1:C:919:ILE:HD12	2.01	0.42
1:C:1181:ILE:O	1:C:1185:ILE:HG13	2.19	0.42
1:C:2260:LEU:O	1:C:2264:LEU:HG	2.19	0.42
1:B:996:ARG:NH1	1:B:1084:ASP:OD2	2.52	0.42
1:B:2196:TYR:CE2	1:B:2246:SER:HA	2.54	0.42
1:A:979:LYS:HD3	1:A:979:LYS:HA	1.91	0.42
1:A:1230:MET:HE3	1:A:1230:MET:HB3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2272:ALA:N	1:A:2299:LEU:HD11	2.35	0.42
1:C:1122:ILE:CD1	4:C:2606:P5S:N	2.79	0.42
1:C:1388:ILE:HG21	1:C:1394:ALA:HA	2.00	0.42
1:C:2181:PHE:HD1	1:C:2280:ARG:HA	1.85	0.42
1:B:984:ILE:HD13	1:B:984:ILE:HA	1.89	0.42
1:B:1302:TYR:N	1:B:1302:TYR:CD1	2.86	0.42
1:B:2377:MET:HE1	1:B:2386:LEU:HD23	2.00	0.42
1:A:980:PHE:HE1	4:A:2607:P5S:O15	1.97	0.42
1:A:1158:TRP:CH2	1:A:1190:GLY:HA2	2.53	0.42
1:A:1990:VAL:HG13	1:A:2096:LEU:HD11	2.00	0.42
1:C:1710:ILE:O	1:C:1713:VAL:HG12	2.20	0.42
1:C:2210:GLU:O	1:C:2213:SER:OG	2.34	0.42
2:C:2603:PLX:H142	2:C:2603:PLX:H111	1.84	0.42
1:B:963:LYS:HD2	1:B:964:ASP:HB2	2.01	0.42
1:B:2099:VAL:HG21	1:A:2150:GLY:HA3	2.01	0.42
1:A:977:PHE:CE2	1:A:1093:ARG:HB3	2.55	0.42
1:A:1061:GLU:O	1:A:1065:ARG:NH2	2.52	0.42
1:A:1179:TYR:OH	1:A:1212:ASN:ND2	2.31	0.42
1:A:1710:ILE:O	1:A:1713:VAL:HG12	2.19	0.42
1:A:1997:LEU:HD23	1:A:1997:LEU:HA	1.86	0.42
1:C:1007:TRP:O	1:C:1010:VAL:HG12	2.20	0.42
1:C:1554:PHE:O	1:C:1558:ILE:HG12	2.20	0.42
1:C:2263:ASP:HB2	1:C:2268:HIS:HB2	2.01	0.42
1:B:983:GLU:HG3	1:B:1292:ILE:HG13	2.01	0.42
1:B:1984:VAL:O	1:B:1988:LEU:HG	2.20	0.42
1:B:2113:MET:HE3	1:B:2481:ILE:HG21	2.02	0.42
1:B:2188:ARG:HA	1:B:2194:PRO:HA	2.01	0.42
1:B:2366:LYS:HB2	1:B:2366:LYS:HE2	1.78	0.42
1:B:2373:LEU:HD12	1:B:2391:ARG:O	2.20	0.42
1:A:1774:TYR:HD1	2:A:2604:PLX:H191	1.85	0.42
1:C:1059:PHE:HB3	1:C:1228:LEU:HD22	2.02	0.42
1:C:1061:GLU:O	1:C:1065:ARG:NH2	2.52	0.42
1:C:1335:ARG:HG3	1:C:1928:LEU:HD13	2.02	0.42
1:C:1986:PHE:CE1	3:C:2605:PEE:H60	2.55	0.42
1:B:1552:TYR:CZ	1:B:1556:ASN:ND2	2.87	0.42
2:B:2602:PLX:H142	2:B:2602:PLX:H111	1.83	0.42
1:A:2119:ASN:O	1:A:2123:ILE:HG13	2.20	0.42
1:A:2188:ARG:HA	1:A:2194:PRO:HA	2.02	0.42
2:A:2603:PLX:H261	1:C:2147:LEU:HD21	2.02	0.42
1:C:813:ILE:HG12	1:C:928:ALA:HA	2.02	0.42
1:C:2251:ASN:OD1	1:C:2251:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:TYR:HA	1:B:1097:ILE:HD13	2.01	0.41
1:A:979:LYS:O	1:A:1296:ARG:NH1	2.52	0.41
1:A:1059:PHE:HB3	1:A:1228:LEU:HD22	2.02	0.41
1:C:1305:HIS:CD2	1:C:1305:HIS:H	2.36	0.41
1:C:1738:VAL:HG13	1:C:2038:ILE:HD12	2.02	0.41
1:B:813:ILE:HG12	1:B:928:ALA:HA	2.02	0.41
1:B:2158:VAL:HA	1:B:2161:ILE:HG22	2.01	0.41
1:A:923:ILE:HD13	1:A:923:ILE:HA	1.94	0.41
1:A:2162:TRP:CD1	1:A:2162:TRP:N	2.88	0.41
1:A:2263:ASP:HB2	1:A:2268:HIS:HB2	2.01	0.41
1:A:2377:MET:HG3	1:A:2388:TRP:CZ2	2.55	0.41
1:A:2393:TYR:CE2	1:A:2396:ASP:HB2	2.55	0.41
1:A:2403:LEU:HD13	1:A:2406:PHE:CE2	2.56	0.41
3:A:2606:PEE:H66	3:A:2606:PEE:H60	1.86	0.41
1:C:1754:LEU:CB	2:C:2604:PLX:H281	2.50	0.41
1:B:1788:LYS:O	1:B:1791:TRP:N	2.54	0.41
1:B:2044:LYS:C	1:B:2048:MET:HE2	2.45	0.41
1:A:2403:LEU:HD13	1:A:2406:PHE:CD2	2.55	0.41
1:C:1928:LEU:HD23	1:C:1928:LEU:HA	1.88	0.41
1:C:1987:LEU:HD12	2:C:2602:PLX:H172	2.03	0.41
1:C:2119:ASN:O	1:C:2123:ILE:HG13	2.20	0.41
1:C:2192:TYR:HD2	1:C:2256:ASP:CB	2.34	0.41
1:C:2229:ILE:HD11	1:C:2363:LEU:HD21	2.03	0.41
1:B:979:LYS:O	1:B:1296:ARG:NH1	2.53	0.41
1:B:1148:LEU:CD2	4:B:2605:P5S:H41A	2.51	0.41
1:B:1213:VAL:HA	1:B:1216:ILE:HG22	2.02	0.41
1:B:2036:PRO:HB2	1:B:2037:PRO:HD3	2.03	0.41
1:B:2377:MET:CE	1:B:2386:LEU:HD23	2.50	0.41
1:A:2281:LYS:HA	1:A:2281:LYS:HD2	1.86	0.41
1:C:1746:LEU:CD1	1:C:2016:HIS:HD2	2.33	0.41
1:B:2263:ASP:HB2	1:B:2268:HIS:HB2	2.02	0.41
1:B:2273:ARG:HD3	1:B:2273:ARG:HA	1.93	0.41
1:A:1350:MET:HE3	1:A:1350:MET:HB3	1.91	0.41
2:A:2601:PLX:H321	2:A:2601:PLX:H171	2.03	0.41
1:C:1243:MET:HE3	1:C:1243:MET:HB3	1.91	0.41
1:C:1993:ARG:NE	3:C:2605:PEE:O5	2.53	0.41
1:C:2202:ASP:OD1	1:C:2202:ASP:N	2.51	0.41
1:B:923:ILE:HD13	1:B:923:ILE:HA	1.94	0.41
1:B:2067:PHE:HB3	3:B:2604:PEE:H2	2.02	0.41
1:A:1360:MET:HE2	1:A:1360:MET:HB3	1.84	0.41
1:A:2182:HIS:HB2	1:A:2201:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2185:LEU:HD23	1:C:2186:SER:N	2.34	0.41
1:C:2369:ASP:OD1	1:C:2369:ASP:N	2.54	0.41
1:B:2181:PHE:HD1	1:B:2280:ARG:HA	1.85	0.41
1:A:1554:PHE:O	1:A:1558:ILE:HG12	2.19	0.41
1:A:1751:MET:HE2	1:A:1751:MET:HB2	1.89	0.41
1:A:2097:ASP:O	1:A:2101:ILE:HB	2.20	0.41
1:C:2097:ASP:O	1:C:2101:ILE:HB	2.21	0.41
1:C:2273:ARG:HD3	1:C:2273:ARG:HA	1.92	0.41
1:B:1997:LEU:HD23	1:B:1997:LEU:HA	1.87	0.41
1:A:1063:ILE:CG2	1:A:1069:LEU:HD12	2.47	0.41
1:A:1064:GLN:HG3	1:A:1065:ARG:HD3	2.02	0.41
1:A:1983:LEU:HD13	1:C:2162:TRP:CH2	2.56	0.41
1:A:2086:ILE:CD1	3:A:2606:PEE:H37	2.51	0.41
1:A:2399:TYR:HE2	1:A:2411:CYS:HB2	1.86	0.41
1:A:2417:MET:SD	1:A:2417:MET:N	2.94	0.41
1:C:2211:MET:CE	1:C:2407:ALA:HA	2.46	0.41
1:B:926:MET:SD	1:B:926:MET:C	3.04	0.41
1:B:1166:LEU:HD23	1:B:1166:LEU:HA	1.82	0.41
1:B:1942:VAL:HG11	2:B:2601:PLX:H201	2.02	0.41
1:B:2212:TYR:CD2	1:B:2234:ALA:HA	2.56	0.41
1:B:2215:MET:SD	1:B:2406:PHE:HA	2.61	0.41
1:B:2307:ALA:HA	1:B:2310:ILE:HD12	2.03	0.41
1:B:2417:MET:SD	1:B:2417:MET:N	2.93	0.41
1:A:818:TYR:CZ	1:A:840:CYS:HB3	2.55	0.41
1:A:984:ILE:HD13	1:A:984:ILE:HA	1.88	0.41
1:A:1223:GLN:NE2	1:A:1249:THR:OG1	2.45	0.41
1:A:2080:PHE:O	1:A:2084:MET:HG2	2.20	0.41
1:A:2260:LEU:O	1:A:2264:LEU:HG	2.19	0.41
1:C:801:PHE:HA	1:C:804:VAL:HG12	2.03	0.41
1:C:957:ILE:HG12	1:C:958:ARG:H	1.85	0.41
1:C:1003:VAL:O	1:C:1006:LEU:HG	2.21	0.41
1:C:1064:GLN:HG3	1:C:1065:ARG:HD3	2.02	0.41
1:C:1155:GLY:HA2	1:C:1158:TRP:HD1	1.86	0.41
1:C:1781:ILE:HD13	1:C:1781:ILE:HA	1.87	0.41
1:C:2136:MET:HB3	1:C:2139:GLN:HE22	1.85	0.41
1:C:2188:ARG:HA	1:C:2194:PRO:HA	2.02	0.41
1:B:1023:TRP:HB3	1:B:1095:LYS:HE2	2.03	0.41
1:B:1078:VAL:O	1:B:1082:ILE:HG23	2.21	0.41
1:B:2150:GLY:HA3	1:C:2099:VAL:HG21	2.01	0.41
1:A:916:THR:HA	1:A:919:ILE:HD12	2.02	0.41
1:A:1078:VAL:O	1:A:1082:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2241:ARG:HG2	1:A:2416:VAL:CG1	2.51	0.41
1:C:1173:ASP:OD2	1:C:1245:GLY:HA3	2.21	0.41
1:C:2272:ALA:CB	1:C:2299:LEU:HD11	2.50	0.41
1:B:1007:TRP:O	1:B:1010:VAL:HG12	2.20	0.40
1:B:1322:ASP:O	1:B:1325:GLU:HG3	2.21	0.40
1:A:2212:TYR:CD2	1:A:2234:ALA:HA	2.57	0.40
1:A:2439:GLY:HA2	1:A:2442:THR:HG22	2.02	0.40
1:C:1712:GLU:O	1:C:1715:ILE:HG22	2.20	0.40
1:C:2307:ALA:HA	1:C:2310:ILE:HD12	2.03	0.40
1:C:2308:ALA:O	1:C:2311:HIS:N	2.54	0.40
1:C:2439:GLY:HA2	1:C:2442:THR:HG22	2.02	0.40
1:B:1350:MET:HE2	1:B:1350:MET:HB2	1.89	0.40
1:A:801:PHE:HA	1:A:804:VAL:HG12	2.03	0.40
1:A:1023:TRP:HB3	1:A:1095:LYS:HE2	2.04	0.40
1:A:1179:TYR:HD1	1:A:1211:PHE:CE2	2.39	0.40
1:A:1216:ILE:CG1	1:A:1284:ASP:HB3	2.51	0.40
1:C:979:LYS:O	1:C:1296:ARG:NH1	2.53	0.40
1:C:1078:VAL:O	1:C:1082:ILE:HG23	2.21	0.40
1:B:916:THR:HA	1:B:919:ILE:HD12	2.02	0.40
1:B:2260:LEU:HA	1:B:2263:ASP:OD2	2.22	0.40
1:B:2393:TYR:CE2	1:B:2396:ASP:HB2	2.56	0.40
1:A:1322:ASP:O	1:A:1325:GLU:HG3	2.20	0.40
1:A:2018:TRP:CD1	1:A:2018:TRP:C	2.99	0.40
1:C:1945:PHE:HZ	3:C:2605:PEE:H44	1.87	0.40
1:C:2122:LEU:HD12	1:C:2122:LEU:HA	1.82	0.40
1:C:2377:MET:HG3	1:C:2388:TRP:CE2	2.57	0.40
1:B:1302:TYR:N	1:B:1302:TYR:HD1	2.18	0.40
1:B:2352:LEU:HB2	1:B:2356:ASP:OD1	2.21	0.40
1:A:1335:ARG:HG3	1:A:1928:LEU:HD13	2.04	0.40
1:A:1746:LEU:CD1	1:A:2016:HIS:HD2	2.33	0.40
1:C:1552:TYR:CZ	1:C:1556:ASN:ND2	2.84	0.40
1:C:2349:ILE:HD12	1:C:2358:ALA:O	2.21	0.40
1:A:995:TYR:CE2	1:A:1079:PRO:HB2	2.57	0.40
1:A:999:ILE:O	1:A:1003:VAL:HG23	2.22	0.40
1:A:1825:LEU:HD23	1:A:1825:LEU:HA	1.91	0.40
1:C:1300:SER:HA	4:C:2606:P5S:HNA	1.87	0.40
1:C:1322:ASP:O	1:C:1325:GLU:HG3	2.21	0.40
1:C:1736:ASN:ND2	1:C:1820:ASP:OD1	2.52	0.40
1:C:2228:PHE:C	1:C:2228:PHE:CD1	2.99	0.40
3:C:2605:PEE:H60	3:C:2605:PEE:H66	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1277/2551 (50%)	1240 (97%)	36 (3%)	1 (0%)	48	81
1	B	1277/2551 (50%)	1239 (97%)	37 (3%)	1 (0%)	48	81
1	C	1277/2551 (50%)	1236 (97%)	40 (3%)	1 (0%)	48	81
All	All	3831/7653 (50%)	3715 (97%)	113 (3%)	3 (0%)	49	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1929	ALA
1	A	1929	ALA
1	C	1929	ALA

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	1091/2268 (48%)	1071 (98%)	20 (2%)	51	67
1	B	1091/2268 (48%)	1079 (99%)	12 (1%)	65	74
1	C	1091/2268 (48%)	1074 (98%)	17 (2%)	55	69
All	All	3273/6804 (48%)	3224 (98%)	49 (2%)	55	70

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1220	THR
1	B	1406	MET
1	B	1541	LEU
1	B	1746	LEU
1	B	2018	TRP
1	B	2030	THR
1	B	2270	LEU
1	B	2345	ILE
1	B	2411	CYS
1	B	2415	ILE
1	B	2438	ILE
1	B	2443	THR
1	A	1068	MET
1	A	1144	TYR
1	A	1209	LEU
1	A	1217	LEU
1	A	1302	TYR
1	A	1305	HIS
1	A	1416	HIS
1	A	1541	LEU
1	A	1718	TRP
1	A	1983	LEU
1	A	2105	MET
1	A	2155	LEU
1	A	2183	VAL
1	A	2242	LEU
1	A	2341	ILE
1	A	2345	ILE
1	A	2373	LEU
1	A	2403	LEU
1	A	2438	ILE
1	A	2443	THR
1	C	1014	LEU
1	C	1195	LEU
1	C	1246	ILE
1	C	1302	TYR
1	C	1305	HIS
1	C	1402	MET
1	C	1541	LEU
1	C	1983	LEU
1	C	2018	TRP
1	C	2032	ASN
1	C	2197	THR

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Mol	Chain	Res	Type
1	C	2240	VAL
1	C	2309	LEU
1	C	2312	MET
1	C	2345	ILE
1	C	2373	LEU
1	C	2443	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1027	GLN
1	B	1150	ASN
1	B	1189	GLN
1	B	1301	HIS
1	B	1341	GLN
1	B	1696	ASN
1	B	1701	ASN
1	B	1837	GLN
1	B	1957	GLN
1	B	1958	GLN
1	B	2199	ASN
1	B	2295	HIS
1	A	1027	GLN
1	A	1092	ASN
1	A	1094	GLN
1	A	1189	GLN
1	A	1301	HIS
1	A	1341	GLN
1	A	1357	GLN
1	A	1696	ASN
1	A	1701	ASN
1	A	1837	GLN
1	A	2295	HIS
1	C	1027	GLN
1	C	1092	ASN
1	C	1189	GLN
1	C	1199	HIS
1	C	1301	HIS
1	C	1341	GLN
1	C	1701	ASN
1	C	1837	GLN
1	C	1958	GLN

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Mol	Chain	Res	Type
1	C	2295	HIS
1	C	2476	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLX	A	2601	-	51,51,51	0.32	0	55,59,59	0.49	1 (1%)
2	PLX	C	2604	-	51,51,51	0.36	0	55,59,59	0.58	2 (3%)
3	PEE	B	2604	-	50,50,50	0.35	0	53,55,55	0.40	0
2	PLX	C	2602	-	51,51,51	0.34	0	55,59,59	0.58	1 (1%)
3	PEE	C	2605	-	50,50,50	0.42	0	53,55,55	0.66	2 (3%)
4	P5S	C	2606	-	52,53,53	0.48	1 (1%)	56,60,60	0.44	0
4	P5S	B	2605	-	52,53,53	0.45	1 (1%)	56,60,60	0.42	0
3	PEE	A	2606	-	50,50,50	0.41	0	53,55,55	0.88	2 (3%)
2	PLX	A	2604	-	51,51,51	0.36	0	55,59,59	0.42	0
2	PLX	A	2605	-	51,51,51	0.35	0	55,59,59	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	P5S	A	2607	-	52,53,53	0.53	1 (1%)	56,60,60	0.47	0
2	PLX	B	2601	-	51,51,51	0.31	0	55,59,59	0.50	1 (1%)
2	PLX	A	2602	-	51,51,51	0.31	0	55,59,59	0.40	0
2	PLX	C	2601	-	51,51,51	0.30	0	55,59,59	0.41	0
2	PLX	C	2603	-	51,51,51	0.36	0	55,59,59	0.42	0
2	PLX	B	2603	-	51,51,51	0.38	0	55,59,59	0.61	1 (1%)
2	PLX	A	2603	-	51,51,51	0.34	0	55,59,59	0.49	0
2	PLX	B	2602	-	51,51,51	0.36	0	55,59,59	0.40	0

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	A	2601	-	-	13/55/55/55	-
2	PLX	C	2604	-	-	8/55/55/55	-
3	PEE	B	2604	-	-	16/54/54/54	-
2	PLX	C	2602	-	-	13/55/55/55	-
3	PEE	C	2605	-	-	18/54/54/54	-
4	P5S	C	2606	-	-	22/59/59/59	-
4	P5S	B	2605	-	-	26/59/59/59	-
3	PEE	A	2606	-	-	20/54/54/54	-
2	PLX	A	2604	-	-	20/55/55/55	-
2	PLX	A	2605	-	-	10/55/55/55	-
4	P5S	A	2607	-	-	25/59/59/59	-
2	PLX	B	2601	-	-	15/55/55/55	-
2	PLX	A	2602	-	-	13/55/55/55	-
2	PLX	C	2601	-	-	10/55/55/55	-
2	PLX	C	2603	-	-	17/55/55/55	-
2	PLX	B	2603	-	-	5/55/55/55	-
2	PLX	A	2603	-	-	11/55/55/55	-
2	PLX	B	2602	-	-	22/55/55/55	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2607	P5S	OXT-C	-2.79	1.21	1.30
4	B	2605	P5S	OXT-C	-2.32	1.22	1.30
4	C	2606	P5S	OXT-C	-2.09	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2606	PEE	O2-C10-C11	4.55	121.30	111.50
2	B	2603	PLX	O8-C5-C4	-3.24	103.09	110.90
2	C	2602	PLX	C6-O6-C4	-3.11	108.99	115.20
3	C	2605	PEE	O2-C10-C11	3.11	118.20	111.50
3	A	2606	PEE	O2-C10-O4	-3.07	116.29	123.70
2	C	2604	PLX	O8-C5-C4	-2.23	105.52	110.90
2	A	2601	PLX	C26-C25-C24	-2.09	108.54	113.38
3	C	2605	PEE	O2-C10-O4	-2.07	118.71	123.70
2	B	2601	PLX	C26-C25-C24	-2.02	108.70	113.38
2	C	2604	PLX	C26-C25-C24	-2.00	108.76	113.38

There are no chirality outliers.

All (284) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2601	PLX	O7-C6-C7-C8
2	B	2601	PLX	O7-C6-O6-C4
2	B	2601	PLX	C2-O1-P1-O2
2	B	2602	PLX	C5-C4-O6-C6
2	B	2602	PLX	C3-O4-P1-O3
2	A	2601	PLX	C3-O4-P1-O1
2	A	2602	PLX	O7-C6-O6-C4
2	A	2602	PLX	C2-O1-P1-O2
2	A	2604	PLX	O9-C24-O8-C5
2	A	2605	PLX	C3-O4-P1-O2
2	C	2601	PLX	O7-C6-O6-C4
2	C	2601	PLX	C2-O1-P1-O2
2	C	2602	PLX	C3-O4-P1-O1
2	C	2602	PLX	C3-O4-P1-O2
2	C	2602	PLX	C2-O1-P1-O2
2	C	2604	PLX	C3-O4-P1-O2
3	B	2604	PEE	C4-O4P-P-O1P
3	A	2606	PEE	C1-O3P-P-O1P
3	A	2606	PEE	C1-O3P-P-O4P
3	A	2606	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
3	A	2606	PEE	O4P-C4-C5-N
3	C	2605	PEE	C4-O4P-P-O1P
3	C	2605	PEE	O4P-C4-C5-N
4	B	2605	P5S	C2-C3-O16-P12
4	B	2605	P5S	N-CA-CB-OG
4	B	2605	P5S	CB-OG-P12-O13
4	B	2605	P5S	C3-O16-P12-O13
4	A	2607	P5S	O-C-CA-CB
4	A	2607	P5S	N-CA-CB-OG
4	A	2607	P5S	C39-C38-O37-C2
4	C	2606	P5S	C2-C3-O16-P12
4	C	2606	P5S	CB-OG-P12-O13
4	C	2606	P5S	C3-O16-P12-OG
4	C	2606	P5S	C3-O16-P12-O13
4	C	2606	P5S	C3-O16-P12-O15
4	A	2607	P5S	O47-C38-O37-C2
3	C	2605	PEE	C31-C30-O3-C3
3	C	2605	PEE	O5-C30-O3-C3
2	A	2601	PLX	C2-C1-N1-C1A
3	A	2606	PEE	C31-C30-O3-C3
3	B	2604	PEE	C30-C31-C32-C33
3	C	2605	PEE	C30-C31-C32-C33
2	A	2605	PLX	C14-C15-C16-C17
2	A	2603	PLX	C11-C10-C9-C8
3	A	2606	PEE	O5-C30-O3-C3
2	B	2602	PLX	C11-C12-C13-C14
2	C	2603	PLX	C32-C33-C34-C35
3	A	2606	PEE	C30-C31-C32-C33
2	A	2601	PLX	C2-C1-N1-C1C
2	A	2604	PLX	C2-C1-N1-C1A
4	A	2607	P5S	C38-C39-C40-C41
4	C	2606	P5S	C46-C48-C49-C50
2	A	2603	PLX	C14-C15-C16-C17
2	B	2602	PLX	C3-O4-P1-O1
2	A	2601	PLX	C2-O1-P1-O4
2	A	2602	PLX	C2-O1-P1-O4
2	A	2603	PLX	C3-O4-P1-O1
2	C	2604	PLX	C3-O4-P1-O1
4	B	2605	P5S	C3-O16-P12-OG
2	C	2603	PLX	O6-C6-C7-C8
4	A	2607	P5S	C1-C2-O37-C38
2	A	2604	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	A	2607	P5S	C2-C3-O16-P12
2	C	2603	PLX	C14-C15-C16-C17
3	B	2604	PEE	C32-C33-C34-C35
2	C	2601	PLX	C11-C12-C13-C14
2	C	2603	PLX	C33-C34-C35-C36
2	B	2602	PLX	C15-C16-C17-C18
2	B	2602	PLX	C10-C11-C12-C13
2	C	2602	PLX	C7-C8-C9-C10
2	B	2603	PLX	C9-C10-C11-C12
4	A	2607	P5S	C20-C21-C22-C23
4	A	2607	P5S	O19-C1-C2-C3
4	C	2606	P5S	C38-C39-C40-C41
2	B	2602	PLX	O7-C6-C7-C8
2	B	2602	PLX	O9-C24-C25-C26
2	A	2602	PLX	O7-C6-C7-C8
2	A	2603	PLX	O7-C6-C7-C8
2	A	2604	PLX	O7-C6-C7-C8
2	C	2601	PLX	O7-C6-C7-C8
2	C	2603	PLX	O7-C6-C7-C8
3	B	2604	PEE	C33-C34-C35-C36
3	B	2604	PEE	C11-C12-C13-C14
2	A	2601	PLX	C2-C1-N1-C1B
2	A	2604	PLX	C2-C1-N1-C1C
2	B	2602	PLX	C30-C31-C32-C33
3	C	2605	PEE	C39-C40-C41-C42
2	B	2602	PLX	C32-C33-C34-C35
2	A	2604	PLX	C25-C26-C27-C28
2	B	2602	PLX	C14-C15-C16-C17
4	C	2606	P5S	C2-C1-O19-C17
2	C	2603	PLX	C10-C11-C12-C13
4	B	2605	P5S	C-CA-CB-OG
4	A	2607	P5S	C-CA-CB-OG
2	C	2603	PLX	C11-C12-C13-C14
4	C	2606	P5S	C39-C38-O37-C2
2	A	2604	PLX	C2-C1-N1-C1B
3	A	2606	PEE	C39-C40-C41-C42
4	B	2605	P5S	O-C-CA-CB
4	A	2607	P5S	OXT-C-CA-CB
2	A	2604	PLX	C32-C33-C34-C35
4	C	2606	P5S	C17-C20-C21-C22
4	C	2606	P5S	O47-C38-O37-C2
2	A	2604	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
3	A	2606	PEE	C4-O4P-P-O3P
2	A	2604	PLX	C13-C14-C15-C16
2	C	2603	PLX	C3-C4-C5-O8
3	B	2604	PEE	C1-C2-C3-O3
4	B	2605	P5S	O19-C1-C2-C3
4	B	2605	P5S	C48-C49-C50-C51
3	B	2604	PEE	C31-C32-C33-C34
2	A	2602	PLX	C12-C13-C14-C15
3	C	2605	PEE	C14-C15-C16-C17
3	A	2606	PEE	C17-C18-C19-C20
4	B	2605	P5S	O19-C1-C2-O37
3	C	2605	PEE	O2-C10-C11-C12
4	C	2606	P5S	C39-C40-C41-C42
2	B	2601	PLX	C7-C8-C9-C10
2	A	2604	PLX	C14-C15-C16-C17
3	C	2605	PEE	O3P-C1-C2-C3
2	C	2601	PLX	C26-C27-C28-C29
4	C	2606	P5S	C20-C21-C22-C23
4	B	2605	P5S	C20-C17-O19-C1
3	C	2605	PEE	C2-C1-O3P-P
2	A	2605	PLX	C31-C32-C33-C34
2	B	2602	PLX	C3-C4-C5-O8
2	A	2604	PLX	C15-C16-C17-C18
2	B	2601	PLX	C11-C12-C13-C14
2	B	2601	PLX	C2-O1-P1-O4
2	A	2604	PLX	C5-C4-O6-C6
2	A	2605	PLX	C3-O4-P1-O1
2	C	2603	PLX	C3-O4-P1-O1
4	C	2606	P5S	CB-OG-P12-O16
4	C	2606	P5S	C40-C41-C42-C43
2	A	2604	PLX	O9-C24-C25-C26
2	A	2605	PLX	O9-C24-C25-C26
2	C	2602	PLX	C11-C12-C13-C14
2	A	2601	PLX	O4-C3-C4-O6
2	A	2603	PLX	O4-C3-C4-O6
2	C	2603	PLX	C13-C14-C15-C16
2	A	2602	PLX	C26-C27-C28-C29
3	A	2606	PEE	O2-C10-C11-C12
2	B	2601	PLX	O6-C4-C5-O8
2	B	2602	PLX	O6-C4-C5-O8
2	C	2604	PLX	C11-C12-C13-C14
2	B	2603	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	A	2603	PLX	C4-C3-O4-P1
4	A	2607	P5S	C40-C41-C42-C43
3	A	2606	PEE	C33-C34-C35-C36
2	B	2602	PLX	O6-C6-C7-C8
2	A	2604	PLX	O6-C6-C7-C8
2	A	2601	PLX	O4-C3-C4-C5
4	B	2605	P5S	C1-C2-C3-O16
4	C	2606	P5S	C20-C17-O19-C1
4	C	2606	P5S	C1-C2-O37-C38
3	B	2604	PEE	C34-C35-C36-C37
2	C	2604	PLX	C12-C13-C14-C15
2	A	2604	PLX	C3-C4-C5-O8
2	B	2601	PLX	C16-C17-C18-C19
4	A	2607	P5S	O37-C2-C3-O16
4	C	2606	P5S	O37-C2-C3-O16
4	A	2607	P5S	O19-C1-C2-O37
4	C	2606	P5S	O18-C17-O19-C1
2	C	2602	PLX	C2-C1-N1-C1A
2	C	2603	PLX	C2-C1-N1-C1A
4	A	2607	P5S	CA-CB-OG-P12
4	B	2605	P5S	O18-C17-O19-C1
4	B	2605	P5S	OXT-C-CA-CB
3	C	2605	PEE	C4-O4P-P-O3P
4	B	2605	P5S	CB-OG-P12-O16
3	A	2606	PEE	C2-C1-O3P-P
2	A	2601	PLX	C3-O4-P1-O3
2	A	2601	PLX	C2-O1-P1-O2
2	A	2602	PLX	C2-O1-P1-O3
2	A	2603	PLX	C3-O4-P1-O2
2	A	2604	PLX	C3-O4-P1-O3
2	A	2605	PLX	C3-O4-P1-O3
2	C	2602	PLX	C2-C1-N1-C1B
2	C	2603	PLX	C2-C1-N1-C1B
2	C	2604	PLX	C3-O4-P1-O3
4	B	2605	P5S	C3-O16-P12-O15
2	A	2603	PLX	O4-C3-C4-C5
2	C	2602	PLX	O4-C3-C4-C5
4	A	2607	P5S	C1-C2-C3-O16
2	B	2601	PLX	C1-C2-O1-P1
2	A	2602	PLX	C1-C2-O1-P1
2	C	2601	PLX	C1-C2-O1-P1
3	A	2606	PEE	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
2	A	2602	PLX	C16-C17-C18-C19
2	C	2602	PLX	O4-C3-C4-O6
3	C	2605	PEE	O3P-C1-C2-O2
4	B	2605	P5S	O37-C2-C3-O16
2	C	2603	PLX	C15-C16-C17-C18
3	B	2604	PEE	C36-C37-C38-C39
3	B	2604	PEE	O5-C30-O3-C3
2	B	2602	PLX	C2-C1-N1-C1A
2	B	2601	PLX	C3-C4-C5-O8
2	B	2601	PLX	N1-C1-C2-O1
2	A	2602	PLX	N1-C1-C2-O1
2	C	2601	PLX	N1-C1-C2-O1
2	C	2603	PLX	O6-C4-C5-O8
3	B	2604	PEE	O2-C2-C3-O3
4	B	2605	P5S	C21-C22-C23-C24
3	A	2606	PEE	C18-C19-C20-C21
2	B	2602	PLX	C25-C26-C27-C28
2	B	2601	PLX	O6-C6-C7-C8
2	C	2602	PLX	O9-C24-C25-C26
2	C	2603	PLX	O9-C24-C25-C26
2	C	2604	PLX	O7-C6-C7-C8
4	A	2607	P5S	C21-C22-C23-C24
4	C	2606	P5S	C1-C2-C3-O16
4	B	2605	P5S	C26-C27-C28-C29
3	B	2604	PEE	C31-C30-O3-C3
3	A	2606	PEE	C11-C10-O2-C2
2	A	2605	PLX	C27-C28-C29-C30
2	A	2603	PLX	C2-O1-P1-O4
2	C	2601	PLX	C2-O1-P1-O4
2	C	2602	PLX	C2-O1-P1-O4
3	B	2604	PEE	C4-O4P-P-O3P
3	C	2605	PEE	C1-O3P-P-O4P
4	A	2607	P5S	CB-OG-P12-O16
3	B	2604	PEE	C18-C19-C20-C21
3	A	2606	PEE	C14-C15-C16-C17
2	B	2601	PLX	C10-C11-C12-C13
2	A	2601	PLX	C16-C17-C18-C19
2	A	2602	PLX	C30-C31-C32-C33
3	C	2605	PEE	O4-C10-C11-C12
2	B	2602	PLX	C27-C28-C29-C30
2	C	2602	PLX	C2-C1-N1-C1C
2	C	2603	PLX	C2-C1-N1-C1C

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Mol	Chain	Res	Type	Atoms
3	A	2606	PEE	C16-C17-C18-C19
2	C	2604	PLX	C5-C4-O6-C6
2	B	2602	PLX	C9-C10-C11-C12
3	B	2604	PEE	C16-C17-C18-C19
2	B	2603	PLX	C29-C30-C31-C32
4	B	2605	P5S	C42-C43-C44-C45
4	A	2607	P5S	O18-C17-O19-C1
2	B	2602	PLX	C11-C10-C9-C8
2	A	2604	PLX	C9-C10-C11-C12
2	B	2601	PLX	C24-C25-C26-C27
2	A	2602	PLX	C18-C19-C20-C21
2	C	2604	PLX	C27-C28-C29-C30
4	A	2607	P5S	C20-C17-O19-C1
2	B	2602	PLX	C2-C1-N1-C1B
4	A	2607	P5S	C42-C43-C44-C45
3	C	2605	PEE	C16-C17-C18-C19
2	A	2601	PLX	C12-C13-C14-C15
2	C	2601	PLX	O4-C3-C4-C5
3	A	2606	PEE	C42-C43-C44-C45
4	B	2605	P5S	C39-C40-C41-C42
4	C	2606	P5S	C21-C22-C23-C24
2	B	2602	PLX	C2-C1-N1-C1C
2	B	2603	PLX	O7-C6-C7-C8
2	A	2601	PLX	O7-C6-C7-C8
2	A	2601	PLX	O9-C24-C25-C26
2	A	2603	PLX	O9-C24-C25-C26
2	A	2605	PLX	O7-C6-C7-C8
2	A	2604	PLX	C27-C28-C29-C30
2	C	2602	PLX	C4-C3-O4-P1
4	B	2605	P5S	O37-C38-C39-C40
2	B	2601	PLX	C17-C18-C19-C20
2	B	2602	PLX	O8-C24-C25-C26
2	A	2604	PLX	C30-C31-C32-C33
4	B	2605	P5S	C39-C38-O37-C2
2	A	2605	PLX	C24-C25-C26-C27
4	B	2605	P5S	O47-C38-O37-C2
2	A	2603	PLX	C2-O1-P1-O2
2	C	2603	PLX	C3-O4-P1-O3
3	C	2605	PEE	C1-O3P-P-O1P
4	A	2607	P5S	CB-OG-P12-O13
2	A	2602	PLX	C13-C14-C15-C16
2	B	2603	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
3	C	2605	PEE	C5-C4-O4P-P
4	B	2605	P5S	O47-C38-C39-C40
4	C	2606	P5S	O37-C38-C39-C40
4	A	2607	P5S	O37-C38-C39-C40
4	B	2605	P5S	OXT-C-CA-N
2	C	2601	PLX	O4-C3-C4-O6
3	B	2604	PEE	C13-C14-C15-C16
4	A	2607	P5S	O47-C38-C39-C40
3	A	2606	PEE	O3-C30-C31-C32
3	C	2605	PEE	O3-C30-C31-C32
2	A	2605	PLX	C12-C13-C14-C15
4	A	2607	P5S	O19-C17-C20-C21

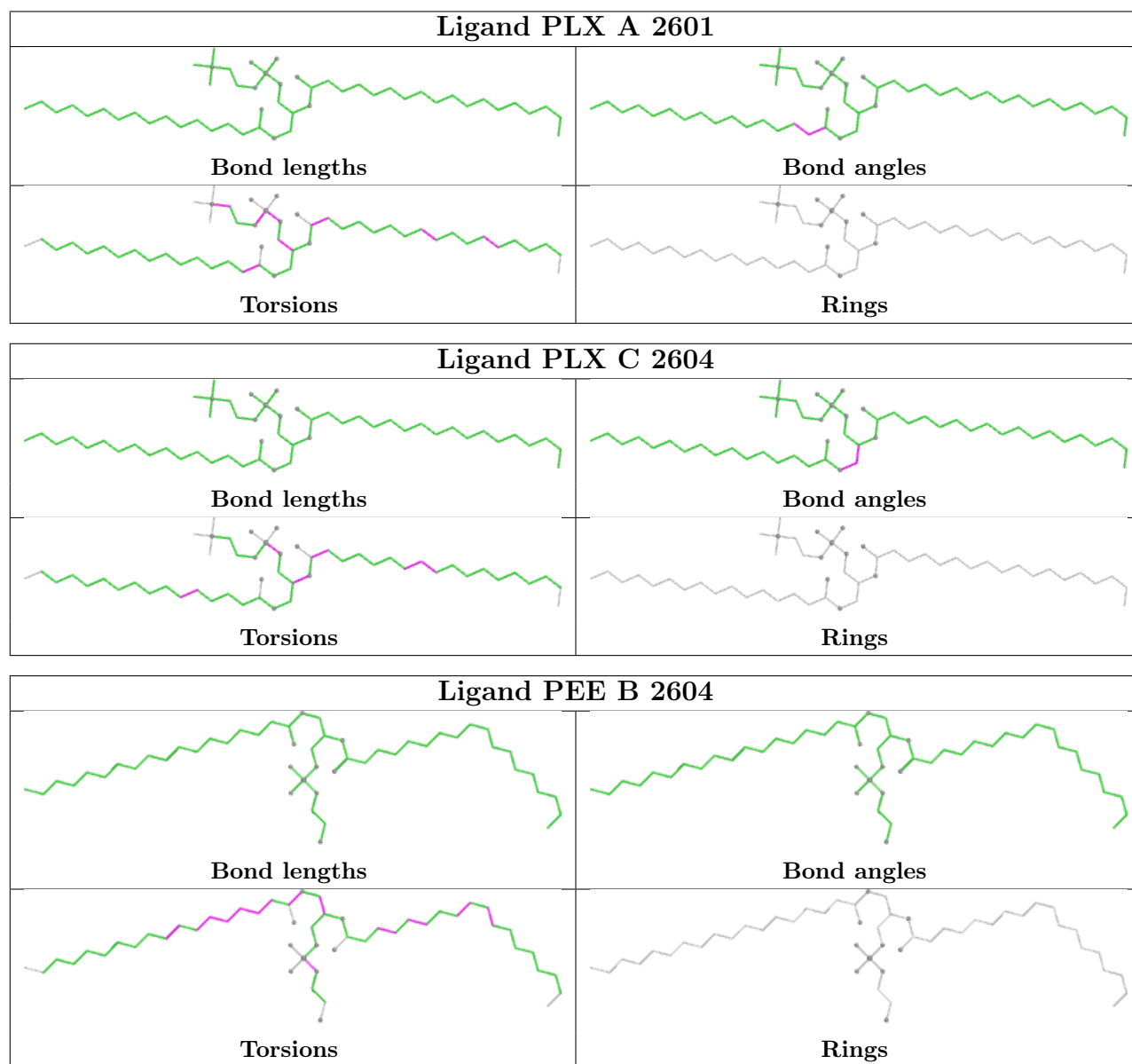
There are no ring outliers.

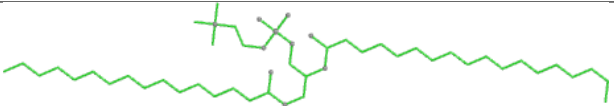
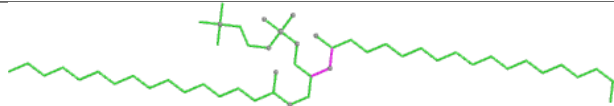
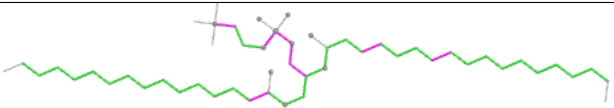
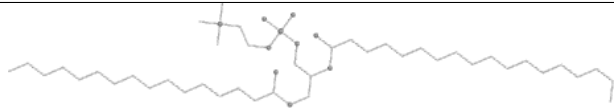
18 monomers are involved in 115 short contacts:

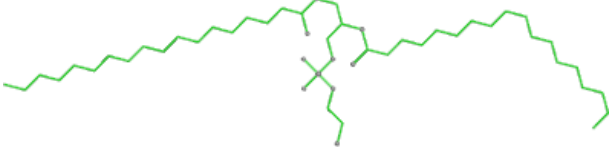
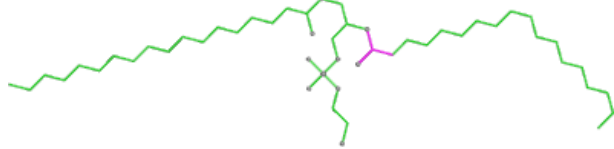
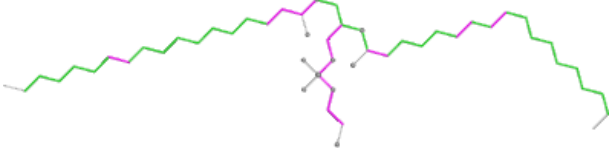
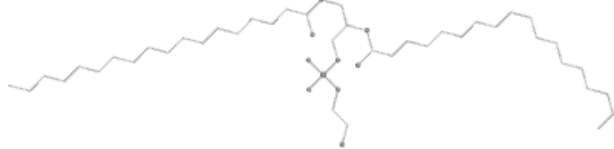
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	PLX	4	0
2	C	2604	PLX	7	0
3	B	2604	PEE	8	0
2	C	2602	PLX	5	0
3	C	2605	PEE	15	0
4	C	2606	P5S	11	0
4	B	2605	P5S	3	0
3	A	2606	PEE	12	0
2	A	2604	PLX	6	0
2	A	2605	PLX	1	0
4	A	2607	P5S	9	0
2	B	2601	PLX	4	0
2	A	2602	PLX	3	0
2	C	2601	PLX	3	0
2	C	2603	PLX	6	0
2	B	2603	PLX	2	0
2	A	2603	PLX	10	0
2	B	2602	PLX	6	0

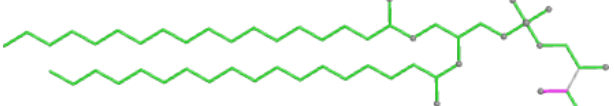
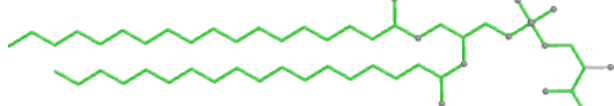
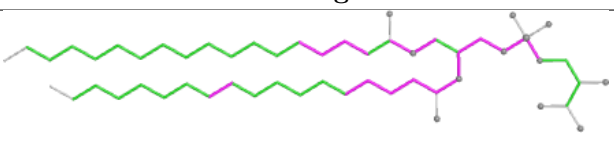
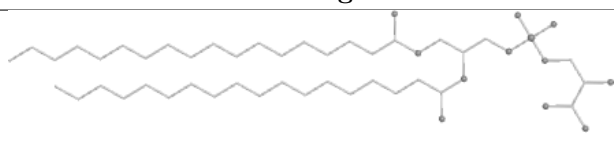
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

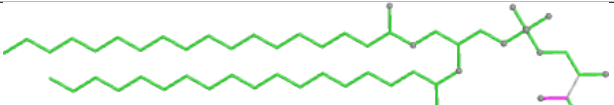
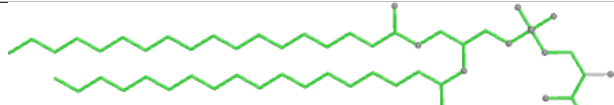
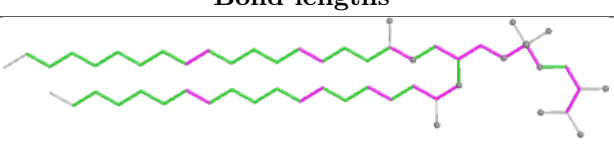
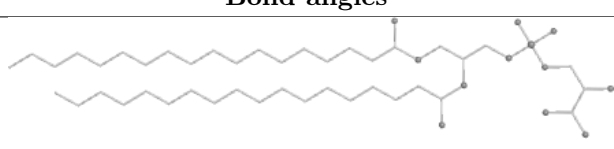
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

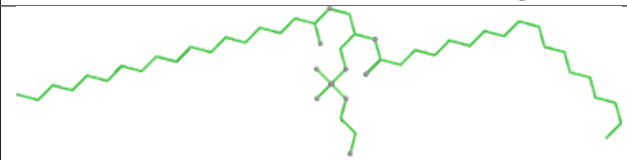
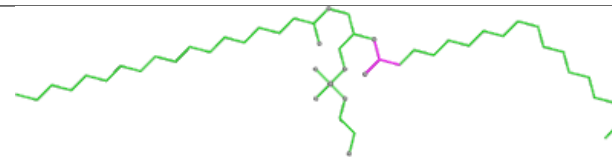
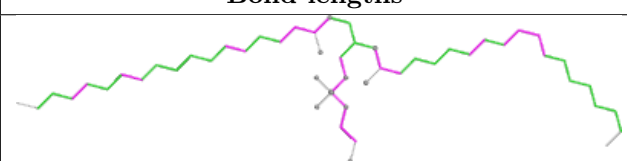
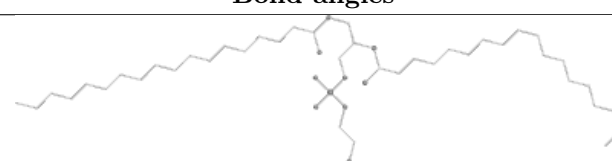


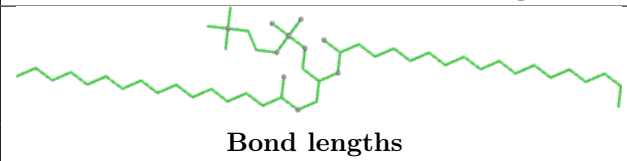
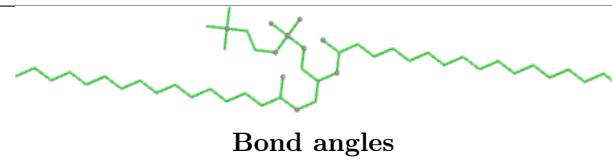
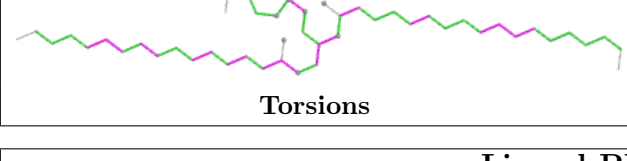

Ligand PLX C 2602	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

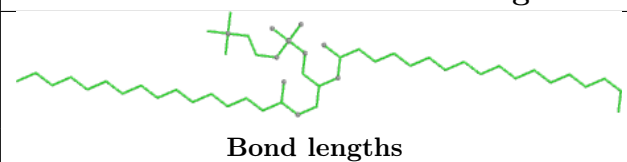
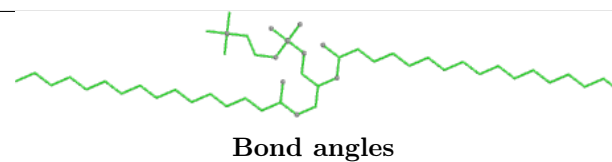
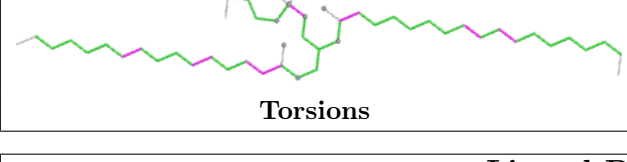

Ligand PEE C 2605	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

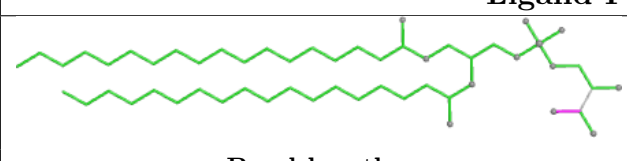
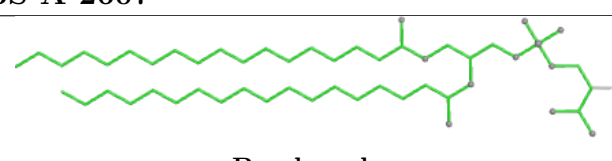
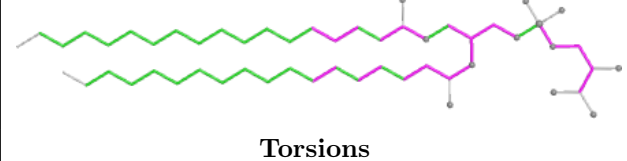
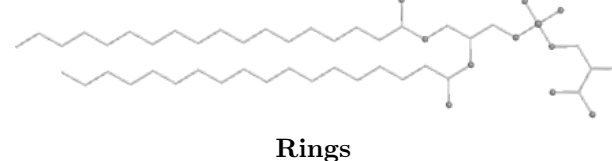
Ligand P5S C 2606	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

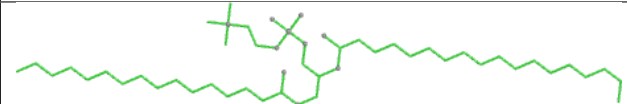
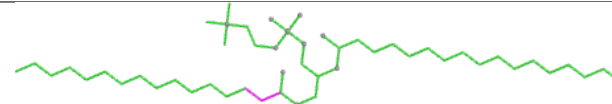
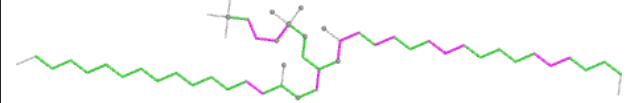
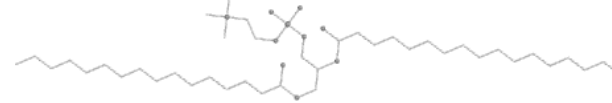
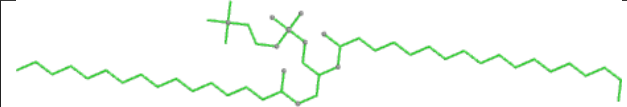
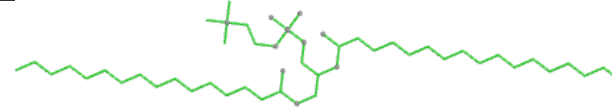
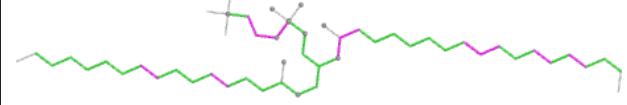
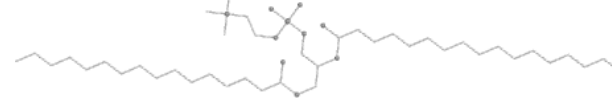
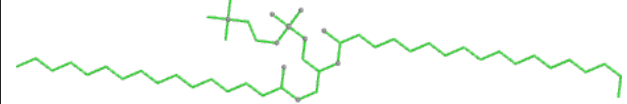
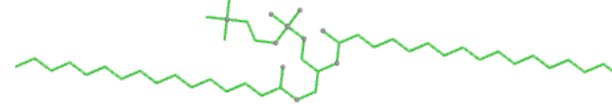
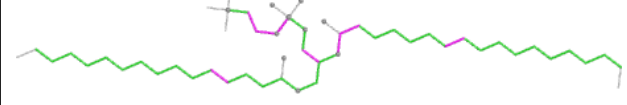
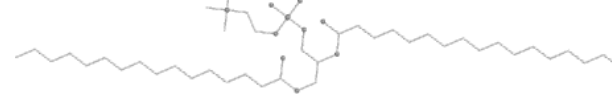
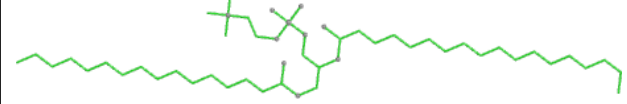
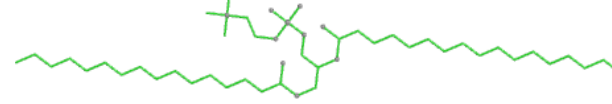
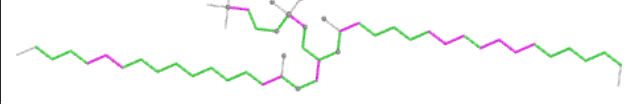
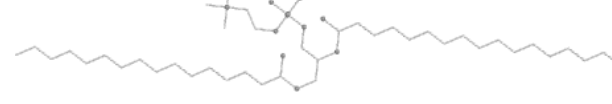
Ligand P5S B 2605	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

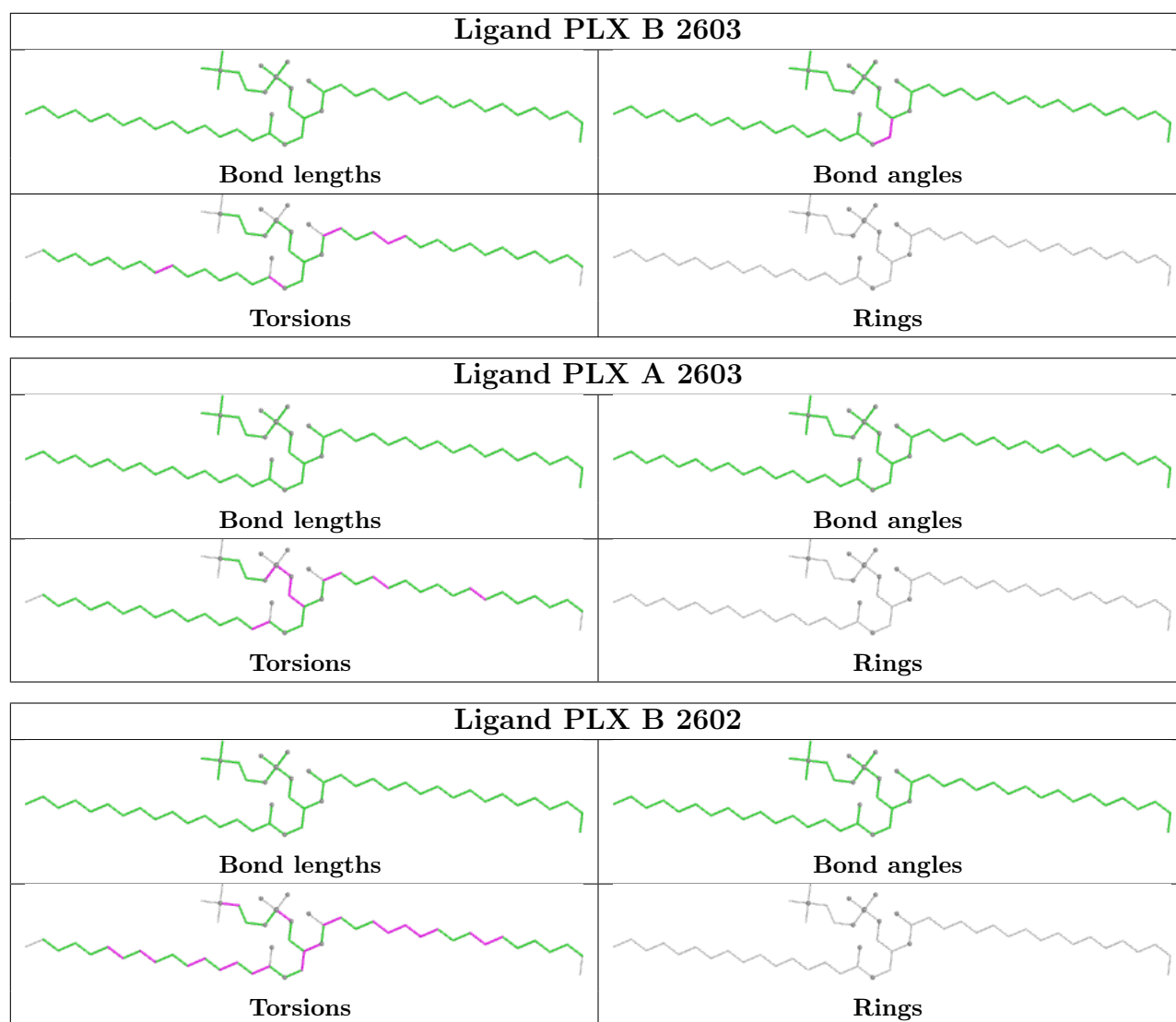
Ligand PEE A 2606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX A 2604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX A 2605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand P5S A 2607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX B 2601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX A 2602	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX C 2601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PLX C 2603	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



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.

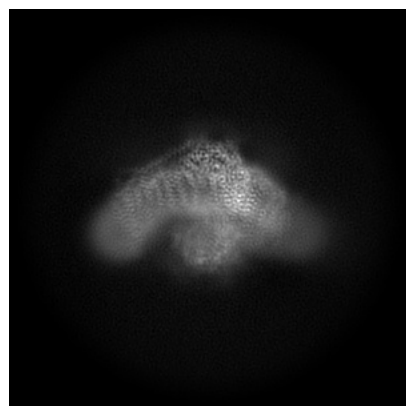
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65735. These allow visual inspection of the internal detail of the map and identification of artifacts.

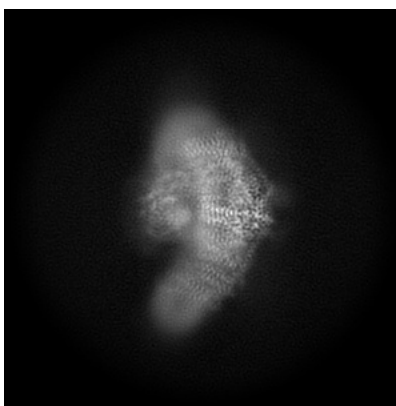
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

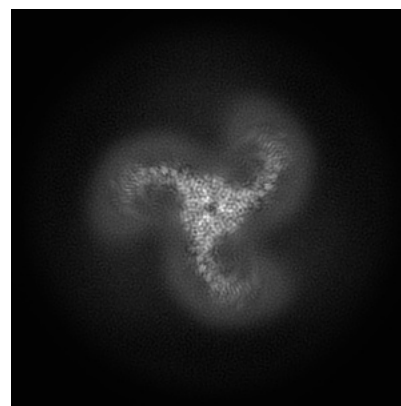
6.1.1 Primary map



X

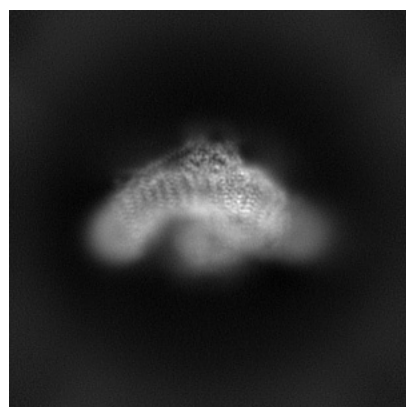


Y

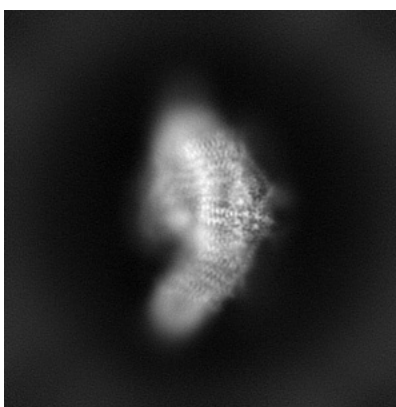


Z

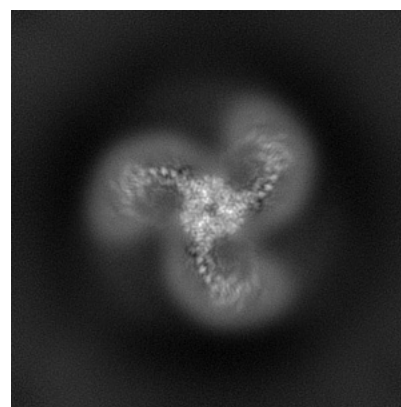
6.1.2 Raw map



X



Y

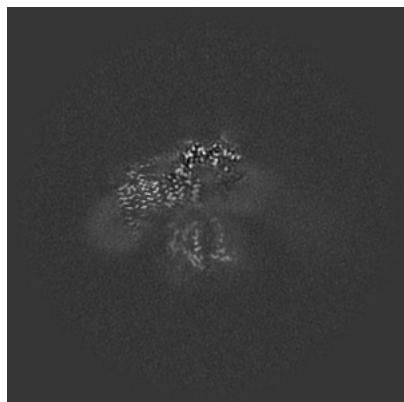


Z

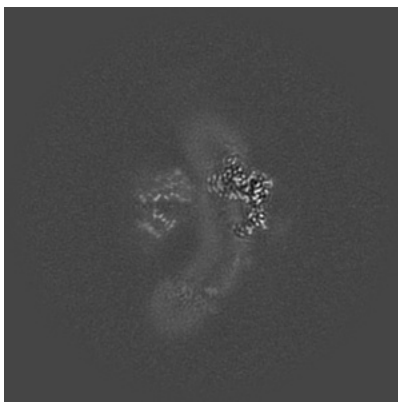
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

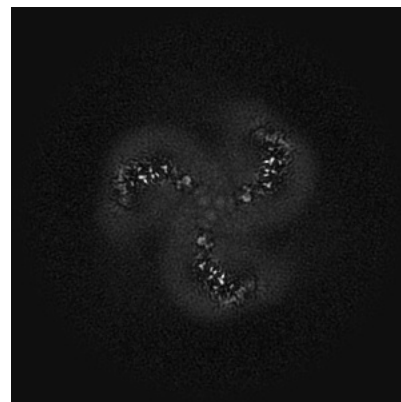
6.2.1 Primary map



X Index: 150

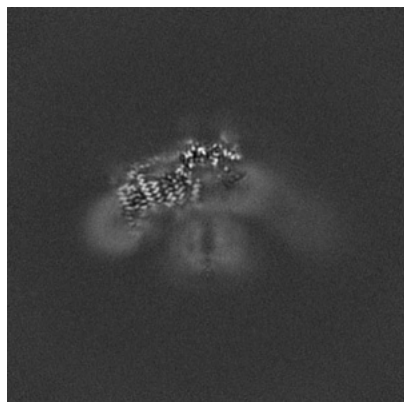


Y Index: 150

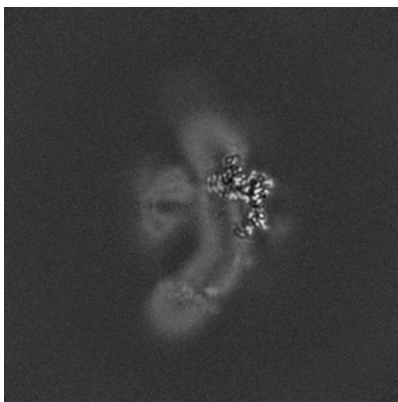


Z Index: 150

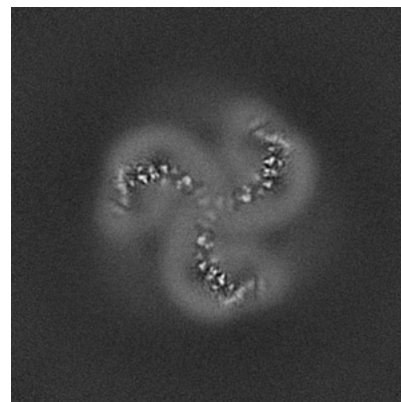
6.2.2 Raw map



X Index: 150



Y Index: 150

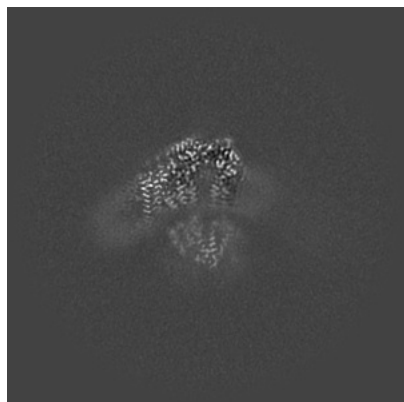


Z Index: 150

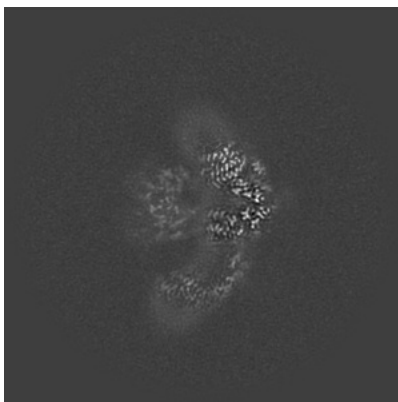
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

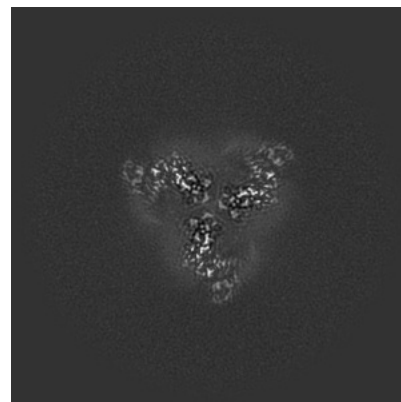
6.3.1 Primary map



X Index: 142

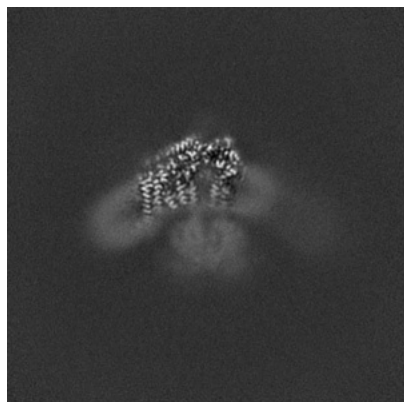


Y Index: 161

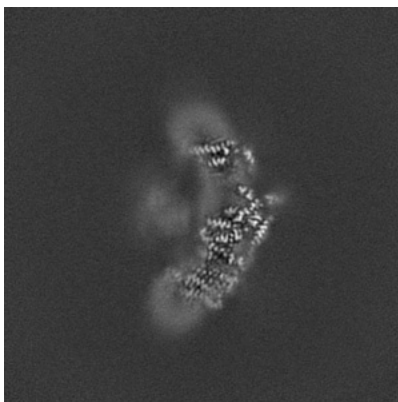


Z Index: 170

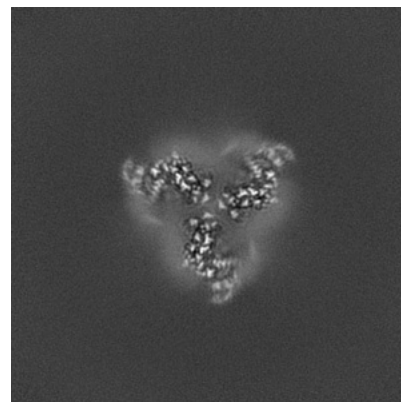
6.3.2 Raw map



X Index: 142



Y Index: 168

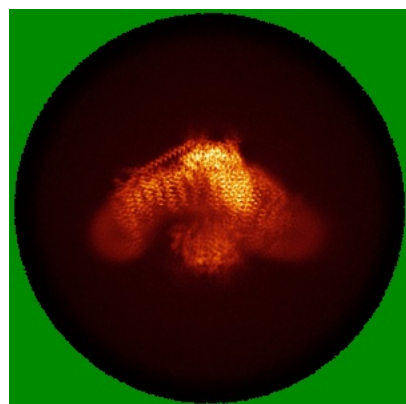


Z Index: 170

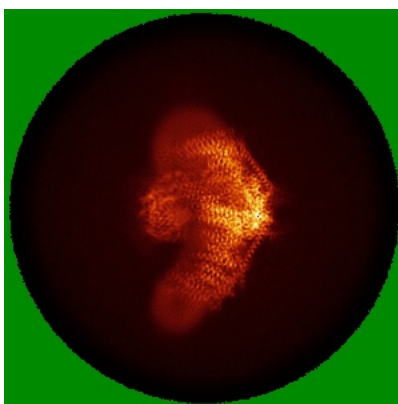
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

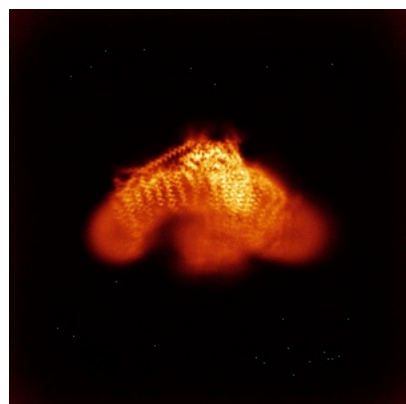


Y

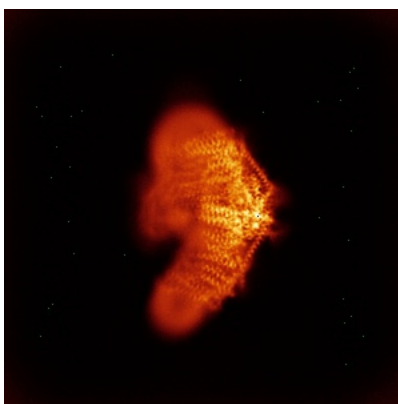


Z

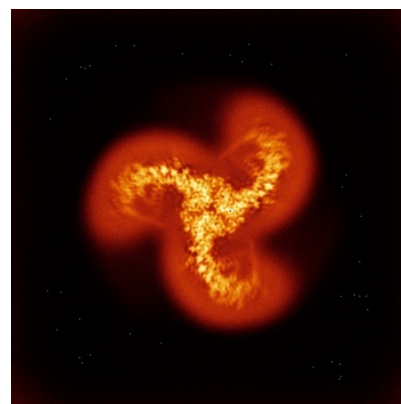
6.4.2 Raw map



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



The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

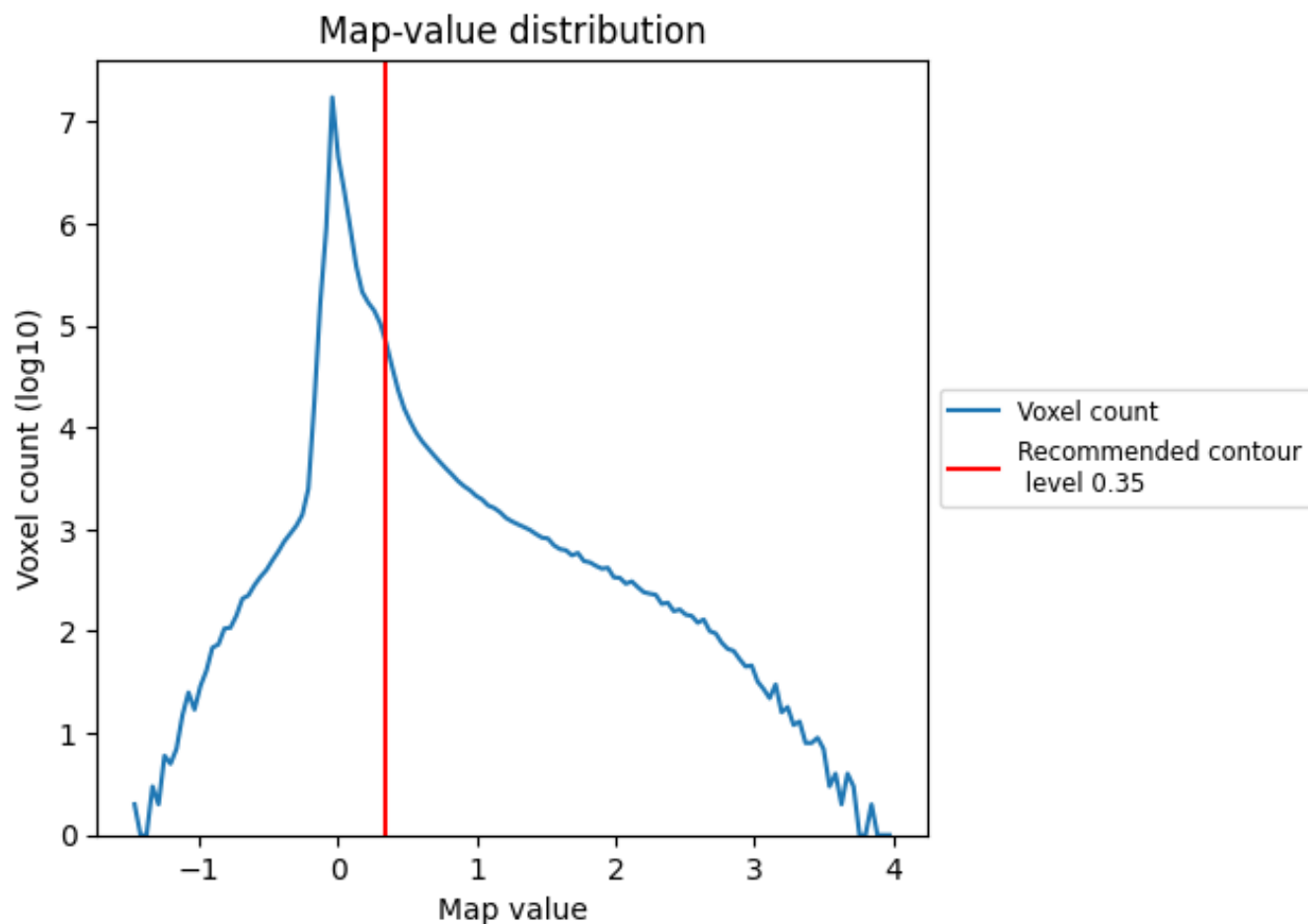
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

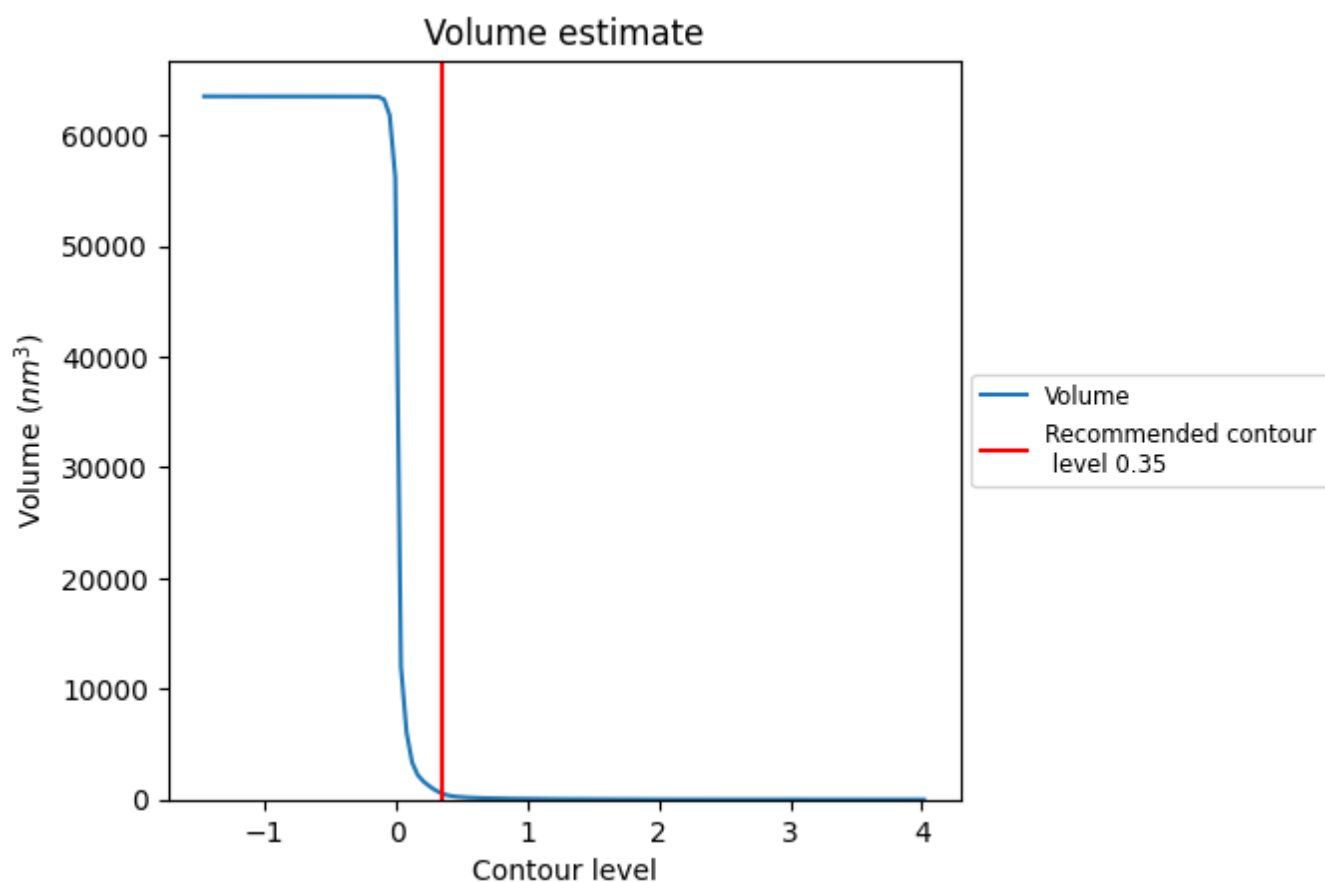
This section contains the results of statistical analysis of the map.

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.

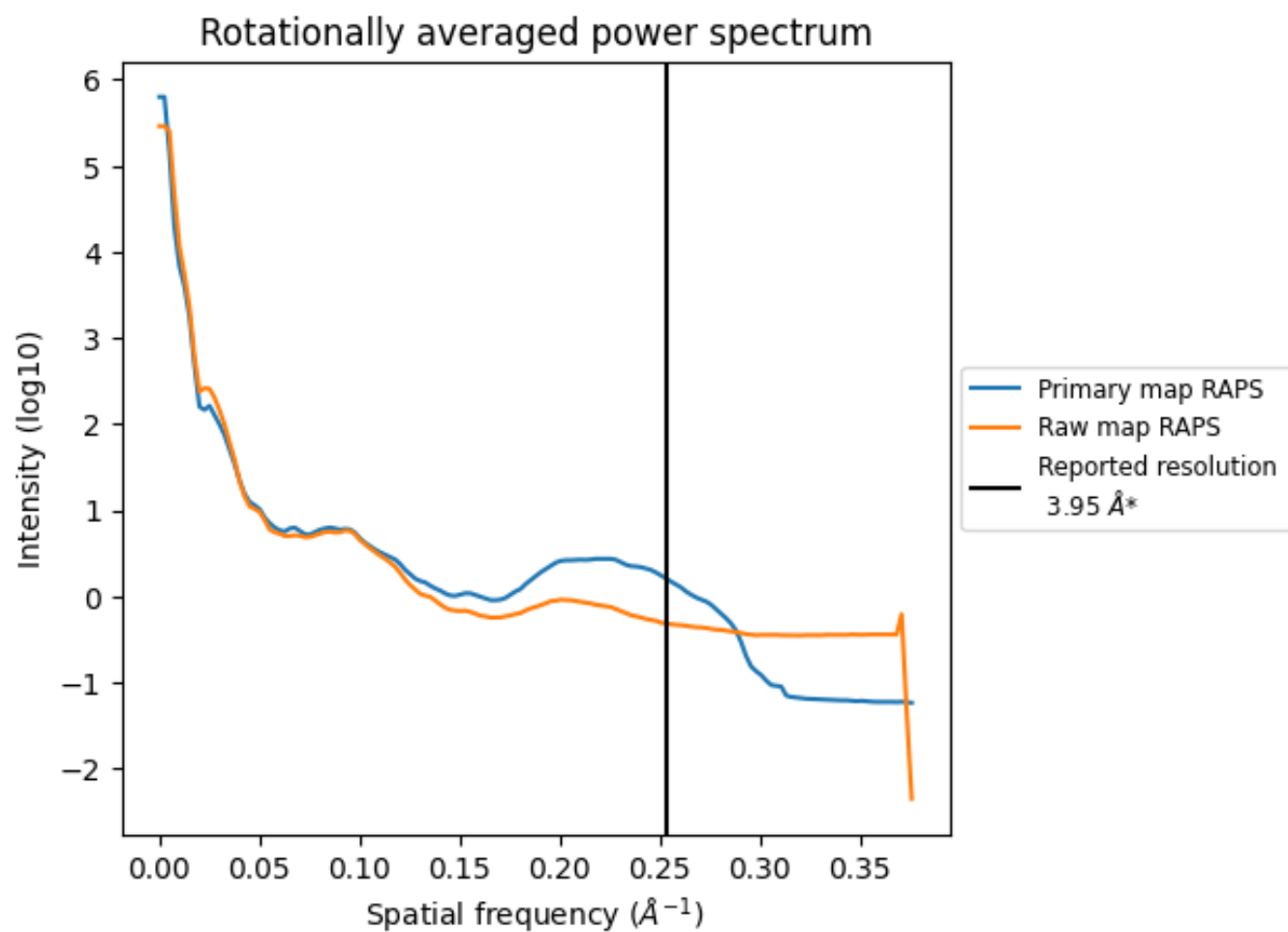
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 551 nm^3 ; this corresponds to an approximate mass of 498 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 ⓘ

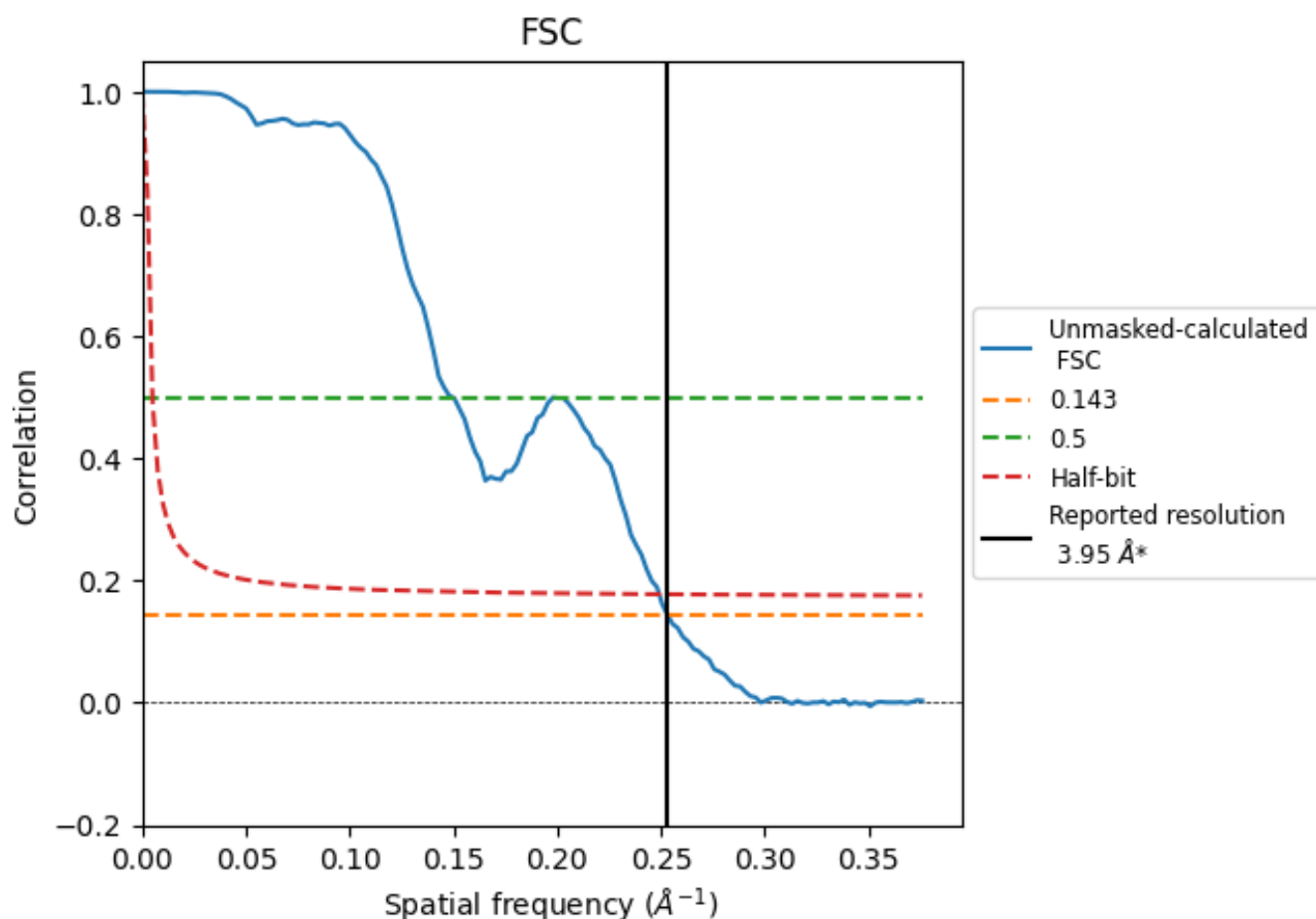


*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	6.69	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

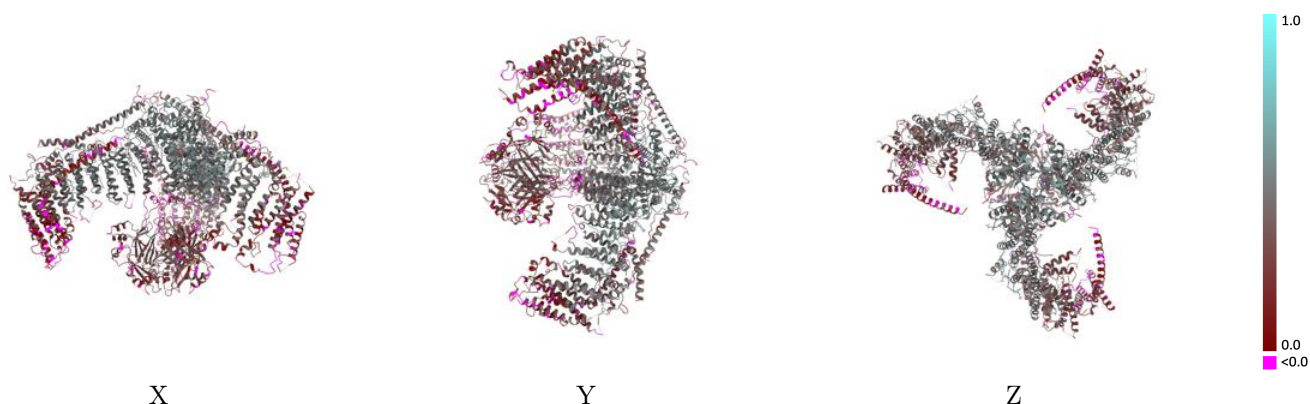
This section contains information regarding the fit between EMDB map EMD-65735 and PDB model 9W7X. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



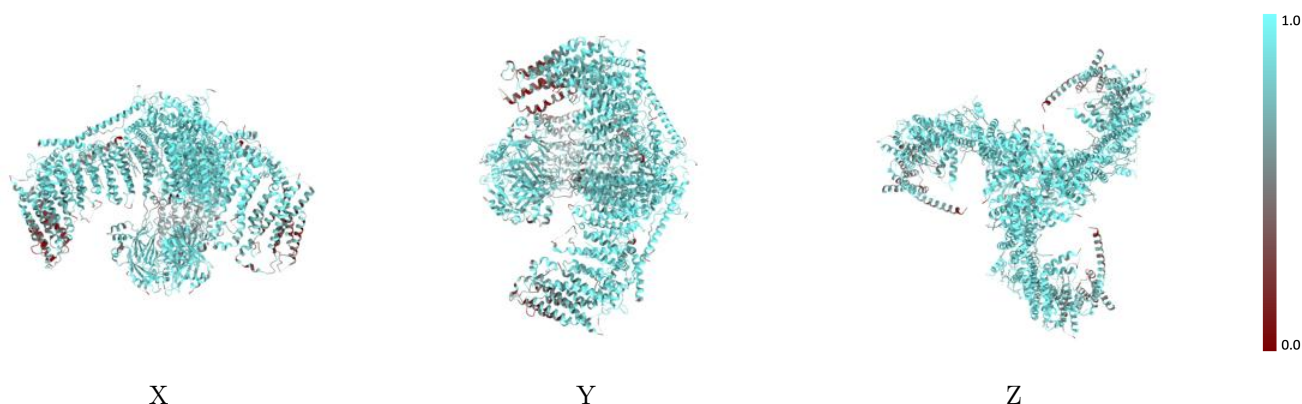
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



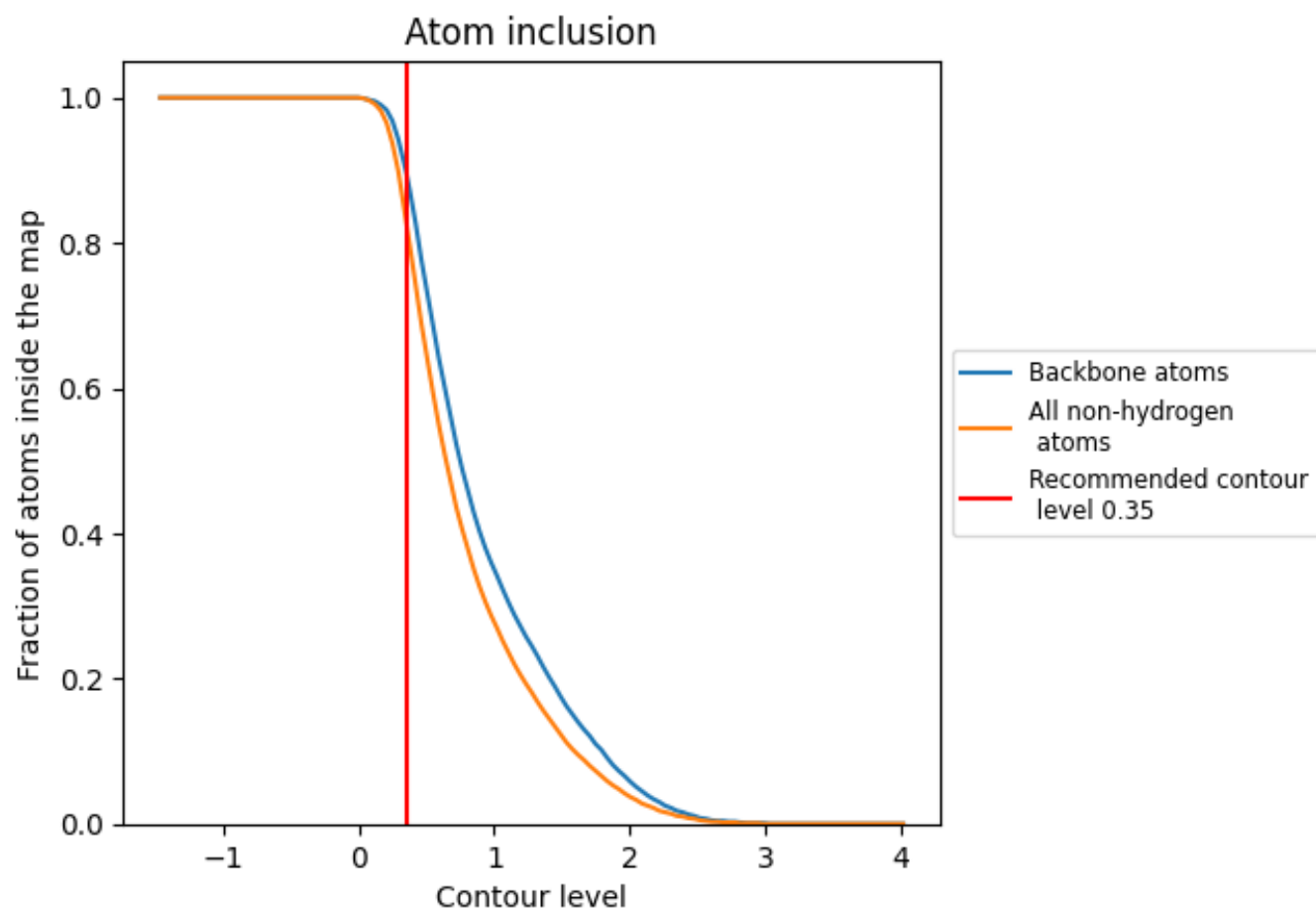
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8320	<div></div> 0.3530
A	<div></div> 0.8310	<div></div> 0.3530
B	<div></div> 0.8330	<div></div> 0.3540
C	<div></div> 0.8340	<div></div> 0.3530

