



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:48 AM UTC

PDB ID : 4WW3 / pdb_00004ww3
Title : Crystal structure of the lumi intermediate of squid rhodopsin
Authors : Murakami, M.; Kouyama, T.
Deposited on : 2014-11-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

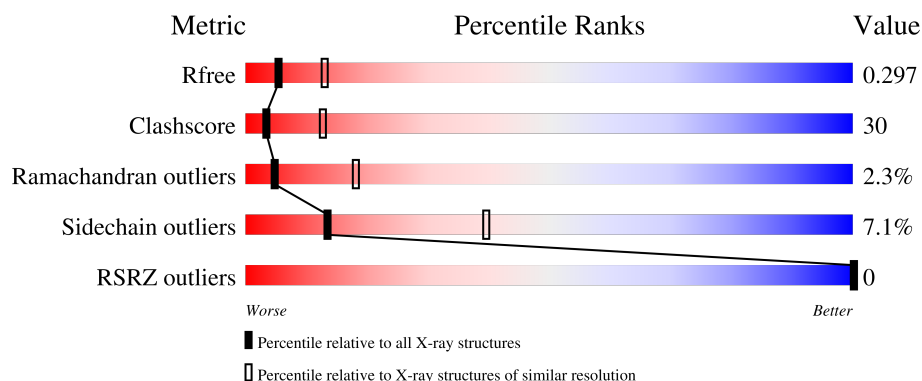
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

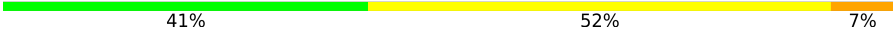
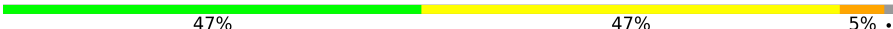
The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	350	 41% 52% 7%
1	B	350	 47% 47% 5%

2 Entry composition [i](#)

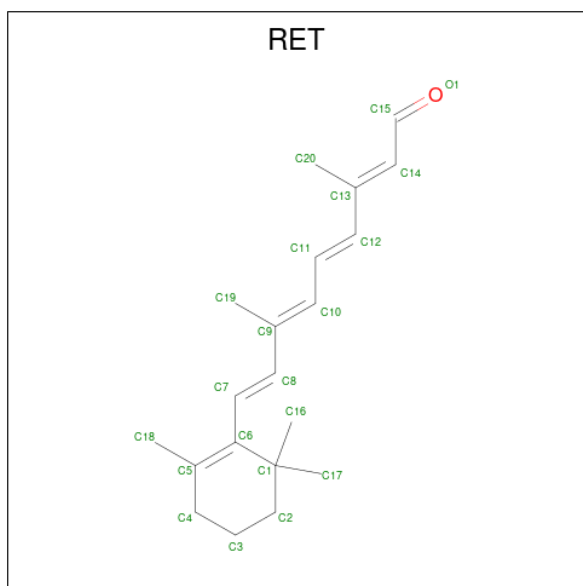
There are 8 unique types of molecules in this entry. The entry contains 5838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2781	1838	443	474	26			
1	B	347	Total	C	N	O	S	0	0	0
			2762	1828	440	468	26			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).

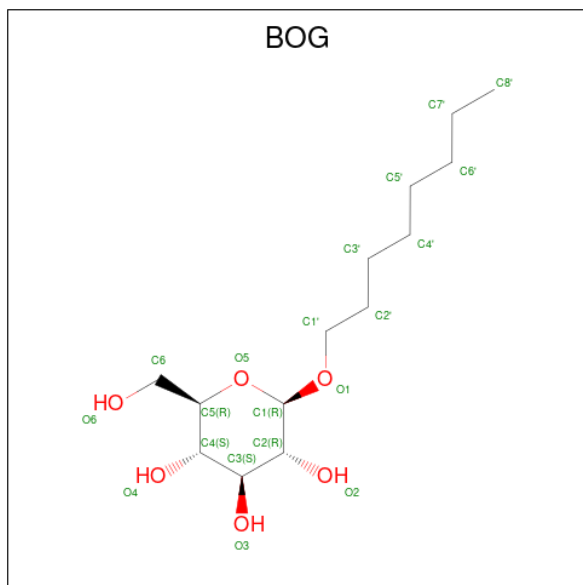


- Molecule 4 is DOCOSANE (CCD ID: TWT) (formula: $C_{22}H_{46}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			22	22		
4	B	1	Total	C	0	0
			22	22		

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



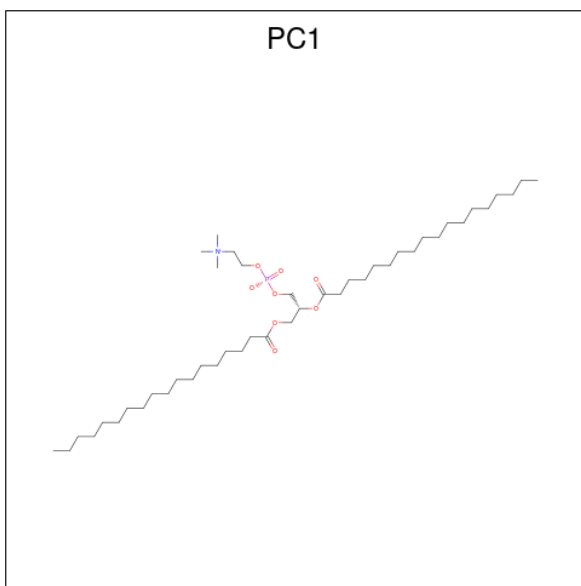
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	P	0	0
			39	30	8	1		

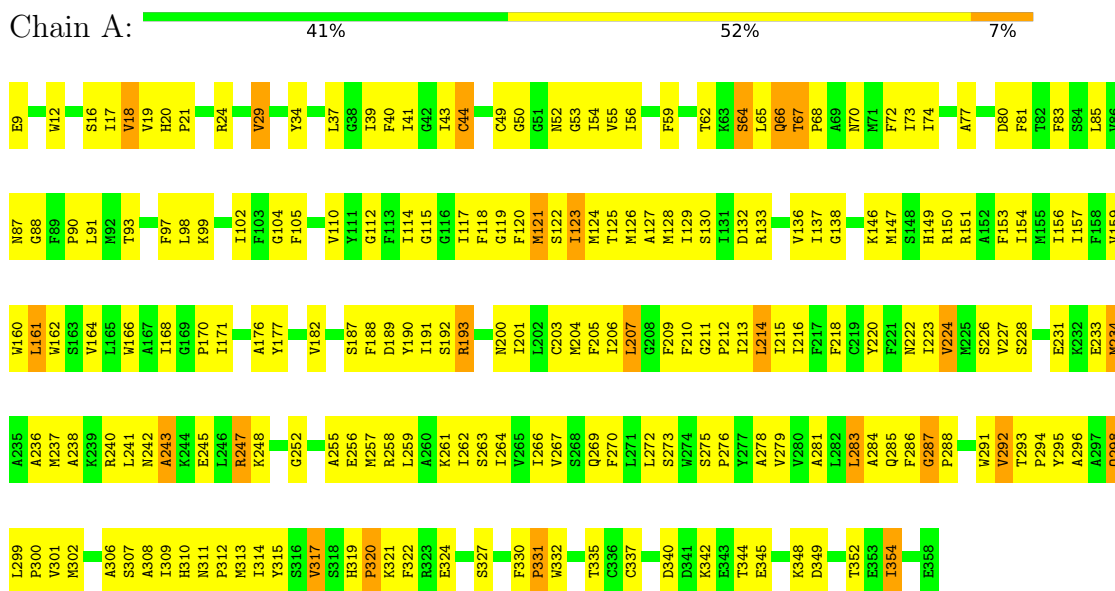
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	29	Total 29	O 29	0	0
8	B	30	Total 30	O 30	0	0

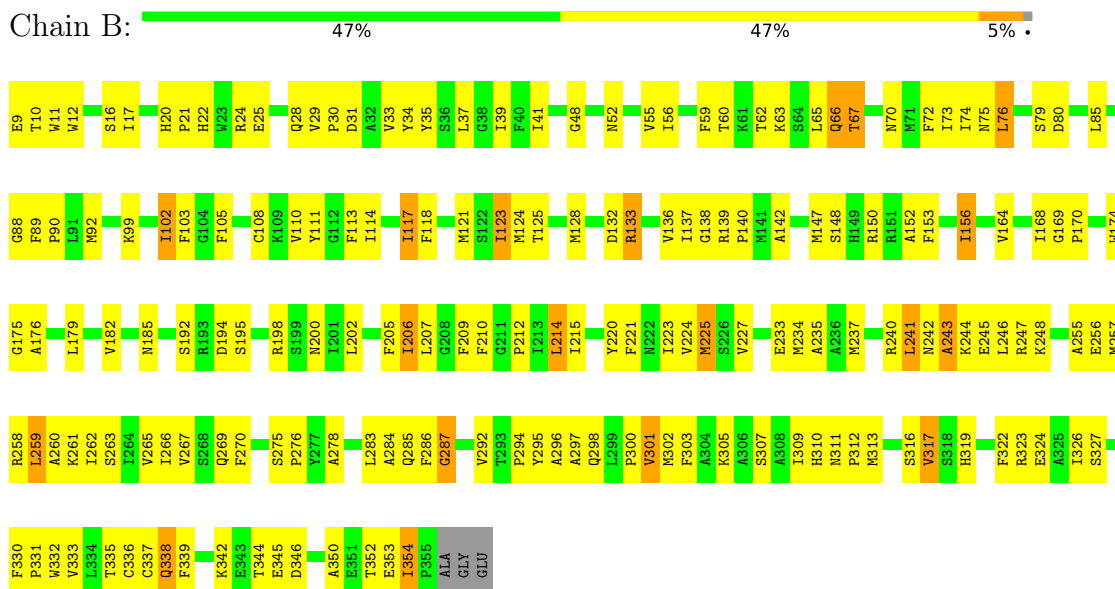
3 Residue-property plots

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

• Molecule 1: Rhodopsin



• Molecule 1: Rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	122.39Å 122.39Å 158.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.08 – 2.80 44.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.5 (44.08-2.80) 83.6 (44.08-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.296 0.290 , 0.297	Depositor DCC
R_{free} test set	1351 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.127 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, BOG, PC1, SO4, PLM, TWT

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	0.54	0/2866	1.01	14/3889 (0.4%)
1	B	0.54	0/2847	1.02	10/3865 (0.3%)
All	All	0.54	0/5713	1.01	24/7754 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	LYS	N-CA-C	-8.06	103.66	113.97
1	A	119	GLY	N-CA-C	-7.01	104.37	112.50
1	B	287	GLY	CA-C-N	6.29	127.71	119.84
1	B	287	GLY	C-N-CA	6.29	127.71	119.84
1	A	193	ARG	N-CA-C	5.96	119.61	112.93
1	A	324	GLU	N-CA-C	-5.93	104.72	111.07
1	A	53	GLY	N-CA-C	-5.76	105.40	112.77
1	B	175	GLY	N-CA-C	-5.75	103.54	112.45
1	A	44	CYS	N-CA-C	-5.68	105.17	111.36
1	A	67	THR	CA-C-N	5.62	126.86	119.84
1	A	67	THR	C-N-CA	5.62	126.86	119.84
1	A	224	VAL	N-CA-C	-5.57	105.68	111.58
1	A	125	THR	N-CA-C	-5.45	104.98	111.69
1	B	29	VAL	CA-C-N	5.37	125.13	119.76
1	B	29	VAL	C-N-CA	5.37	125.13	119.76
1	A	287	GLY	CA-C-N	5.30	126.47	119.84
1	A	287	GLY	C-N-CA	5.30	126.47	119.84
1	B	206	ILE	N-CA-C	5.29	115.43	110.30
1	B	103	PHE	N-CA-C	5.28	119.44	113.15
1	B	221	PHE	N-CA-C	-5.20	105.26	111.03
1	B	267	VAL	N-CA-C	-5.19	105.35	111.00
1	A	283	LEU	N-CA-C	-5.12	105.60	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	VAL	CA-C-N	5.05	124.97	119.76
1	A	29	VAL	C-N-CA	5.05	124.97	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2781	0	2766	202	0
1	B	2762	0	2752	150	0
2	A	20	0	27	3	0
2	B	20	0	27	0	0
3	A	34	0	62	1	0
3	B	34	0	62	1	0
4	A	22	0	46	0	0
4	B	22	0	46	0	0
5	A	20	0	28	5	0
5	B	20	0	28	2	0
6	B	5	0	0	0	0
7	B	39	0	49	1	0
8	A	29	0	0	8	0
8	B	30	0	0	3	0
All	All	5838	0	5893	350	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 30.

All (350) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HB2	1:B:121:MET:HE2	1.29	1.14
1:A:21:PRO:HA	1:A:24:ARG:HD3	1.32	1.11
1:A:59:PHE:HB3	1:A:74:ILE:HD11	1.36	1.06
1:A:284:ALA:HB2	1:A:292:VAL:HG21	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:H	1:B:150:ARG:HD2	1.28	0.96
1:B:113:PHE:O	1:B:117:ILE:HG22	1.69	0.91
1:A:298:GLN:O	1:A:301:VAL:HG12	1.72	0.87
1:A:20:HIS:ND1	1:A:21:PRO:HD2	1.92	0.85
1:A:218:PHE:O	1:A:222:ASN:HB2	1.79	0.82
1:B:234:MET:HA	1:B:237:MET:HE3	1.61	0.82
1:A:21:PRO:CA	1:A:24:ARG:HD3	2.08	0.82
1:A:220:TYR:OH	1:A:263:SER:HB3	1.82	0.79
1:B:170:PRO:HB3	1:B:176:ALA:CA	2.13	0.79
1:B:75:ASN:HD21	1:B:121:MET:HE3	1.48	0.78
1:A:115:GLY:HA3	2:A:401:RET:H203	1.66	0.78
1:B:117:ILE:HD12	1:B:164:VAL:HG22	1.64	0.78
1:B:150:ARG:HD2	1:B:150:ARG:N	2.02	0.75
1:A:209:PHE:CE2	1:A:213:ILE:HD11	2.22	0.75
1:B:137:ILE:HD11	1:B:256:GLU:HB3	1.69	0.75
1:B:354:ILE:HD13	1:B:354:ILE:H	1.51	0.74
1:A:212:PRO:HA	1:A:215:ILE:HD12	1.68	0.74
1:A:146:LYS:HE2	5:A:405:BOG:H61	1.68	0.74
1:B:258:ARG:O	1:B:262:ILE:HG13	1.88	0.74
1:B:75:ASN:ND2	1:B:121:MET:HE3	2.03	0.73
1:A:201:ILE:HD12	1:A:285:GLN:HE21	1.54	0.73
1:A:299:LEU:HD12	1:A:299:LEU:H	1.53	0.72
1:B:150:ARG:H	1:B:150:ARG:CD	2.00	0.72
1:B:311:ASN:HB2	1:B:312:PRO:HD3	1.69	0.72
1:A:293:THR:H	1:A:296:ALA:HB3	1.54	0.71
1:A:201:ILE:HD12	1:A:285:GLN:NE2	2.06	0.71
1:B:63:LYS:HD2	1:B:66:GLN:NE2	2.07	0.70
1:B:257:MET:HG3	1:B:261:LYS:HE3	1.74	0.69
1:A:133:ARG:HA	1:A:133:ARG:NE	2.07	0.69
1:A:209:PHE:O	1:A:213:ILE:HG13	1.94	0.68
1:A:233:GLU:HG2	1:A:237:MET:HE3	1.73	0.68
1:A:73:ILE:HD11	5:A:405:BOG:H7'2	1.75	0.68
1:A:284:ALA:CB	1:A:292:VAL:HG21	2.23	0.67
1:B:63:LYS:HD2	1:B:66:GLN:HE22	1.58	0.67
1:B:202:LEU:HD12	7:B:406:PC1:H361	1.75	0.67
1:B:298:GLN:O	1:B:301:VAL:HG12	1.93	0.67
1:A:200:ASN:OD1	1:A:204:MET:HE2	1.95	0.67
1:A:201:ILE:CD1	1:A:285:GLN:HE21	2.08	0.67
1:B:284:ALA:HB2	1:B:292:VAL:HG21	1.77	0.67
1:A:126:MET:HE1	1:A:270:PHE:HB2	1.77	0.66
1:A:121:MET:HE1	1:A:160:TRP:CZ2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ALA:O	1:A:281:ALA:HB3	1.95	0.66
1:A:190:TYR:HA	1:A:201:ILE:HD11	1.77	0.66
1:A:306:ALA:O	1:A:309:ILE:HG12	1.97	0.65
1:A:188:PHE:CE1	1:A:190:TYR:HB3	2.32	0.65
1:A:12:TRP:CD2	1:A:24:ARG:HG2	2.32	0.64
1:A:37:LEU:CD2	1:A:302:MET:HE2	2.28	0.64
1:A:188:PHE:HE1	1:A:190:TYR:HB3	1.63	0.64
1:B:110:VAL:O	1:B:114:ILE:HG13	1.98	0.64
1:A:137:ILE:HD11	1:A:256:GLU:HB2	1.80	0.64
1:A:50:GLY:O	1:A:54:ILE:HG13	1.97	0.64
1:B:170:PRO:HB3	1:B:176:ALA:N	2.12	0.63
1:A:37:LEU:HD22	1:A:302:MET:HE2	1.78	0.63
1:A:311:ASN:HB2	1:A:312:PRO:HD3	1.80	0.63
1:B:52:ASN:HD21	1:B:80:ASP:HB3	1.64	0.63
1:B:170:PRO:HB3	1:B:176:ALA:HA	1.80	0.63
1:A:340:ASP:OD2	1:A:342:LYS:HB2	1.98	0.63
1:A:20:HIS:CE1	1:A:21:PRO:HD2	2.33	0.63
1:B:136:VAL:O	1:B:137:ILE:HD13	1.99	0.63
1:A:21:PRO:HA	1:A:24:ARG:CD	2.21	0.63
1:B:248:LYS:HE3	1:B:350:ALA:O	1.99	0.62
1:A:133:ARG:NH2	1:A:136:VAL:HG11	2.15	0.62
1:A:263:SER:O	1:A:267:VAL:HG23	2.00	0.62
1:B:20:HIS:ND1	1:B:21:PRO:HD2	2.15	0.61
1:B:324:GLU:HG3	1:B:339:PHE:CE2	2.35	0.61
1:B:118:PHE:HA	1:B:121:MET:HB3	1.82	0.61
1:B:41:ILE:HG13	1:B:88:GLY:HA2	1.82	0.61
1:A:59:PHE:HB3	1:A:74:ILE:CD1	2.22	0.61
1:A:293:THR:N	1:A:296:ALA:HB3	2.16	0.61
1:B:313:MET:O	1:B:317:VAL:HG23	2.00	0.60
1:A:150:ARG:HD3	1:A:150:ARG:N	2.16	0.60
1:A:34:TYR:CD1	1:A:99:LYS:HG2	2.37	0.60
1:B:52:ASN:HA	1:B:55:VAL:HG12	1.82	0.60
1:A:137:ILE:HG22	1:A:223:ILE:HG23	1.82	0.60
1:B:276:PRO:HB2	8:B:501:HOH:O	2.01	0.59
1:B:79:SER:HB2	1:B:121:MET:CE	2.20	0.59
1:A:209:PHE:CZ	1:A:213:ILE:HD11	2.37	0.58
1:A:354:ILE:HD12	1:A:354:ILE:O	2.02	0.58
1:B:153:PHE:O	1:B:156:ILE:HG13	2.02	0.58
1:B:132:ASP:OD2	1:B:147:MET:HB2	2.02	0.58
1:A:177:TYR:HA	1:A:187:SER:O	2.03	0.58
1:B:72:PHE:HE2	1:B:147:MET:HE3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ALA:O	1:B:300:PRO:HG2	2.04	0.58
1:A:283:LEU:O	1:A:287:GLY:N	2.34	0.57
1:B:33:VAL:O	1:B:37:LEU:HG	2.05	0.56
1:A:170:PRO:HB3	1:A:176:ALA:CA	2.36	0.56
1:A:122:SER:O	1:A:126:MET:HG3	2.05	0.56
1:A:224:VAL:HA	1:A:227:VAL:HG23	1.88	0.56
1:B:11:TRP:HB2	1:B:28:GLN:OE1	2.06	0.56
1:A:114:ILE:O	1:A:117:ILE:HG22	2.06	0.56
1:A:12:TRP:CE3	1:A:24:ARG:HG2	2.40	0.56
1:A:257:MET:O	1:A:261:LYS:HG3	2.05	0.56
1:B:102:ILE:HD13	1:B:102:ILE:H	1.70	0.56
1:A:313:MET:O	1:A:317:VAL:HG22	2.06	0.56
1:B:240:ARG:HD3	1:B:241:LEU:HD13	1.87	0.56
1:A:236:ALA:O	1:A:240:ARG:HB2	2.06	0.55
1:B:322:PHE:CE2	1:B:326:ILE:HD11	2.42	0.55
1:A:29:VAL:HG22	8:A:519:HOH:O	2.06	0.55
1:A:269:GLN:NE2	1:A:307:SER:OG	2.40	0.55
1:B:48:GLY:HA3	1:B:309:ILE:HG22	1.88	0.55
1:B:297:ALA:O	1:B:300:PRO:HD2	2.07	0.55
1:B:48:GLY:CA	1:B:309:ILE:HG22	2.37	0.55
1:A:12:TRP:HA	8:A:521:HOH:O	2.07	0.55
1:B:113:PHE:CZ	1:B:168:ILE:HD12	2.42	0.55
1:A:263:SER:O	1:A:266:ILE:HG12	2.07	0.54
1:A:77:ALA:HA	8:A:518:HOH:O	2.07	0.54
1:A:49:CYS:HB3	1:A:81:PHE:HE1	1.72	0.54
1:A:190:TYR:HA	1:A:201:ILE:CD1	2.37	0.54
1:A:49:CYS:HB3	1:A:81:PHE:CE1	2.43	0.54
1:B:324:GLU:OE2	1:B:344:THR:HG21	2.07	0.54
1:B:297:ALA:C	1:B:300:PRO:HD2	2.32	0.53
1:A:52:ASN:HA	1:A:55:VAL:HG12	1.88	0.53
1:B:220:TYR:O	1:B:224:VAL:HG23	2.08	0.53
1:B:248:LYS:NZ	1:B:353:GLU:HA	2.24	0.53
1:A:342:LYS:HA	1:A:345:GLU:HG3	1.91	0.53
1:B:319:HIS:HB3	1:B:322:PHE:HB3	1.89	0.53
1:A:327:SER:O	1:A:331:PRO:HB3	2.09	0.53
1:A:55:VAL:O	1:A:59:PHE:HB2	2.08	0.53
1:A:19:VAL:O	1:A:24:ARG:HD2	2.09	0.53
1:A:12:TRP:HZ2	1:B:25:GLU:HB2	1.74	0.52
1:B:72:PHE:CE2	1:B:147:MET:HE3	2.43	0.52
1:B:237:MET:O	1:B:242:ASN:HB2	2.09	0.52
1:B:322:PHE:CZ	1:B:326:ILE:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:HIS:HB3	1:A:322:PHE:HB3	1.92	0.52
1:B:257:MET:O	1:B:261:LYS:HG3	2.09	0.52
1:A:72:PHE:HE2	1:A:147:MET:HE3	1.74	0.52
1:A:110:VAL:O	1:A:114:ILE:HG12	2.10	0.52
1:A:259:LEU:HD12	5:A:405:BOG:H6'1	1.91	0.52
1:A:291:TRP:O	1:A:293:THR:HG23	2.10	0.52
1:B:205:PHE:HE1	1:B:278:ALA:HB1	1.75	0.52
1:B:34:TYR:CG	1:B:99:LYS:HG2	2.45	0.52
1:A:67:THR:HG21	5:A:405:BOG:H5	1.92	0.52
1:A:295:TYR:HB3	1:A:299:LEU:HD13	1.92	0.52
1:A:293:THR:HB	1:A:294:PRO:HD2	1.91	0.51
1:A:170:PRO:HB3	1:A:176:ALA:HA	1.92	0.51
1:A:293:THR:H	1:A:296:ALA:CB	2.21	0.51
1:A:344:THR:O	1:A:348:LYS:HG3	2.11	0.51
1:A:40:PHE:HD2	1:A:302:MET:HE3	1.75	0.51
1:A:153:PHE:CE2	1:A:157:ILE:HD11	2.46	0.51
1:A:228:SER:HA	1:A:231:GLU:HB2	1.91	0.51
1:A:279:VAL:O	1:A:283:LEU:HD13	2.11	0.51
1:B:133:ARG:HA	1:B:133:ARG:NH1	2.26	0.51
1:A:243:ALA:HB3	1:A:245:GLU:OE2	2.11	0.51
1:A:98:LEU:HD12	1:A:102:ILE:HD13	1.93	0.50
1:A:206:ILE:HA	1:A:210:PHE:CD2	2.46	0.50
1:B:207:LEU:N	1:B:207:LEU:HD22	2.25	0.50
1:B:125:THR:O	1:B:128:MET:HB2	2.11	0.50
1:A:133:ARG:HA	1:A:133:ARG:HE	1.74	0.50
1:A:234:MET:HE2	1:A:237:MET:SD	2.51	0.50
1:B:22:HIS:O	1:B:25:GLU:HG2	2.12	0.50
1:B:263:SER:O	1:B:266:ILE:HG12	2.12	0.50
1:B:336:CYS:SG	3:B:404:PLM:H21	2.51	0.50
1:A:342:LYS:O	1:A:345:GLU:HG3	2.11	0.50
1:B:275:SER:HB2	1:B:276:PRO:HD3	1.93	0.50
1:B:330:PHE:N	1:B:331:PRO:CD	2.75	0.50
1:A:293:THR:HB	1:A:294:PRO:CD	2.42	0.50
1:B:133:ARG:HG2	1:B:260:ALA:HA	1.93	0.50
1:A:112:GLY:HA2	2:A:401:RET:H202	1.93	0.50
1:B:182:VAL:HG22	1:B:298:GLN:OE1	2.12	0.49
1:B:248:LYS:HZ2	1:B:353:GLU:HA	1.77	0.49
1:A:330:PHE:N	1:A:331:PRO:CD	2.75	0.49
1:B:48:GLY:O	1:B:52:ASN:HB2	2.12	0.49
1:A:345:GLU:HA	1:A:348:LYS:HD2	1.95	0.49
1:B:12:TRP:CD1	1:B:12:TRP:H	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:O	1:A:87:ASN:HB2	2.12	0.49
1:B:247:ARG:O	1:B:247:ARG:HD3	2.12	0.49
1:B:316:SER:O	1:B:323:ARG:NH1	2.40	0.49
1:A:233:GLU:O	1:A:237:MET:HG2	2.13	0.49
1:B:137:ILE:HD11	1:B:256:GLU:CB	2.39	0.49
1:B:337:CYS:O	1:B:338:GLN:C	2.56	0.49
1:A:247:ARG:HH21	1:A:247:ARG:HB2	1.78	0.49
1:B:76:LEU:HD13	1:B:311:ASN:HD22	1.77	0.49
1:B:259:LEU:HB3	5:B:407:BOG:H6'1	1.95	0.48
1:B:327:SER:O	1:B:331:PRO:HB3	2.13	0.48
1:A:127:ALA:HB3	1:A:128:MET:HE2	1.95	0.48
1:B:30:PRO:O	1:B:31:ASP:C	2.56	0.48
1:A:273:SER:HB3	1:A:307:SER:HB2	1.95	0.48
1:B:269:GLN:NE2	1:B:307:SER:OG	2.44	0.48
1:A:20:HIS:ND1	1:A:21:PRO:CD	2.70	0.48
1:A:176:ALA:O	1:A:189:ASP:N	2.46	0.48
1:B:132:ASP:OD1	1:B:133:ARG:NH1	2.46	0.48
1:B:206:ILE:HA	1:B:210:PHE:CD2	2.48	0.48
1:B:123:ILE:HG12	1:B:270:PHE:CZ	2.48	0.48
1:B:192:SER:HB3	1:B:194:ASP:OD1	2.14	0.48
1:A:157:ILE:HG22	1:A:161:LEU:HD23	1.96	0.48
1:A:311:ASN:OD1	8:A:501:HOH:O	2.20	0.48
1:A:16:SER:HB2	1:A:17:ILE:HD12	1.95	0.48
1:A:288:PRO:O	1:A:291:TRP:HB2	2.13	0.48
1:B:275:SER:O	1:B:276:PRO:C	2.57	0.48
1:A:153:PHE:CZ	1:A:157:ILE:HD11	2.49	0.47
1:B:214:LEU:HD23	1:B:215:ILE:N	2.28	0.47
1:B:67:THR:O	1:B:70:ASN:HB2	2.13	0.47
1:B:235:ALA:C	1:B:237:MET:H	2.22	0.47
1:A:40:PHE:CD2	1:A:302:MET:HE3	2.49	0.47
1:B:92:MET:HG3	1:B:185:ASN:HB3	1.96	0.47
1:A:216:ILE:HD13	1:A:267:VAL:HG11	1.95	0.47
1:A:224:VAL:O	1:A:227:VAL:HG23	2.14	0.47
1:A:49:CYS:HA	1:A:81:PHE:CD1	2.49	0.47
1:A:52:ASN:O	1:A:56:ILE:HG13	2.15	0.47
1:A:67:THR:HB	8:A:527:HOH:O	2.14	0.47
1:B:52:ASN:O	1:B:55:VAL:HG12	2.15	0.47
1:B:89:PHE:CD2	1:B:90:PRO:HA	2.49	0.47
1:B:255:ALA:O	1:B:259:LEU:HD22	2.15	0.47
1:A:62:THR:HG22	1:A:64:SER:H	1.80	0.47
1:A:146:LYS:HE2	5:A:405:BOG:C6	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HH11	1:A:286:PHE:C	2.22	0.47
1:B:41:ILE:HB	1:B:302:MET:HE1	1.97	0.47
1:A:205:PHE:CE1	1:A:278:ALA:HB1	2.50	0.47
1:A:288:PRO:HB2	1:A:291:TRP:CG	2.50	0.46
1:B:332:TRP:O	1:B:335:THR:HG23	2.14	0.46
1:A:193:ARG:HH11	1:A:286:PHE:CA	2.28	0.46
1:B:35:TYR:O	1:B:39:ILE:HG12	2.15	0.46
1:A:218:PHE:CD1	1:A:218:PHE:C	2.93	0.46
1:A:240:ARG:HH11	1:A:241:LEU:HD13	1.80	0.46
1:B:330:PHE:O	1:B:333:VAL:HG23	2.15	0.46
1:A:12:TRP:CZ2	1:B:25:GLU:HB2	2.50	0.46
1:B:324:GLU:CD	1:B:344:THR:HG21	2.40	0.46
1:A:39:ILE:O	1:A:43:ILE:HG13	2.15	0.46
1:A:93:THR:HG22	1:A:97:PHE:CE2	2.51	0.46
1:A:52:ASN:O	1:A:55:VAL:HG12	2.16	0.46
1:A:220:TYR:CD1	1:A:264:ILE:HD11	2.51	0.46
1:B:59:PHE:CD2	1:B:65:LEU:HD13	2.51	0.46
1:A:123:ILE:HG12	1:A:270:PHE:CZ	2.51	0.46
1:A:133:ARG:NE	1:A:133:ARG:CA	2.76	0.46
1:B:234:MET:HE2	1:B:246:LEU:CD1	2.46	0.46
1:B:52:ASN:CA	1:B:55:VAL:HG12	2.46	0.46
1:A:18:VAL:HG12	1:A:18:VAL:O	2.15	0.45
1:A:133:ARG:HE	1:A:133:ARG:CA	2.29	0.45
1:A:150:ARG:N	1:A:150:ARG:CD	2.79	0.45
1:A:224:VAL:C	1:A:226:SER:H	2.24	0.45
1:A:124:MET:HG3	1:A:159:VAL:HG22	1.99	0.45
1:B:124:MET:O	1:B:128:MET:HG2	2.16	0.45
1:A:121:MET:HE1	1:A:160:TRP:CE2	2.52	0.45
1:A:275:SER:O	1:A:276:PRO:C	2.59	0.45
1:B:233:GLU:O	1:B:237:MET:HG3	2.16	0.45
1:B:301:VAL:O	1:B:305:LYS:HG3	2.15	0.45
1:A:270:PHE:O	1:A:273:SER:HB2	2.15	0.45
1:B:21:PRO:HA	1:B:24:ARG:HG3	1.98	0.45
1:B:52:ASN:HA	1:B:55:VAL:CG1	2.46	0.45
1:A:150:ARG:CD	1:A:150:ARG:H	2.30	0.45
1:B:52:ASN:C	1:B:55:VAL:HG12	2.41	0.45
1:B:137:ILE:C	1:B:139:ARG:H	2.25	0.45
1:A:17:ILE:HG13	1:A:105:PHE:CD2	2.52	0.45
1:A:72:PHE:CE2	1:A:147:MET:HE3	2.51	0.45
1:A:147:MET:SD	1:A:151:ARG:HB3	2.56	0.45
1:A:206:ILE:HA	1:A:210:PHE:HD2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:HA	1:A:240:ARG:CB	2.47	0.44
1:B:298:GLN:O	1:B:302:MET:HG2	2.18	0.44
1:B:310:HIS:O	1:B:311:ASN:C	2.60	0.44
1:B:224:VAL:O	1:B:227:VAL:HG22	2.17	0.44
1:A:150:ARG:O	1:A:154:ILE:HG13	2.18	0.44
1:B:148:SER:HB2	1:B:150:ARG:HH21	1.82	0.44
1:B:220:TYR:CD1	1:B:223:ILE:HD12	2.53	0.44
1:B:52:ASN:O	1:B:56:ILE:HG13	2.17	0.44
1:B:35:TYR:N	1:B:35:TYR:CD2	2.86	0.44
1:B:140:PRO:C	1:B:142:ALA:N	2.74	0.44
1:A:114:ILE:C	1:A:117:ILE:HG22	2.42	0.44
1:A:150:ARG:HD3	1:A:150:ARG:H	1.82	0.44
1:A:348:LYS:O	1:A:352:THR:HG23	2.18	0.44
1:B:206:ILE:HG22	1:B:207:LEU:HD22	2.00	0.44
1:A:330:PHE:O	1:A:332:TRP:N	2.51	0.43
1:A:127:ALA:O	1:A:130:SER:OG	2.29	0.43
1:A:214:LEU:O	1:A:215:ILE:C	2.61	0.43
1:A:332:TRP:O	1:A:335:THR:HG23	2.18	0.43
1:B:111:TYR:C	1:B:111:TYR:CD2	2.96	0.43
1:B:133:ARG:CG	1:B:260:ALA:HA	2.48	0.43
1:A:118:PHE:HA	1:A:121:MET:HB3	2.00	0.43
1:A:153:PHE:O	1:A:157:ILE:HG13	2.18	0.43
1:B:52:ASN:ND2	1:B:80:ASP:HB3	2.31	0.43
1:B:33:VAL:HG21	1:B:295:TYR:OH	2.18	0.43
1:B:198:ARG:O	1:B:202:LEU:HG	2.18	0.43
1:A:299:LEU:HB2	1:A:300:PRO:HD3	2.01	0.43
1:A:310:HIS:O	1:A:311:ASN:C	2.62	0.43
1:B:220:TYR:OH	1:B:263:SER:HB3	2.18	0.43
1:A:188:PHE:HB2	1:A:204:MET:HE1	2.01	0.43
1:A:252:GLY:O	1:A:255:ALA:HB3	2.18	0.43
1:A:266:ILE:HG22	1:A:314:ILE:HD12	2.01	0.43
1:A:275:SER:HB2	1:A:276:PRO:HD3	2.00	0.43
1:B:21:PRO:O	1:B:22:HIS:C	2.61	0.43
1:A:29:VAL:HG21	1:A:182:VAL:HG11	1.99	0.43
1:A:191:ILE:O	1:A:192:SER:C	2.62	0.43
1:A:205:PHE:HE1	1:A:278:ALA:HB1	1.83	0.43
1:A:276:PRO:HB2	8:A:502:HOH:O	2.18	0.43
1:B:243:ALA:N	1:B:245:GLU:HG2	2.34	0.42
1:A:41:ILE:HG13	1:A:88:GLY:HA2	1.99	0.42
1:A:240:ARG:HA	1:A:240:ARG:NE	2.33	0.42
1:B:52:ASN:O	1:B:55:VAL:CG1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TRP:CH2	1:A:207:LEU:HD23	2.54	0.42
1:B:55:VAL:HG13	1:B:56:ILE:N	2.34	0.42
1:B:73:ILE:HD11	5:B:407:BOG:H7'2	2.01	0.42
1:B:169:GLY:HA3	8:B:515:HOH:O	2.19	0.42
1:B:72:PHE:CZ	1:B:152:ALA:HA	2.53	0.42
1:A:132:ASP:OD1	1:A:133:ARG:NH2	2.53	0.42
1:B:59:PHE:CE2	1:B:65:LEU:HD13	2.55	0.42
1:B:105:PHE:O	1:B:108:CYS:HB3	2.19	0.42
1:B:285:GLN:NE2	1:B:285:GLN:HA	2.35	0.42
1:A:37:LEU:HD23	1:A:302:MET:HE2	2.01	0.42
1:A:136:VAL:O	1:A:136:VAL:HG22	2.19	0.42
1:A:299:LEU:H	1:A:299:LEU:CD1	2.28	0.42
1:B:17:ILE:CG2	1:B:179:LEU:HD12	2.49	0.42
1:B:20:HIS:CE1	1:B:21:PRO:HD2	2.55	0.42
1:A:120:PHE:CZ	2:A:401:RET:H7	2.55	0.42
1:A:234:MET:O	1:A:238:ALA:HB2	2.20	0.42
1:A:258:ARG:NH2	1:A:258:ARG:HG3	2.35	0.42
1:A:258:ARG:O	1:A:262:ILE:HG13	2.20	0.42
1:B:234:MET:O	1:B:237:MET:HB2	2.20	0.42
1:A:117:ILE:HD11	1:A:164:VAL:HG22	2.01	0.41
1:A:161:LEU:HD13	1:A:161:LEU:HA	1.63	0.41
1:A:170:PRO:HB3	1:A:176:ALA:N	2.35	0.41
1:A:233:GLU:HG2	1:A:233:GLU:O	2.19	0.41
1:B:12:TRP:CH2	1:B:24:ARG:HD3	2.55	0.41
1:A:80:ASP:HB3	1:A:308:ALA:O	2.19	0.41
1:A:90:PRO:O	1:A:91:LEU:C	2.62	0.41
1:A:168:ILE:O	1:A:171:ILE:HB	2.20	0.41
1:A:337:CYS:SG	3:A:403:PLM:O2	2.77	0.41
1:B:60:THR:CG2	1:B:74:ILE:HD13	2.50	0.41
1:A:114:ILE:HA	1:A:117:ILE:HG22	2.02	0.41
1:A:216:ILE:HG23	1:A:220:TYR:CE2	2.54	0.41
1:B:261:LYS:O	1:B:265:VAL:HG23	2.20	0.41
1:A:220:TYR:O	1:A:224:VAL:HG23	2.20	0.41
1:A:65:LEU:HD21	1:A:321:LYS:HB3	2.02	0.41
1:A:68:PRO:HG3	1:A:149:HIS:CE1	2.56	0.41
1:A:114:ILE:HA	1:A:117:ILE:CG2	2.50	0.41
1:A:129:ILE:O	1:A:133:ARG:HG2	2.21	0.41
1:A:258:ARG:HG3	1:A:258:ARG:HH21	1.86	0.41
1:B:55:VAL:O	1:B:56:ILE:C	2.62	0.41
1:A:299:LEU:HD12	1:A:299:LEU:N	2.30	0.41
1:A:312:PRO:HA	1:A:315:TYR:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:MET:HB2	8:B:528:HOH:O	2.20	0.41
1:B:242:ASN:HA	1:B:245:GLU:HG3	2.03	0.41
1:A:44:CYS:HB3	8:A:528:HOH:O	2.21	0.40
1:A:138:GLY:CA	1:A:223:ILE:HG12	2.50	0.40
1:B:133:ARG:HA	1:B:133:ARG:HH11	1.85	0.40
1:A:136:VAL:HG13	1:A:137:ILE:HG12	2.04	0.40
1:A:320:PRO:HG2	8:A:525:HOH:O	2.21	0.40
1:B:283:LEU:O	1:B:287:GLY:N	2.53	0.40
1:A:17:ILE:HD12	1:A:17:ILE:N	2.36	0.40
1:B:174:TRP:CD1	1:B:200:ASN:HB2	2.57	0.40
1:B:202:LEU:HD21	1:B:286:PHE:HZ	1.87	0.40
1:B:209:PHE:O	1:B:212:PRO:HG2	2.21	0.40
1:B:342:LYS:HA	1:B:345:GLU:OE1	2.21	0.40
1:A:166:TRP:CZ3	1:A:207:LEU:HD23	2.56	0.40
1:A:262:ILE:O	1:A:263:SER:C	2.65	0.40
1:A:16:SER:HB3	1:A:104:GLY:HA2	2.04	0.40
1:A:345:GLU:HA	1:A:348:LYS:CD	2.51	0.40
1:B:132:ASP:HB2	1:B:147:MET:HE2	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/350 (99%)	299 (86%)	39 (11%)	10 (3%)	3	13
1	B	345/350 (99%)	306 (89%)	33 (10%)	6 (2%)	7	25
All	All	693/700 (99%)	605 (87%)	72 (10%)	16 (2%)	5	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	A	298	GLN
1	B	241	LEU
1	B	243	ALA
1	B	352	THR
1	A	66	GLN
1	A	162	TRP
1	A	211	GLY
1	A	248	LYS
1	A	331	PRO
1	B	62	THR
1	B	225	MET
1	A	70	ASN
1	A	292	VAL
1	B	138	GLY
1	A	320	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/296 (100%)	277 (94%)	19 (6%)	16	44
1	B	295/296 (100%)	272 (92%)	23 (8%)	11	35
All	All	591/592 (100%)	549 (93%)	42 (7%)	13	39

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	18	VAL
1	A	64	SER
1	A	66	GLN
1	A	85	LEU
1	A	121	MET
1	A	123	ILE
1	A	156	ILE

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	203	CYS
1	A	207	LEU
1	A	214	LEU
1	A	234	MET
1	A	242	ASN
1	A	247	ARG
1	A	272	LEU
1	A	317	VAL
1	A	349	ASP
1	A	354	ILE
1	B	9	GLU
1	B	10	THR
1	B	16	SER
1	B	66	GLN
1	B	67	THR
1	B	76	LEU
1	B	85	LEU
1	B	102	ILE
1	B	117	ILE
1	B	123	ILE
1	B	133	ARG
1	B	156	ILE
1	B	195	SER
1	B	214	LEU
1	B	225	MET
1	B	259	LEU
1	B	294	PRO
1	B	301	VAL
1	B	303	PHE
1	B	317	VAL
1	B	338	GLN
1	B	346	ASP
1	B	354	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	87	ASN
1	A	229	ASN
1	A	230	HIS

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Mol	Chain	Res	Type
1	A	242	ASN
1	A	254	ASN
1	A	269	GLN
1	B	52	ASN
1	B	70	ASN
1	B	149	HIS
1	B	200	ASN
1	B	222	ASN
1	B	229	ASN
1	B	230	HIS
1	B	250	GLN
1	B	254	ASN
1	B	338	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	RET	B	402	1	20,20,21	1.75	5 (25%)	27,27,28	2.34	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PLM	A	402	-	15,16,17	0.37	0	14,15,17	0.57	0
3	PLM	B	404	-	15,16,17	0.25	0	14,15,17	0.65	0
7	PC1	B	406	-	38,38,53	1.64	3 (7%)	41,43,61	1.01	2 (4%)
6	SO4	B	401	-	4,4,4	0.40	0	6,6,6	0.08	0
5	BOG	A	405	-	20,20,20	1.82	8 (40%)	25,25,25	2.78	11 (44%)
3	PLM	A	403	-	15,16,17	0.26	0	14,15,17	0.66	0
4	TWT	B	405	-	21,21,21	0.27	0	20,20,20	1.74	6 (30%)
5	BOG	B	407	-	20,20,20	1.81	8 (40%)	25,25,25	2.75	11 (44%)
3	PLM	B	403	-	15,16,17	0.29	0	14,15,17	0.62	0
4	TWT	A	404	-	21,21,21	0.33	0	20,20,20	1.68	4 (20%)
2	RET	A	401	1	20,20,21	2.17	5 (25%)	27,27,28	2.40	8 (29%)

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	RET	B	402	1	-	2/13/30/31	0/1/1/1
3	PLM	A	402	-	-	5/14/14/15	-
3	PLM	B	404	-	-	8/14/14/15	-
7	PC1	B	406	-	-	14/42/42/57	-
5	BOG	A	405	-	-	4/11/31/31	0/1/1/1
3	PLM	A	403	-	-	7/14/14/15	-
4	TWT	B	405	-	-	8/19/19/19	-
5	BOG	B	407	-	-	6/11/31/31	0/1/1/1
3	PLM	B	403	-	-	4/14/14/15	-
4	TWT	A	404	-	-	9/19/19/19	-
2	RET	A	401	1	-	2/13/30/31	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	406	PC1	O21-C21	7.54	1.55	1.34
2	A	401	RET	C1-C6	5.79	1.61	1.53
2	A	401	RET	C14-C13	5.16	1.37	1.33
2	B	402	RET	C1-C6	4.39	1.59	1.53
7	B	406	PC1	O31-C31	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	RET	C2-C3	-3.85	1.43	1.52
5	A	405	BOG	O5-C1	3.69	1.51	1.41
5	B	407	BOG	O5-C1	3.67	1.51	1.41
2	B	402	RET	C2-C3	-3.58	1.44	1.52
2	B	402	RET	C14-C13	3.24	1.36	1.33
5	A	405	BOG	C4-C3	2.66	1.59	1.52
5	B	407	BOG	C4-C3	2.65	1.59	1.52
2	A	401	RET	C7-C6	2.57	1.53	1.45
5	A	405	BOG	O6-C6	2.56	1.53	1.42
5	B	407	BOG	O6-C6	2.54	1.53	1.42
5	B	407	BOG	C4-C5	-2.52	1.47	1.53
5	A	405	BOG	O2-C2	2.28	1.48	1.43
2	B	402	RET	C7-C6	2.24	1.52	1.45
5	A	405	BOG	C3-C2	-2.18	1.46	1.52
2	A	401	RET	C5-C6	2.16	1.38	1.34
5	B	407	BOG	O2-C2	2.15	1.48	1.43
5	A	405	BOG	C6-C5	2.14	1.59	1.51
5	A	405	BOG	O1-C1	-2.14	1.36	1.40
5	A	405	BOG	C4-C5	-2.14	1.48	1.53
7	B	406	PC1	P-O14	2.12	1.58	1.50
5	B	407	BOG	C6-C5	2.12	1.58	1.51
5	B	407	BOG	C3-C2	-2.11	1.46	1.52
2	B	402	RET	C5-C6	2.06	1.38	1.34
5	B	407	BOG	O1-C1	-2.00	1.36	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	407	BOG	C1'-O1-C1	-7.96	100.08	113.68
5	A	405	BOG	C1'-O1-C1	-7.89	100.20	113.68
2	A	401	RET	C11-C10-C9	7.07	137.19	127.28
2	B	402	RET	C11-C10-C9	5.91	135.57	127.28
2	B	402	RET	C7-C8-C9	5.75	134.74	126.23
2	B	402	RET	C8-C9-C10	-5.65	110.12	119.01
2	A	401	RET	C7-C8-C9	5.61	134.54	126.23
2	A	401	RET	C8-C9-C10	-5.36	110.57	119.01
5	A	405	BOG	O1-C1-C2	-4.98	100.70	108.27
5	B	407	BOG	O1-C1-C2	-4.48	101.47	108.27
5	A	405	BOG	O5-C5-C4	-4.37	101.83	109.70
5	B	407	BOG	C1-C2-C3	-4.32	100.92	110.01
5	B	407	BOG	O5-C5-C4	-4.19	102.15	109.70
5	A	405	BOG	C1-C2-C3	-4.12	101.34	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	BOG	O3-C3-C2	-3.75	101.55	110.38
5	B	407	BOG	O3-C3-C2	-3.69	101.68	110.38
4	B	405	TWT	C14-C13-C12	-3.38	97.28	114.37
4	A	404	TWT	C14-C13-C12	-3.32	97.57	114.37
2	B	402	RET	C19-C9-C8	3.32	123.16	118.09
4	A	404	TWT	C16-C15-C14	-3.13	98.55	114.37
7	B	406	PC1	O21-C21-C22	3.04	118.06	111.48
4	B	405	TWT	C16-C15-C14	-3.01	99.14	114.37
4	B	405	TWT	C12-C11-C10	-3.00	99.21	114.37
4	B	405	TWT	C18-C17-C16	-2.97	99.34	114.37
2	A	401	RET	C19-C9-C10	2.97	127.62	122.82
4	A	404	TWT	C12-C11-C10	-2.94	99.49	114.37
5	B	407	BOG	O4-C4-C5	-2.85	102.30	109.32
5	A	405	BOG	O4-C4-C5	-2.69	102.69	109.32
4	A	404	TWT	C18-C17-C16	-2.66	100.90	114.37
5	B	407	BOG	C4'-C3'-C2'	-2.65	100.97	114.37
5	B	407	BOG	C3'-C2'-C1'	-2.64	102.01	113.47
5	A	405	BOG	C3'-C2'-C1'	-2.59	102.19	113.47
5	A	405	BOG	C4'-C3'-C2'	-2.58	101.32	114.37
2	B	402	RET	C10-C11-C12	-2.57	115.75	123.20
5	A	405	BOG	C6'-C5'-C4'	-2.56	101.45	114.37
5	A	405	BOG	O1-C1'-C2'	-2.54	100.73	109.37
4	B	405	TWT	C20-C19-C18	-2.54	101.51	114.37
5	B	407	BOG	C6'-C5'-C4'	-2.48	101.82	114.37
2	A	401	RET	C10-C11-C12	-2.48	116.01	123.20
2	A	401	RET	C19-C9-C8	2.44	121.81	118.09
2	B	402	RET	C19-C9-C10	2.41	126.72	122.82
2	B	402	RET	C8-C7-C6	-2.27	120.93	127.00
2	A	401	RET	C11-C12-C13	2.16	132.30	126.36
5	B	407	BOG	O1-C1'-C2'	-2.15	102.06	109.37
5	B	407	BOG	C5'-C4'-C3'	-2.14	103.53	114.37
2	B	402	RET	C18-C5-C6	2.12	126.80	124.48
2	A	401	RET	C18-C5-C6	2.11	126.78	124.48
4	B	405	TWT	C10-C9-C8	-2.10	103.77	114.37
5	A	405	BOG	C5'-C4'-C3'	-2.09	103.78	114.37
7	B	406	PC1	C2-O21-C21	2.03	122.65	117.80

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	PLM	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	403	PLM	C1-C2-C3-C4
3	B	403	PLM	C1-C2-C3-C4
7	B	406	PC1	C1-O11-P-O12
7	B	406	PC1	C1-O11-P-O14
7	B	406	PC1	C1-O11-P-O13
7	B	406	PC1	C32-C31-O31-C3
7	B	406	PC1	C21-C22-C23-C24
7	B	406	PC1	O32-C31-O31-C3
5	A	405	BOG	O1-C1'-C2'-C3'
5	B	407	BOG	O1-C1'-C2'-C3'
3	A	402	PLM	C7-C8-C9-CA
3	A	403	PLM	CB-CC-CD-CE
4	B	405	TWT	C6-C7-C8-C9
4	A	404	TWT	C3-C4-C5-C6
3	B	404	PLM	CB-CC-CD-CE
3	A	402	PLM	C9-CA-CB-CC
3	B	403	PLM	C7-C8-C9-CA
3	B	404	PLM	C8-C9-CA-CB
3	A	403	PLM	CC-CD-CE-CF
3	B	404	PLM	C2-C3-C4-C5
3	B	404	PLM	C6-C7-C8-C9
3	A	403	PLM	C7-C8-C9-CA
3	B	403	PLM	C2-C3-C4-C5
3	B	404	PLM	CC-CD-CE-CF
4	A	404	TWT	C6-C7-C8-C9
7	B	406	PC1	C22-C23-C24-C25
3	B	403	PLM	C6-C7-C8-C9
4	B	405	TWT	C4-C5-C6-C7
7	B	406	PC1	C26-C27-C28-C29
4	B	405	TWT	C7-C8-C9-C10
4	A	404	TWT	C15-C16-C17-C18
4	B	405	TWT	C3-C4-C5-C6
3	A	403	PLM	C8-C9-CA-CB
4	A	404	TWT	C4-C5-C6-C7
5	A	405	BOG	C3'-C4'-C5'-C6'
4	A	404	TWT	C7-C8-C9-C10
5	B	407	BOG	C3'-C4'-C5'-C6'
7	B	406	PC1	C23-C24-C25-C26
3	A	402	PLM	C8-C9-CA-CB
7	B	406	PC1	C2B-C2C-C2D-C2E
3	B	404	PLM	C4-C5-C6-C7
7	B	406	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
4	A	404	TWT	C14-C15-C16-C17
3	A	403	PLM	C6-C7-C8-C9
2	A	401	RET	C1-C6-C7-C8
2	B	402	RET	C1-C6-C7-C8
4	B	405	TWT	C15-C16-C17-C18
4	B	405	TWT	C14-C15-C16-C17
3	B	404	PLM	C7-C8-C9-CA
7	B	406	PC1	C32-C33-C34-C35
4	A	404	TWT	C11-C10-C9-C8
4	B	405	TWT	C5-C6-C7-C8
5	A	405	BOG	C5'-C6'-C7'-C8'
4	B	405	TWT	C12-C13-C14-C15
3	A	403	PLM	C4-C5-C6-C7
3	B	404	PLM	C9-CA-CB-CC
5	B	407	BOG	C1'-C2'-C3'-C4'
2	A	401	RET	C5-C6-C7-C8
5	B	407	BOG	C4-C5-C6-O6
5	B	407	BOG	O5-C5-C6-O6
5	B	407	BOG	C5'-C6'-C7'-C8'
4	A	404	TWT	C5-C6-C7-C8
2	B	402	RET	C5-C6-C7-C8
4	A	404	TWT	C13-C14-C15-C16
7	B	406	PC1	O21-C21-C22-C23
5	A	405	BOG	C1'-C2'-C3'-C4'
3	A	402	PLM	CB-CC-CD-CE
7	B	406	PC1	O22-C21-C22-C23

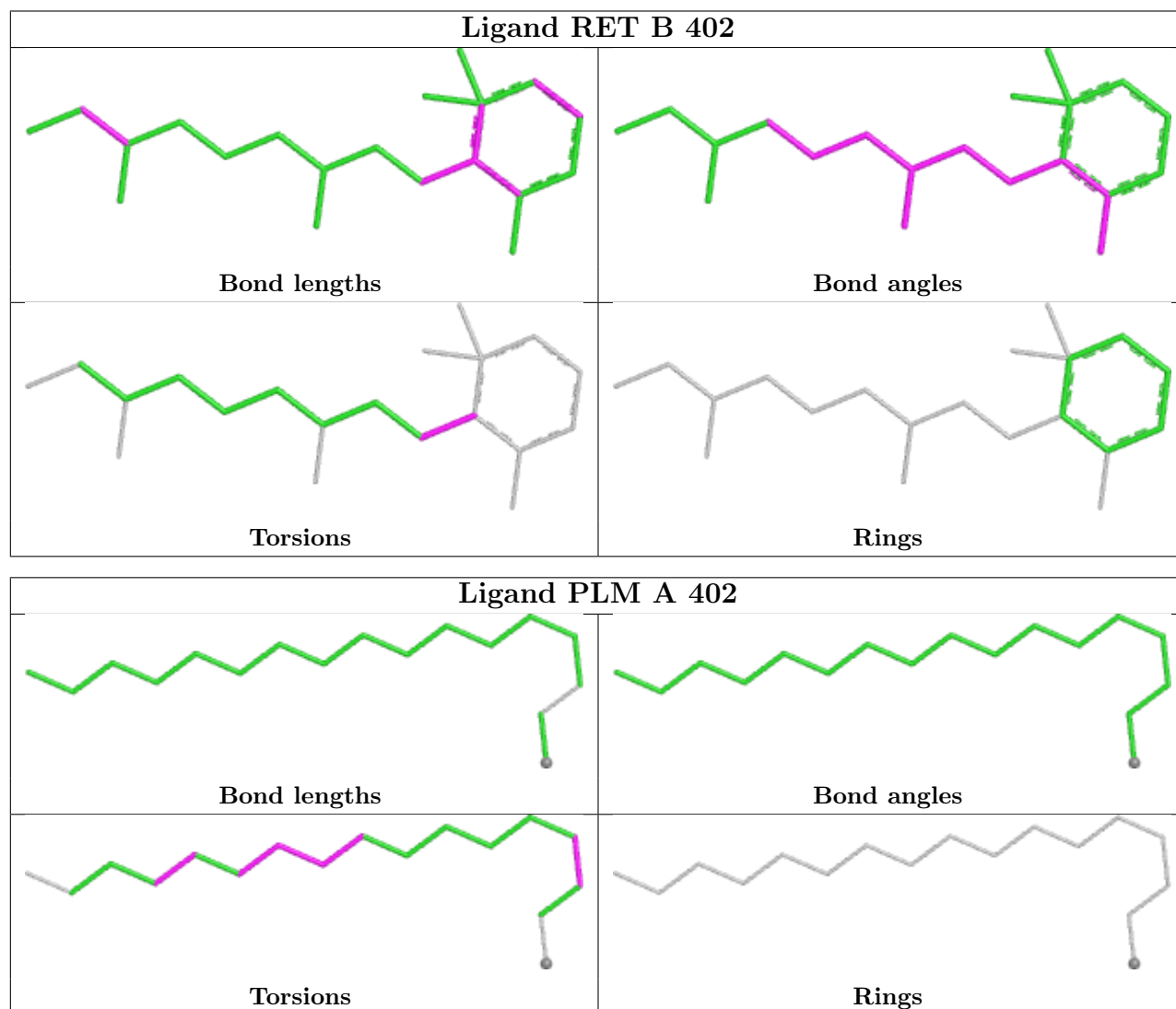
There are no ring outliers.

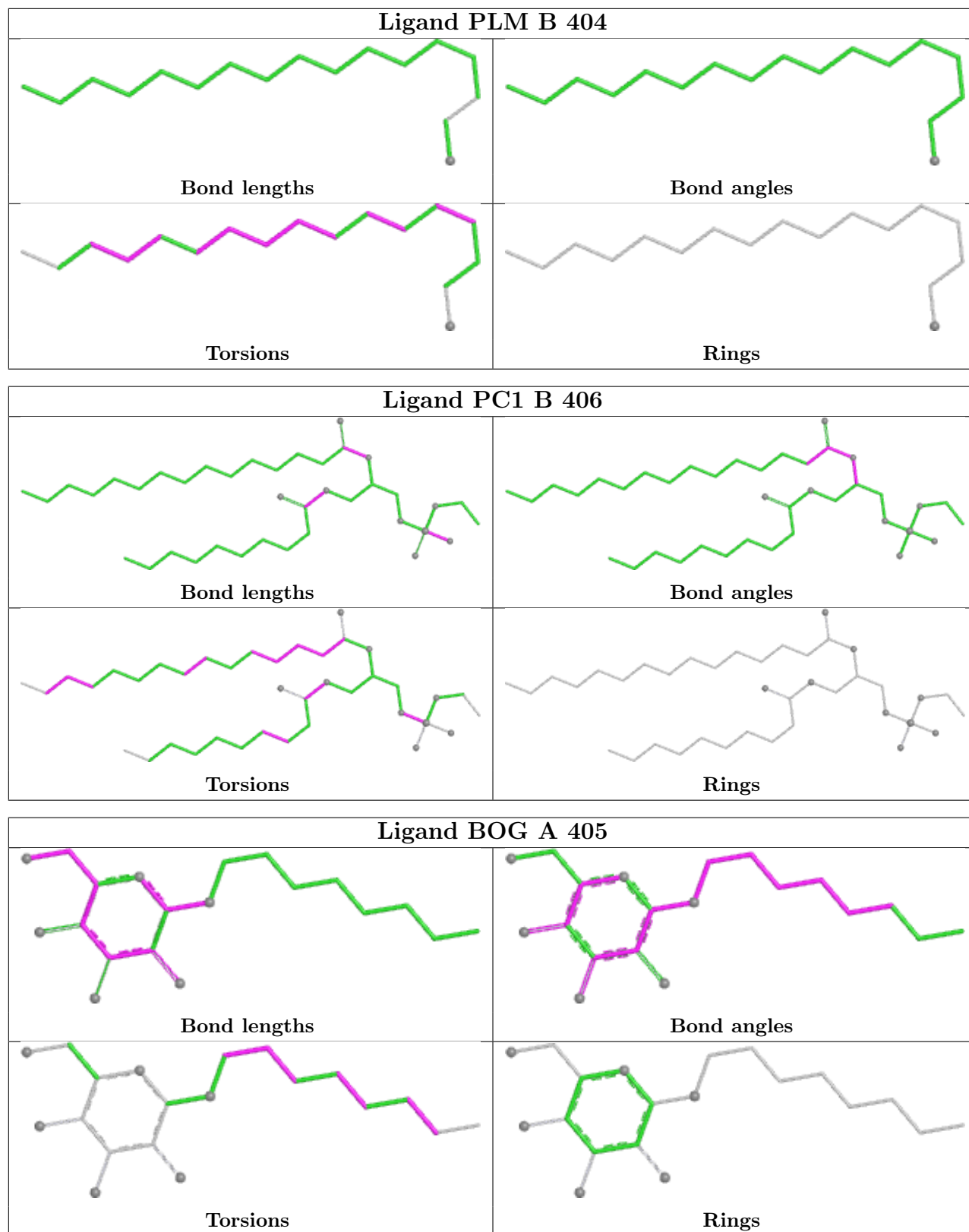
6 monomers are involved in 13 short contacts:

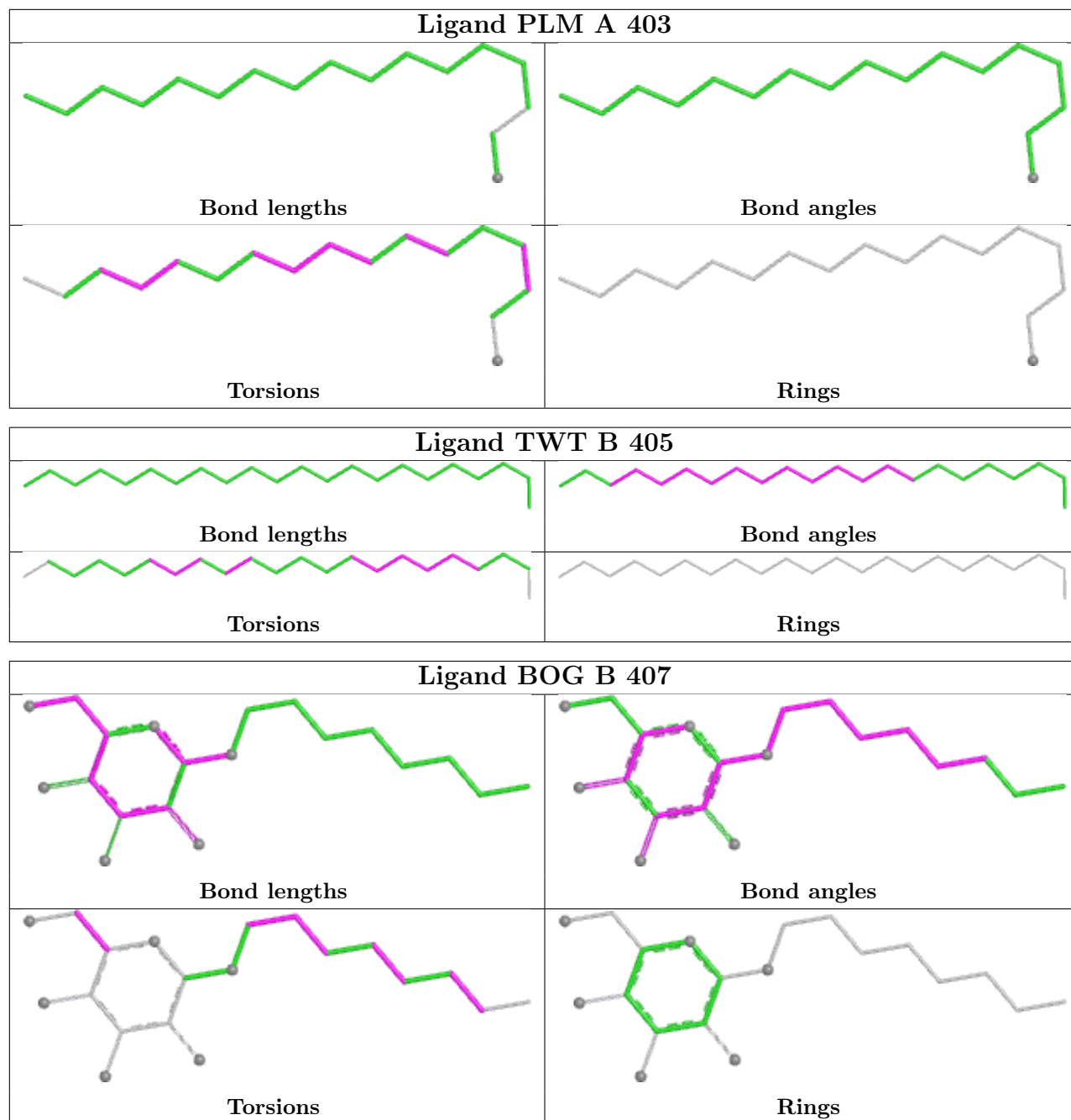
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	PLM	1	0
7	B	406	PC1	1	0
5	A	405	BOG	5	0
3	A	403	PLM	1	0
5	B	407	BOG	2	0
2	A	401	RET	3	0

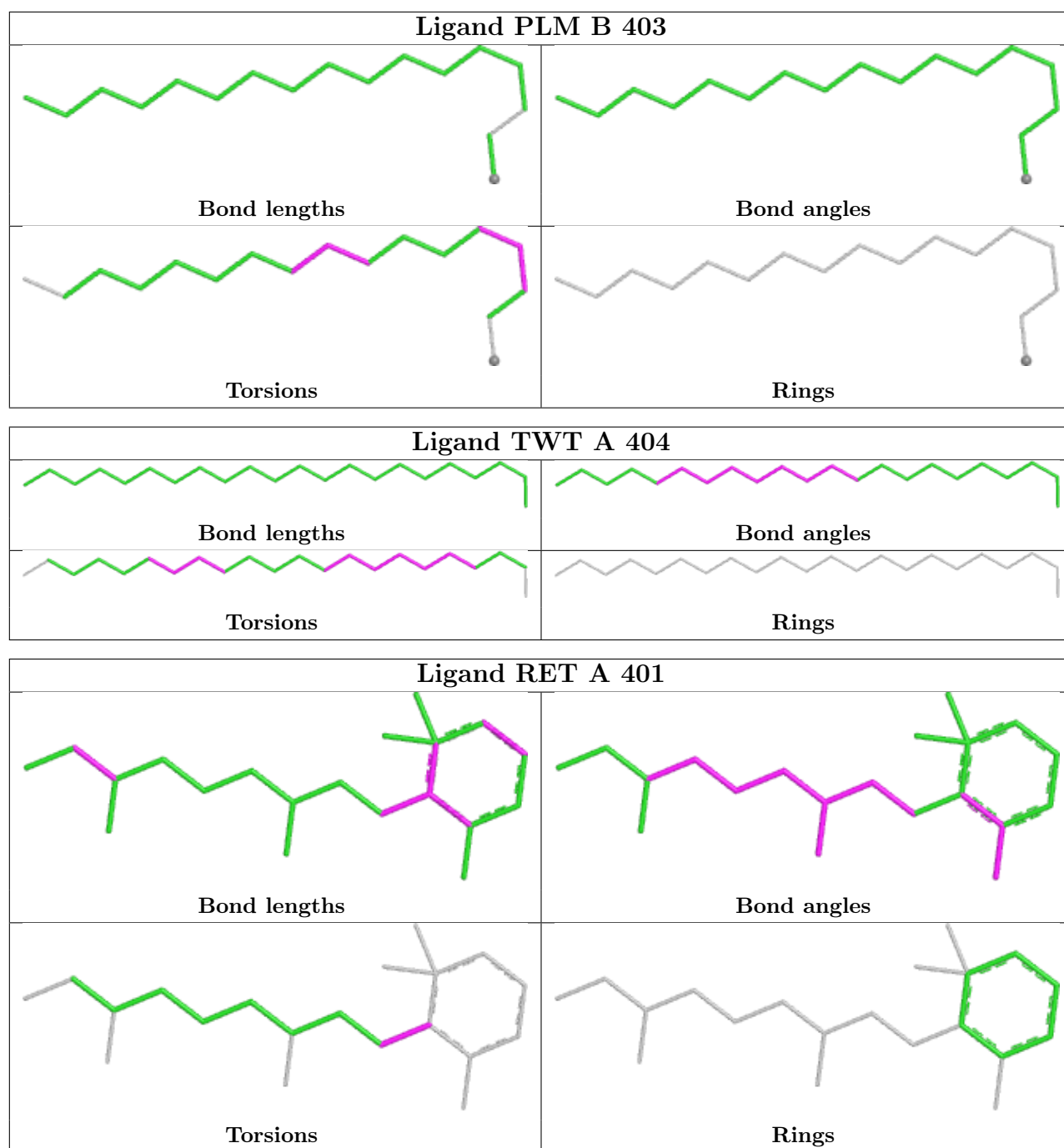
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/350 (100%)	-1.40	0 100 100	33, 62, 145, 158	0
1	B	347/350 (99%)	-1.44	0 100 100	32, 60, 124, 143	0
All	All	697/700 (99%)	-1.42	0 100 100	32, 61, 135, 158	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

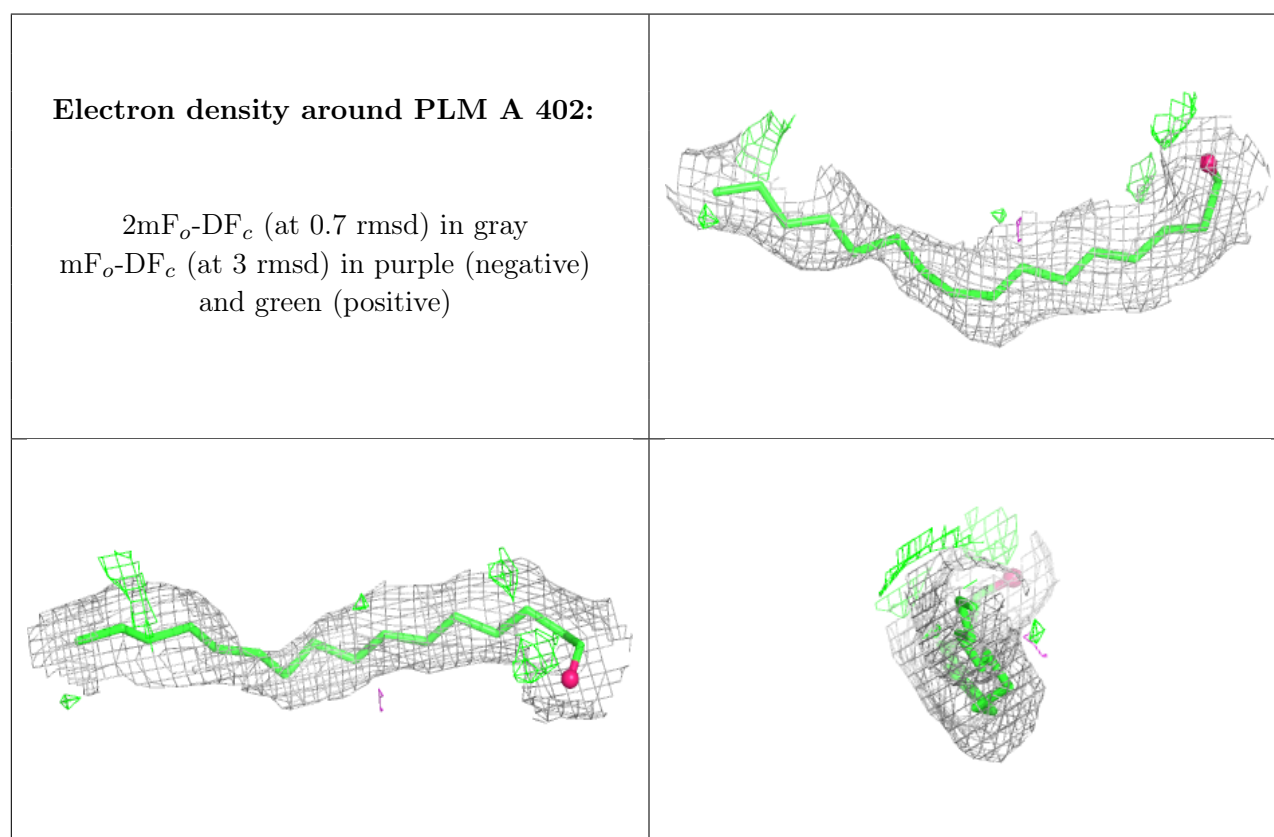
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PLM	A	402	17/18	0.98	0.05	50,57,62,63	0
3	PLM	A	403	17/18	0.98	0.08	98,108,111,111	0
3	PLM	B	404	17/18	0.98	0.09	115,115,117,118	0
3	PLM	B	403	17/18	0.99	0.05	63,69,73,74	0
2	RET	B	402	20/21	0.99	0.04	37,42,46,49	0
4	TWT	A	404	22/22	0.99	0.06	79,92,105,106	0
4	TWT	B	405	22/22	0.99	0.07	82,86,90,90	0

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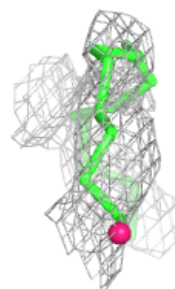
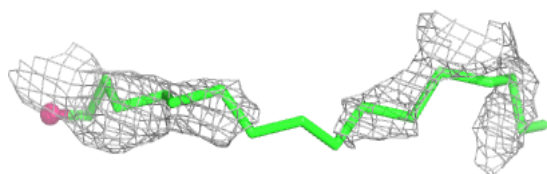
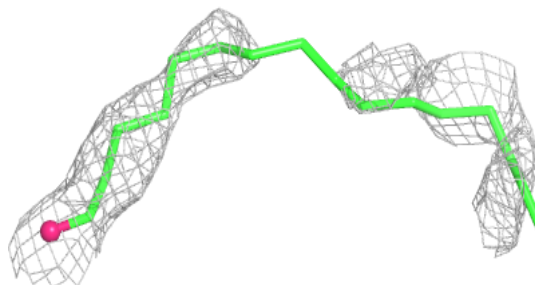
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BOG	A	405	20/20	0.99	0.04	57,105,111,112	0
5	BOG	B	407	20/20	0.99	0.05	102,116,118,119	0
6	SO4	B	401	5/5	0.99	0.05	141,141,142,142	0
7	PC1	B	406	39/54	0.99	0.06	71,88,131,131	0
2	RET	A	401	20/21	1.00	0.04	45,50,53,53	0

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

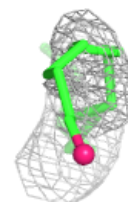
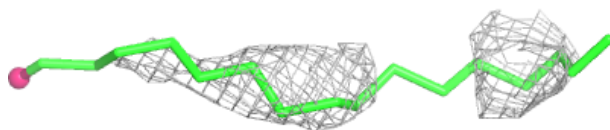
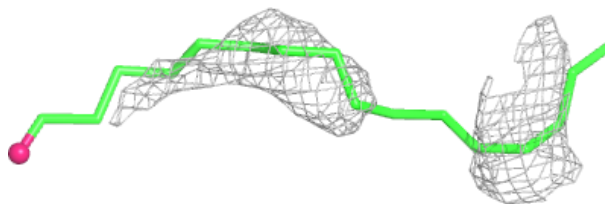


Electron density around PLM A 403:

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

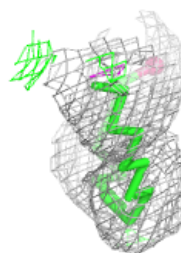
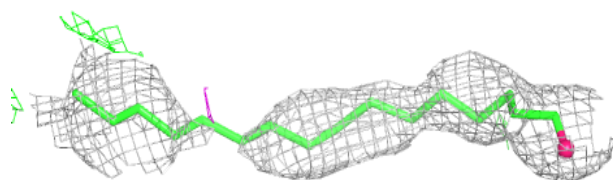
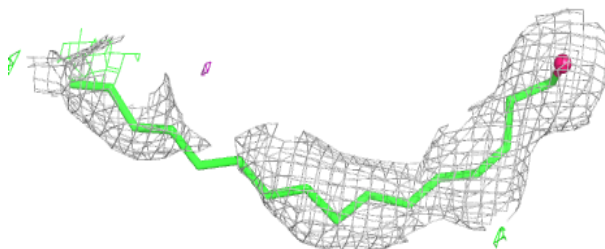
**Electron density around PLM B 404:**

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

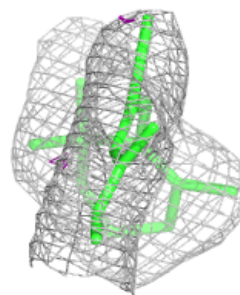
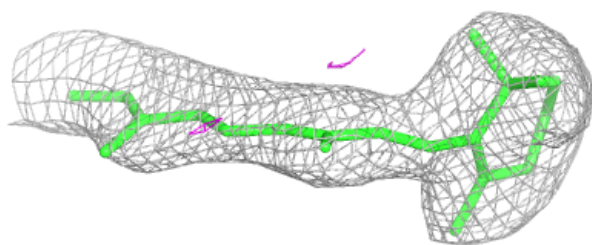
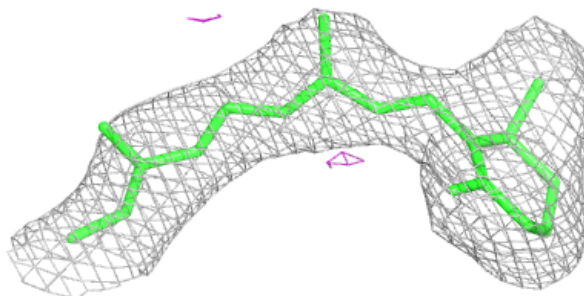


Electron density around PLM B 403:

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

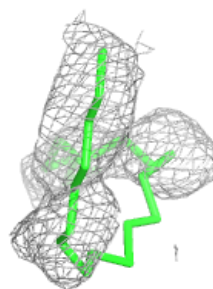
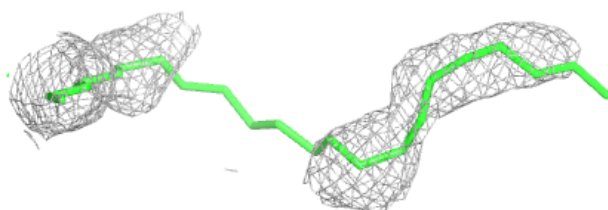
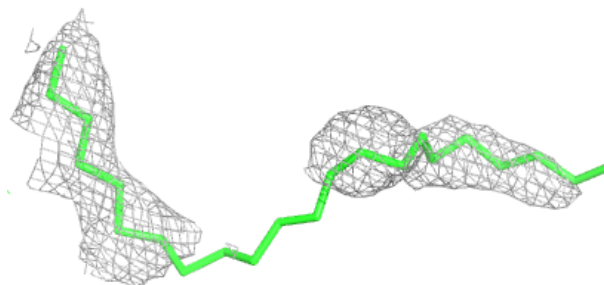
**Electron density around RET B 402:**

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

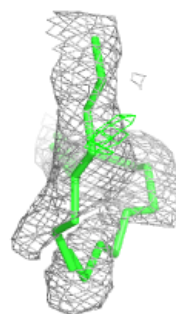
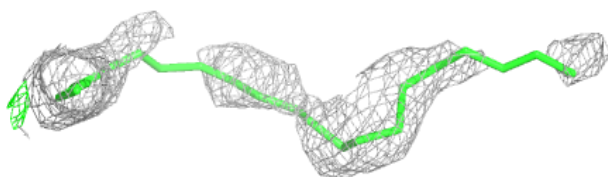
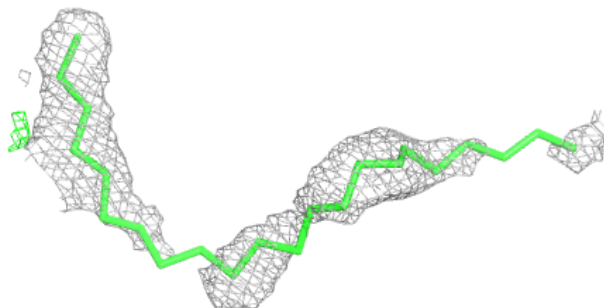


Electron density around TWT A 404:

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

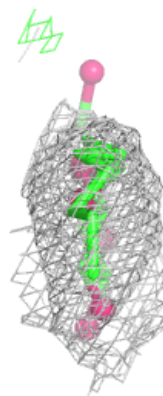
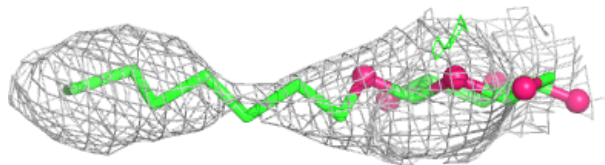
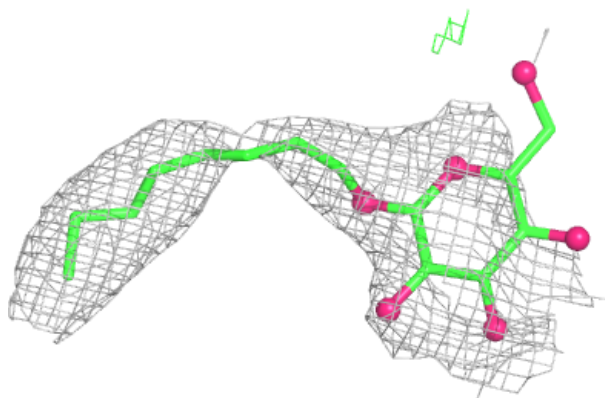
**Electron density around TWT B 405:**

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

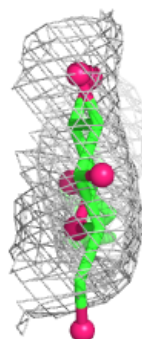
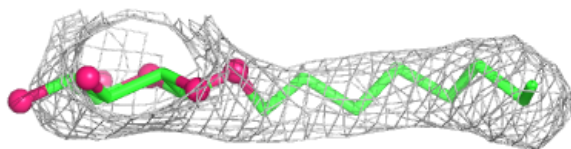
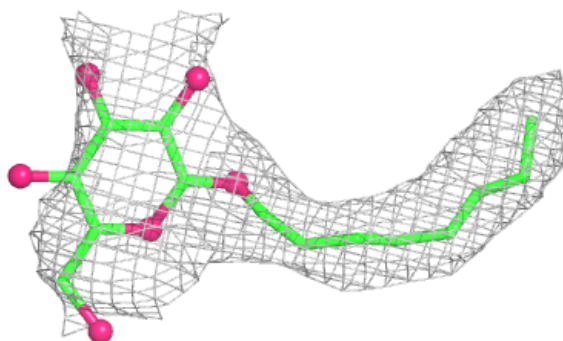


Electron density around BOG A 405:

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

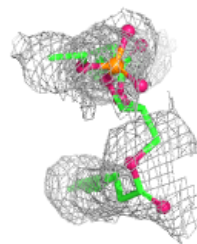
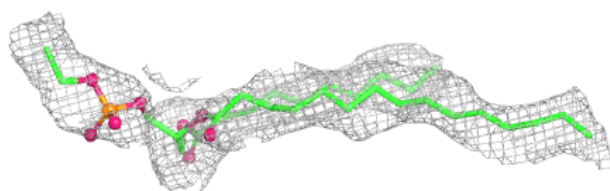
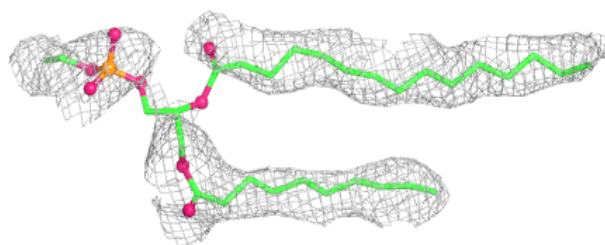
**Electron density around BOG B 407:**

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

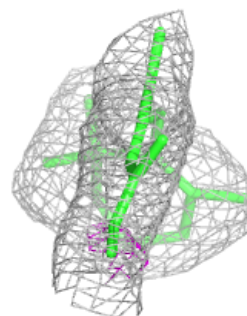
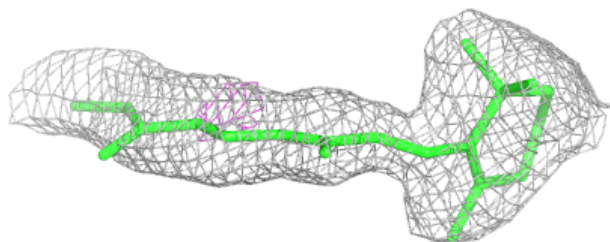
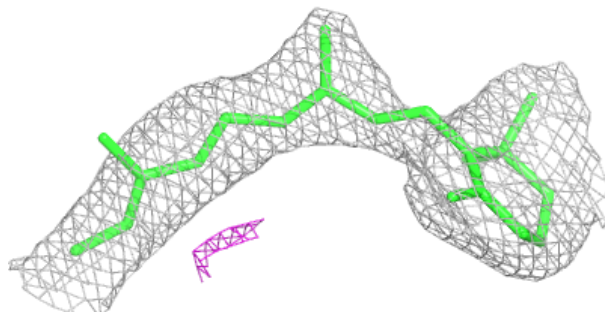


Electron density around PC1 B 406:

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

**Electron density around RET A 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.