Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:37 PM BST

PDB ID	:	3AYN
Title	:	Crystal structure of squid isorhodopsin
Authors	:	Murakami, M.; Kouyama, T.
Deposited on	:	2011-05-09
Resolution	:	2.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

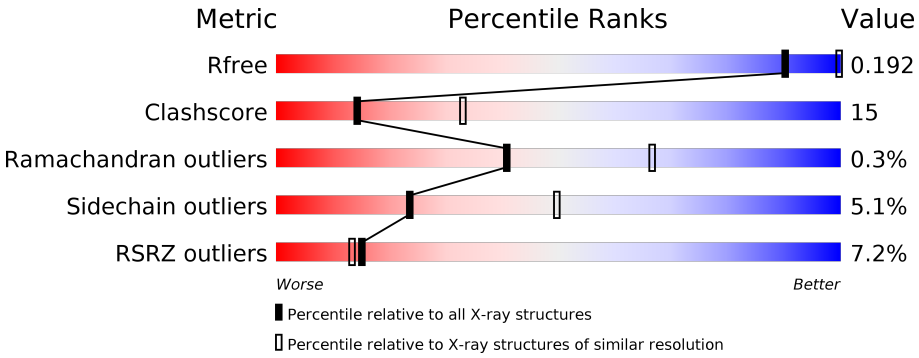
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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 <=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	448	8% 51% 26% • 22%
1	B	448	3% 51% 23% • 23%

2 Entry composition

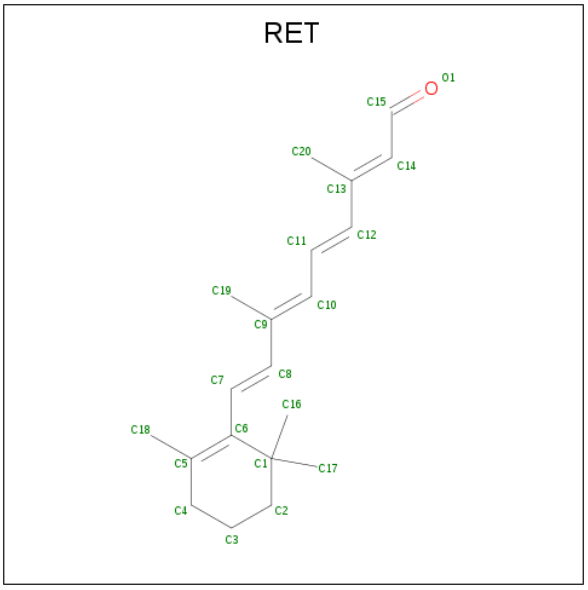
There are 7 unique types of molecules in this entry. The entry contains 5756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

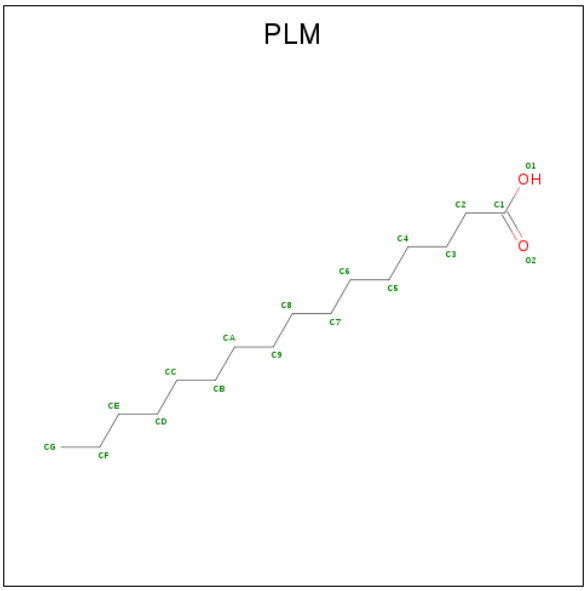
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2780	1838	443	473	26			
1	B	347	Total	C	N	O	S	0	0	0
			2762	1828	440	468	26			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



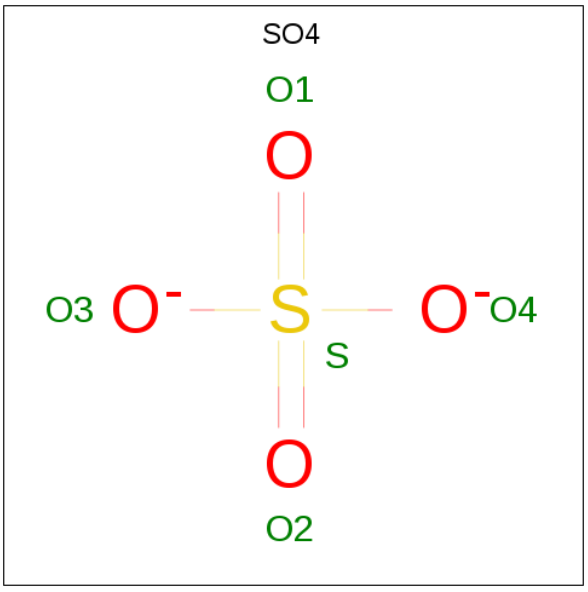
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		
2	B	1	Total	C	0	0
			20	20		

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



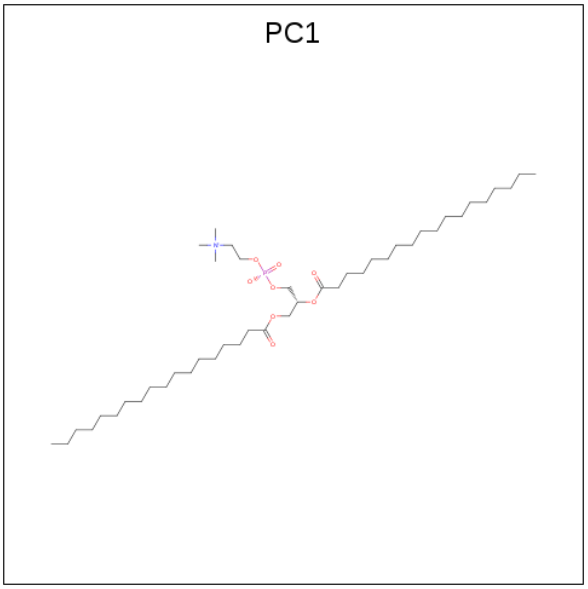
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 17 16 1	0	0
3	A	1	Total C O 17 16 1	0	0
3	B	1	Total C O 17 16 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



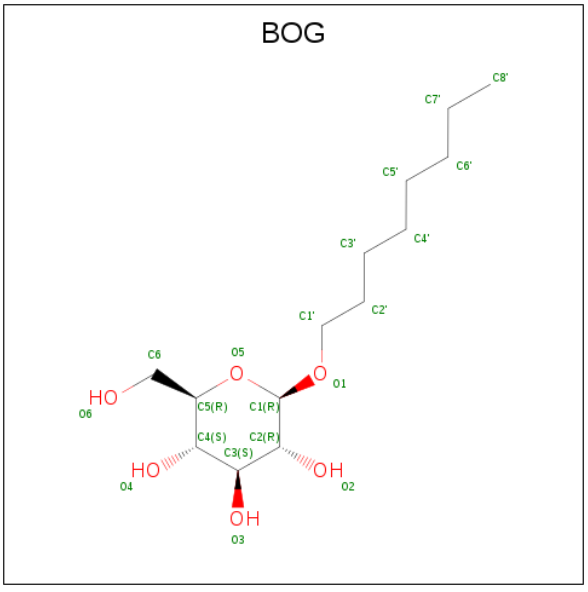
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



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

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 7 is water.

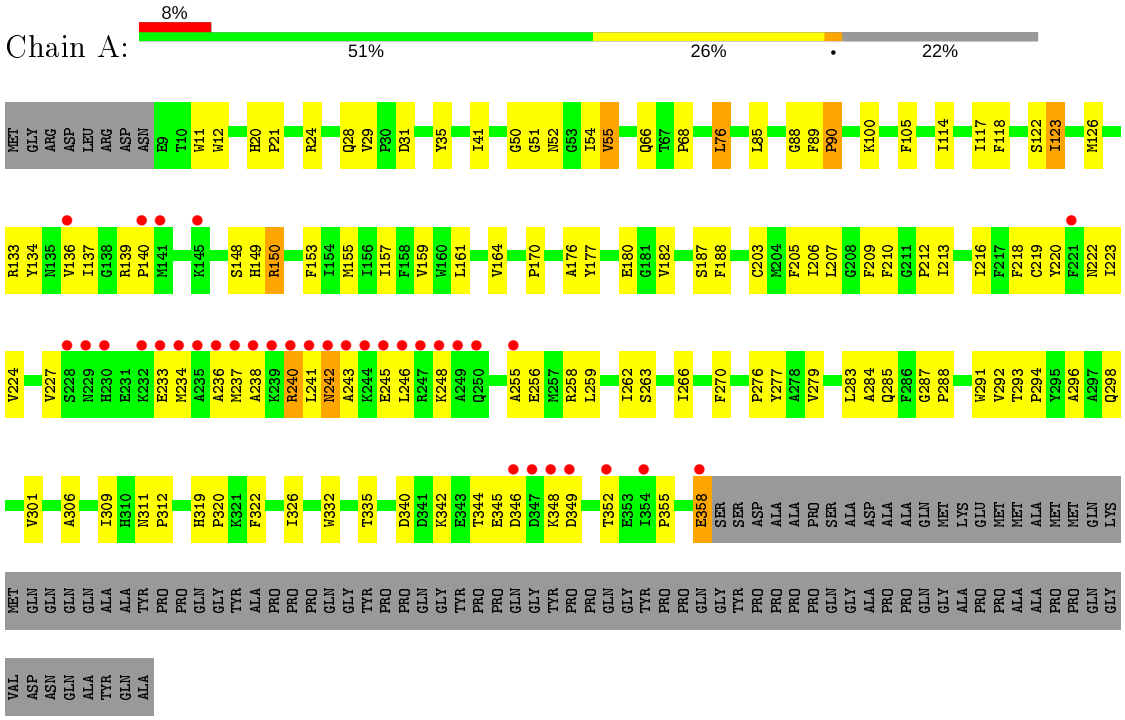
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	29	Total O 29 29	0	0
7	B	30	Total O 30 30	0	0

3 Residue-property plots (i)

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.

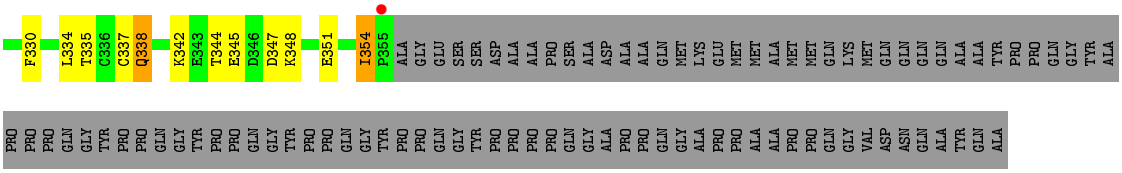
- Molecule 1: Rhodopsin

Chain A:



- Molecule 1: Rhodopsin

Chain B:


F330
L334
T335
C336
C337
Q338
K342
E343
T344
E345
D346
D347
K348
E351
I354
P355
ALA GLY GLU SER SER ASP ALA ALA PRO SER ALA ASP ALA ALA GLN MET LYS GLU MET MET ALA MET MET GLN LYS MET GLN GLN GLN GLN ALA ALA TYR PRO PRO GLN GLY TYR ALA
PRO PRO PRO GLN GLY TYR PRO PRO GLN GLY TYR PRO PRO GLN GLY TYR PRO PRO PRO PRO PRO GLN GLY ALA PRO PRO GLN GLY ALA PRO PRO ALA ALA ALA PRO PRO GLN GLY VAL ASP ASN GLN ALA TYR GLN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	122.54Å 122.54Å 158.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.70 61.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (15.00-2.70) 91.4 (61.27-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.180 , 0.200 0.177 , 0.192	Depositor DCC
R_{free} test set	1679 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 87.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5756	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PLM, PC1, SO4, RET, BOG

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	0.39	0/2865	0.57	0/3889
1	B	0.41	0/2847	0.57	0/3865
All	All	0.40	0/5712	0.57	0/7754

There are no bond length outliers.

There are no bond angle outliers.

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	2780	0	2766	95	0
1	B	2762	0	2752	82	0
2	A	20	0	27	0	0
2	B	20	0	27	1	0
3	A	34	0	62	0	0
3	B	17	0	31	0	0
4	B	5	0	0	0	0
5	B	39	0	49	1	0
6	B	20	0	28	3	0
7	A	29	0	0	3	0
7	B	30	0	0	2	0
All	All	5756	0	5742	177	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 15.

All (177) 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:354:ILE:H	1:B:354:ILE:HD13	1.29	0.98
1:B:150:ARG:H	1:B:150:ARG:HD2	1.29	0.96
1:A:284:ALA:HB2	1:A:292:VAL:HG21	1.47	0.94
1:A:21:PRO:HA	1:A:24:ARG:HD3	1.48	0.93
1:A:117:ILE:HD11	1:A:164:VAL:HG22	1.58	0.84
1:B:113:PHE:O	1:B:117:ILE:HG23	1.87	0.75
1:A:21:PRO:CA	1:A:24:ARG:HD3	2.17	0.73
1:B:237:MET:O	1:B:242:ASN:HB2	1.88	0.73
1:A:218:PHE:O	1:A:222:ASN:HB2	1.90	0.71
1:B:41:ILE:HG13	1:B:88:GLY:HA2	1.73	0.71
1:B:148:SER:HB2	1:B:150:ARG:HH21	1.57	0.69
1:A:298:GLN:O	1:A:301:VAL:HG12	1.93	0.68
1:A:137:ILE:HD11	1:A:256:GLU:HB2	1.76	0.68
1:B:319:HIS:HB3	1:B:322:PHE:HB3	1.76	0.66
1:B:298:GLN:O	1:B:301:VAL:HG12	1.95	0.66
1:B:306:ALA:O	1:B:309:ILE:HG12	1.95	0.65
1:A:241:LEU:N	1:A:241:LEU:HD12	2.12	0.64
1:B:73:ILE:HD11	6:B:1005:BOG:H7'2	1.78	0.64
1:A:306:ALA:O	1:A:309:ILE:HG12	1.98	0.64
1:A:340:ASP:OD2	1:A:342:LYS:HB2	1.98	0.63
1:B:67:THR:HG21	6:B:1005:BOG:H5	1.80	0.61
1:B:150:ARG:CD	1:B:150:ARG:H	2.10	0.61
1:B:242:ASN:ND2	1:B:245:GLU:HG3	2.16	0.60
1:A:320:PRO:HG2	7:A:521:HOH:O	2.02	0.60
1:B:354:ILE:H	1:B:354:ILE:CD1	2.07	0.60
1:B:102:ILE:HD13	1:B:102:ILE:H	1.66	0.60
1:A:139:ARG:HB3	1:A:140:PRO:HD2	1.83	0.58
1:B:123:ILE:HG12	1:B:270:PHE:CZ	2.38	0.58
1:A:133:ARG:NH2	1:A:136:VAL:HG11	2.19	0.57
1:A:122:SER:O	1:A:126:MET:HG3	2.05	0.57
1:B:117:ILE:HG13	1:B:118:PHE:N	2.19	0.57
1:B:52:ASN:HA	1:B:55:VAL:HG12	1.86	0.57
1:A:344:THR:O	1:A:348:LYS:HG3	2.05	0.56
1:A:279:VAL:O	1:A:283:LEU:HD13	2.05	0.56
1:B:301:VAL:O	1:B:305:LYS:HG3	2.05	0.56
1:A:50:GLY:O	1:A:54:ILE:HG13	2.04	0.56
1:B:52:ASN:HA	1:B:55:VAL:CG1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASP:O	1:B:351:GLU:HG2	2.06	0.56
1:B:311:ASN:HB2	1:B:312:PRO:HD3	1.88	0.55
1:A:348:LYS:O	1:A:352:THR:HG23	2.07	0.55
1:B:238:ALA:HA	1:B:246:LEU:HD13	1.90	0.54
1:A:259:LEU:HD13	1:A:262:ILE:HD12	1.90	0.54
1:A:342:LYS:HA	1:A:345:GLU:HG3	1.90	0.54
1:B:60:THR:HG22	1:B:74:ILE:HD13	1.91	0.53
1:A:148:SER:HB2	1:A:150:ARG:HH11	1.73	0.53
1:A:345:GLU:HA	1:A:348:LYS:HD2	1.89	0.53
1:B:284:ALA:HB2	1:B:292:VAL:HG21	1.91	0.53
1:B:323:ARG:HH12	1:B:337:CYS:HB3	1.73	0.53
1:A:52:ASN:O	1:A:55:VAL:HG13	2.09	0.53
1:A:216:ILE:HG23	1:A:220:TYR:CE2	2.44	0.53
1:A:311:ASN:HB2	1:A:312:PRO:HD3	1.91	0.52
1:A:332:TRP:O	1:A:335:THR:HG23	2.09	0.52
1:B:182:VAL:HG22	1:B:298:GLN:OE1	2.09	0.52
1:B:79:SER:HB2	1:B:121:MET:CE	2.40	0.52
1:B:136:VAL:HG23	1:B:137:ILE:HG12	1.92	0.51
1:A:355:PRO:HG2	1:A:358:GLU:HA	1.93	0.51
1:B:63:LYS:HA	1:B:66:GLN:NE2	2.25	0.51
1:A:20:HIS:ND1	1:A:21:PRO:HD2	2.26	0.51
1:A:219:CYS:O	1:A:223:ILE:HG13	2.10	0.51
1:A:206:ILE:HA	1:A:210:PHE:CD2	2.46	0.50
1:A:276:PRO:HB2	7:A:510:HOH:O	2.10	0.50
1:B:87:ASN:HA	1:B:111:TYR:CE1	2.45	0.50
1:A:149:HIS:HB2	1:A:150:ARG:NH2	2.26	0.50
1:A:12:TRP:CD2	1:A:24:ARG:HG2	2.46	0.50
1:B:322:PHE:CE2	1:B:326:ILE:HD11	2.47	0.50
1:A:12:TRP:CE3	1:A:24:ARG:HG2	2.46	0.50
1:B:79:SER:HB2	1:B:121:MET:HE2	1.93	0.50
1:B:323:ARG:HH12	1:B:337:CYS:CB	2.25	0.50
1:B:212:PRO:O	1:B:216:ILE:HG13	2.12	0.50
1:A:237:MET:HA	1:A:240:ARG:HB2	1.93	0.50
1:B:229:ASN:O	1:B:233:GLU:HG3	2.11	0.50
1:A:236:ALA:O	1:A:240:ARG:HB2	2.11	0.50
1:B:197:THR:O	1:B:201:ILE:HG13	2.11	0.49
1:B:219:CYS:O	1:B:223:ILE:HG13	2.13	0.49
1:B:317:VAL:O	1:B:317:VAL:HG12	2.12	0.49
1:A:114:ILE:HA	1:A:117:ILE:HG22	1.95	0.48
1:A:176:ALA:O	1:A:188:PHE:HA	2.14	0.48
1:A:52:ASN:HA	1:A:55:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HB2	1:B:300:PRO:HD3	1.96	0.48
1:A:242:ASN:OD1	1:A:246:LEU:HD13	2.14	0.47
1:A:68:PRO:HG3	1:A:149:HIS:CE1	2.49	0.47
1:B:296:ALA:O	1:B:300:PRO:HG2	2.14	0.47
1:A:207:LEU:HD22	1:A:207:LEU:N	2.29	0.47
1:A:203:CYS:HA	1:A:207:LEU:HD23	1.97	0.47
1:B:138:GLY:HA2	1:B:223:ILE:HA	1.97	0.47
1:B:294:PRO:O	1:B:298:GLN:HB2	2.14	0.47
1:A:284:ALA:CB	1:A:292:VAL:HG21	2.32	0.47
1:B:166:TRP:CZ2	1:B:207:LEU:HG	2.49	0.47
1:B:235:ALA:C	1:B:237:MET:H	2.18	0.47
1:B:243:ALA:N	1:B:245:GLU:OE2	2.47	0.47
1:A:241:LEU:CD1	1:A:241:LEU:N	2.76	0.47
1:A:258:ARG:O	1:A:262:ILE:HG13	2.15	0.47
1:B:247:ARG:O	1:B:251:ALA:HB2	2.15	0.47
1:A:150:ARG:NE	1:A:150:ARG:H	2.13	0.47
1:B:204:MET:SD	2:B:1000:RET:H192	2.55	0.47
1:B:124:MET:O	1:B:128:MET:HG2	2.15	0.47
1:B:176:ALA:O	1:B:188:PHE:HA	2.15	0.46
1:A:212:PRO:O	1:A:216:ILE:HG13	2.15	0.46
1:A:51:GLY:O	1:A:55:VAL:HG12	2.15	0.46
1:A:114:ILE:O	1:A:117:ILE:HG22	2.15	0.46
1:A:155:MET:O	1:A:159:VAL:HG23	2.15	0.46
1:A:177:TYR:HA	1:A:187:SER:O	2.16	0.46
1:B:127:ALA:O	1:B:131:ILE:HG13	2.16	0.46
1:A:161:LEU:HD13	1:A:161:LEU:HA	1.82	0.46
1:A:76:LEU:HD13	1:A:311:ASN:HD22	1.80	0.46
1:B:293:THR:H	1:B:296:ALA:HB3	1.80	0.46
1:A:285:GLN:HE21	1:A:285:GLN:HA	1.80	0.46
1:A:11:TRP:CD2	1:A:28:GLN:HB2	2.52	0.45
1:A:133:ARG:HA	1:A:133:ARG:NE	2.30	0.45
1:B:263:SER:O	1:B:266:ILE:HG12	2.16	0.45
1:A:133:ARG:CZ	1:A:136:VAL:HG11	2.46	0.45
1:A:293:THR:N	1:A:296:ALA:HB3	2.32	0.45
1:B:100:LYS:HB2	1:B:100:LYS:HE2	1.77	0.45
1:A:248:LYS:HG3	1:A:349:ASP:O	2.17	0.45
1:B:202:LEU:HD12	5:B:1004:PC1:H361	1.98	0.45
1:A:123:ILE:HG12	1:A:270:PHE:CZ	2.52	0.45
1:A:322:PHE:CE2	1:A:326:ILE:HD11	2.52	0.45
1:B:105:PHE:O	1:B:109:LYS:HG3	2.16	0.45
1:B:117:ILE:HG22	1:B:167:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HB2	7:B:511:HOH:O	2.17	0.44
1:B:223:ILE:O	1:B:224:VAL:C	2.56	0.44
1:B:344:THR:O	1:B:348:LYS:HG3	2.17	0.44
1:A:220:TYR:OH	1:A:263:SER:HB3	2.18	0.44
1:B:298:GLN:O	1:B:302:MET:HG2	2.17	0.44
1:A:309:ILE:O	1:A:309:ILE:HG13	2.17	0.44
1:A:220:TYR:O	1:A:224:VAL:HG23	2.17	0.44
1:A:31:ASP:HB3	1:A:35:TYR:CE1	2.53	0.44
1:A:224:VAL:O	1:A:227:VAL:HG23	2.18	0.43
1:A:294:PRO:O	1:A:298:GLN:HB2	2.19	0.43
1:B:150:ARG:N	1:B:150:ARG:HD2	2.11	0.43
1:B:322:PHE:CZ	1:B:326:ILE:HD11	2.54	0.43
1:B:55:VAL:HG23	1:B:59:PHE:CD1	2.53	0.43
1:B:342:LYS:HA	1:B:345:GLU:OE1	2.19	0.43
1:A:255:ALA:O	1:A:259:LEU:HD23	2.18	0.43
1:A:134:TYR:O	1:A:139:ARG:HG3	2.19	0.43
1:A:206:ILE:HA	1:A:210:PHE:HD2	1.84	0.43
1:B:297:ALA:O	1:B:300:PRO:HD2	2.19	0.43
1:A:243:ALA:HB3	1:A:245:GLU:OE2	2.19	0.42
1:A:263:SER:O	1:A:266:ILE:HG12	2.19	0.42
1:A:216:ILE:HG23	1:A:220:TYR:HE2	1.83	0.42
1:A:242:ASN:ND2	1:A:245:GLU:HG3	2.34	0.42
1:A:209:PHE:O	1:A:213:ILE:HG13	2.19	0.42
1:A:29:VAL:HG22	7:A:523:HOH:O	2.18	0.42
1:B:326:ILE:O	1:B:330:PHE:N	2.46	0.42
1:A:170:PRO:HB2	1:A:177:TYR:CD2	2.55	0.42
1:B:165:LEU:O	1:B:168:ILE:HG22	2.19	0.42
1:B:136:VAL:HG11	7:B:528:HOH:O	2.19	0.42
1:B:73:ILE:HD11	6:B:1005:BOG:H5'2	2.02	0.42
1:A:233:GLU:O	1:A:237:MET:HG2	2.20	0.41
1:A:153:PHE:O	1:A:157:ILE:HG13	2.20	0.41
1:A:100:LYS:HB2	1:A:100:LYS:HE2	1.93	0.41
1:B:228:SER:O	1:B:231:GLU:HG2	2.19	0.41
1:A:342:LYS:HA	1:A:345:GLU:CG	2.50	0.41
1:B:83:PHE:O	1:B:87:ASN:HB2	2.19	0.41
1:A:89:PHE:HA	1:A:90:PRO:HA	1.88	0.41
1:B:117:ILE:HG22	1:B:167:ALA:CB	2.51	0.41
1:A:117:ILE:HG23	1:A:118:PHE:CD1	2.55	0.41
1:A:238:ALA:HA	1:A:246:LEU:HD22	2.03	0.41
1:A:293:THR:H	1:A:296:ALA:HB3	1.85	0.41
1:B:216:ILE:HG23	1:B:220:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:PRO:HB2	1:A:291:TRP:CD2	2.56	0.41
1:B:31:ASP:HB3	1:B:35:TYR:CZ	2.56	0.41
1:A:182:VAL:HG22	1:A:298:GLN:OE1	2.21	0.41
1:B:354:ILE:N	1:B:354:ILE:HD13	2.13	0.41
1:B:52:ASN:O	1:B:56:ILE:HG13	2.21	0.41
1:B:62:THR:HB	1:B:65:LEU:HD12	2.02	0.41
1:A:180:GLU:OE1	1:A:277:TYR:OH	2.30	0.41
1:A:210:PHE:HA	1:A:213:ILE:HD12	2.02	0.41
1:A:319:HIS:HB3	1:A:322:PHE:HB3	2.02	0.41
1:B:261:LYS:O	1:B:265:VAL:HG23	2.21	0.41
1:B:334:LEU:O	1:B:338:GLN:N	2.37	0.40
1:A:322:PHE:O	1:A:326:ILE:HG13	2.21	0.40
1:B:244:LYS:C	1:B:246:LEU:N	2.75	0.40
1:A:205:PHE:O	1:A:209:PHE:HB3	2.22	0.40
1:B:269:GLN:NE2	1:B:310:HIS:HD2	2.19	0.40
1:A:283:LEU:O	1:A:287:GLY:N	2.48	0.40
1:A:41:ILE:HG13	1:A:88:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	348/448 (78%)	316 (91%)	32 (9%)	0	100 100
1	B	345/448 (77%)	316 (92%)	27 (8%)	2 (1%)	25 50
All	All	693/896 (77%)	632 (91%)	59 (8%)	2 (0%)	41 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLN

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Mol	Chain	Res	Type
1	B	223	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	296/369 (80%)	283 (96%)	13 (4%)	28 56
1	B	295/369 (80%)	278 (94%)	17 (6%)	20 43
All	All	591/738 (80%)	561 (95%)	30 (5%)	24 50

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	66	GLN
1	A	76	LEU
1	A	85	LEU
1	A	90	PRO
1	A	105	PHE
1	A	123	ILE
1	A	150	ARG
1	A	234	MET
1	A	240	ARG
1	A	242	ASN
1	A	346	ASP
1	A	358	GLU
1	B	10	THR
1	B	66	GLN
1	B	76	LEU
1	B	85	LEU
1	B	102	ILE
1	B	105	PHE
1	B	117	ILE
1	B	123	ILE
1	B	133	ARG

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Mol	Chain	Res	Type
1	B	150	ARG
1	B	225	MET
1	B	242	ASN
1	B	245	GLU
1	B	247	ARG
1	B	303	PHE
1	B	335	THR
1	B	354	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	87	ASN
1	A	222	ASN
1	A	229	ASN
1	A	230	HIS
1	A	254	ASN
1	A	269	GLN
1	A	328	GLN
1	B	70	ASN
1	B	135	ASN
1	B	242	ASN
1	B	269	GLN
1	B	328	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
5	PC1	B	1004	-	38,38,53	1.59	3 (7%)	41,43,61	0.97	1 (2%)
2	RET	A	1000	1	20,20,21	1.94	4 (20%)	27,27,28	1.22	3 (11%)
2	RET	B	1000	1	20,20,21	1.78	4 (20%)	27,27,28	1.15	4 (14%)
3	PLM	B	1001	-	16,16,17	0.35	0	15,15,17	0.65	0
3	PLM	A	1004	-	16,16,17	0.31	0	15,15,17	0.66	0
6	BOG	B	1005	-	20,20,20	1.83	7 (35%)	25,25,25	2.84	11 (44%)
4	SO4	B	449	-	4,4,4	0.27	0	6,6,6	0.06	0
3	PLM	A	1001	-	16,16,17	0.31	0	15,15,17	0.68	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
5	PC1	B	1004	-	-	14/42/42/57	-
2	RET	A	1000	1	-	2/13/30/31	0/1/1/1
2	RET	B	1000	1	-	2/13/30/31	0/1/1/1
3	PLM	B	1001	-	-	8/13/14/15	-
3	PLM	A	1004	-	-	6/13/14/15	-
6	BOG	B	1005	-	-	5/11/31/31	0/1/1/1
3	PLM	A	1001	-	-	5/13/14/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	PC1	O21-C21	7.28	1.54	1.34
2	A	1000	RET	C14-C13	5.68	1.38	1.33
2	B	1000	RET	C14-C13	5.29	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	RET	C1-C6	4.68	1.60	1.53
5	B	1004	PC1	O31-C31	4.01	1.45	1.33
2	B	1000	RET	C1-C6	3.88	1.59	1.53
6	B	1005	BOG	O5-C1	3.84	1.51	1.41
6	B	1005	BOG	C4-C3	2.70	1.59	1.52
2	A	1000	RET	C7-C6	2.56	1.54	1.45
6	B	1005	BOG	C4-C5	-2.51	1.47	1.53
2	A	1000	RET	C5-C6	2.51	1.38	1.34
6	B	1005	BOG	O6-C6	2.47	1.52	1.42
2	B	1000	RET	C7-C6	2.43	1.53	1.45
6	B	1005	BOG	O2-C2	2.31	1.48	1.43
2	B	1000	RET	C5-C6	2.23	1.38	1.34
6	B	1005	BOG	O1-C1	-2.17	1.36	1.40
6	B	1005	BOG	C3-C2	-2.11	1.46	1.52
5	B	1004	PC1	P-O14	2.09	1.58	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1005	BOG	C1'-O1-C1	-8.47	99.80	113.84
6	B	1005	BOG	O1-C1-C2	-4.79	100.83	108.30
6	B	1005	BOG	C1-C2-C3	-4.35	100.93	110.00
6	B	1005	BOG	O5-C5-C4	-4.25	101.98	109.69
6	B	1005	BOG	O3-C3-C2	-3.74	101.71	110.35
5	B	1004	PC1	O21-C21-C22	3.14	118.28	111.50
2	A	1000	RET	C19-C9-C10	-3.12	118.55	122.92
2	B	1000	RET	C19-C9-C10	-3.02	118.70	122.92
2	A	1000	RET	C7-C8-C9	2.89	130.60	126.23
6	B	1005	BOG	O4-C4-C5	-2.79	102.37	109.30
6	B	1005	BOG	C4'-C3'-C2'	-2.75	100.44	114.42
2	B	1000	RET	C8-C9-C10	2.66	123.02	118.94
6	B	1005	BOG	C3'-C2'-C1'	-2.60	101.97	113.49
6	B	1005	BOG	C6'-C5'-C4'	-2.57	101.36	114.42
2	A	1000	RET	C8-C9-C10	2.53	122.82	118.94
6	B	1005	BOG	O1-C1'-C2'	-2.41	101.14	109.56
2	B	1000	RET	C7-C8-C9	2.19	129.55	126.23
6	B	1005	BOG	C5'-C4'-C3'	-2.19	103.32	114.42
2	B	1000	RET	C18-C5-C6	2.01	126.78	124.53

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1004	PC1	C1-O11-P-O12
5	B	1004	PC1	C1-O11-P-O14
3	A	1001	PLM	C1-C2-C3-C4
5	B	1004	PC1	C32-C31-O31-C3
5	B	1004	PC1	O32-C31-O31-C3
6	B	1005	BOG	O5-C5-C6-O6
5	B	1004	PC1	C1-O11-P-O13
3	B	1001	PLM	C7-C8-C9-CA
3	A	1004	PLM	C8-C9-CA-CB
5	B	1004	PC1	C22-C23-C24-C25
3	B	1001	PLM	C2-C3-C4-C5
3	A	1004	PLM	C7-C8-C9-CA
3	A	1004	PLM	CC-CD-CE-CF
3	A	1001	PLM	C9-CA-CB-CC
5	B	1004	PC1	C23-C24-C25-C26
3	A	1001	PLM	CC-CD-CE-CF
3	B	1001	PLM	CB-CC-CD-CE
5	B	1004	PC1	C26-C27-C28-C29
6	B	1005	BOG	C4-C5-C6-O6
5	B	1004	PC1	C21-C22-C23-C24
3	B	1001	PLM	C6-C7-C8-C9
3	B	1001	PLM	C4-C5-C6-C7
3	A	1001	PLM	C7-C8-C9-CA
6	B	1005	BOG	C3'-C4'-C5'-C6'
5	B	1004	PC1	C2C-C2D-C2E-C2F
5	B	1004	PC1	C32-C33-C34-C35
3	A	1001	PLM	C8-C9-CA-CB
3	A	1004	PLM	C6-C7-C8-C9
5	B	1004	PC1	C2B-C2C-C2D-C2E
3	B	1001	PLM	C1-C2-C3-C4
3	A	1004	PLM	C1-C2-C3-C4
3	A	1004	PLM	CB-CC-CD-CE
5	B	1004	PC1	C11-O13-P-O11
3	B	1001	PLM	CC-CD-CE-CF
2	A	1000	RET	C11-C10-C9-C19
2	B	1000	RET	C11-C10-C9-C19
6	B	1005	BOG	O5-C1-O1-C1'
2	A	1000	RET	C11-C10-C9-C8
2	B	1000	RET	C11-C10-C9-C8
3	B	1001	PLM	C8-C9-CA-CB
5	B	1004	PC1	C35-C36-C37-C38
6	B	1005	BOG	C2-C1-O1-C1'

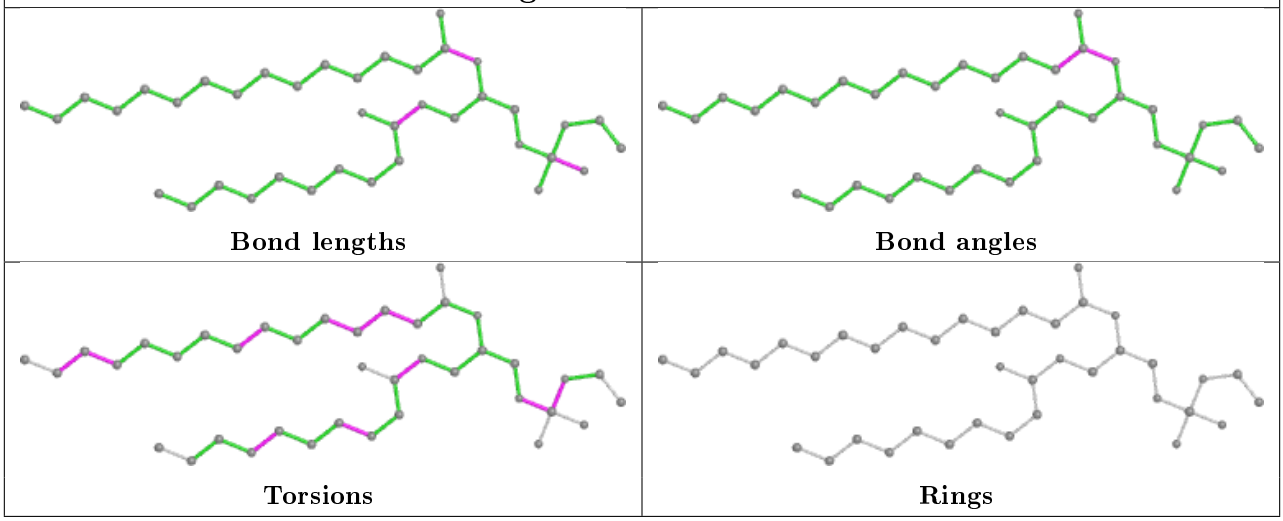
There are no ring outliers.

3 monomers are involved in 5 short contacts:

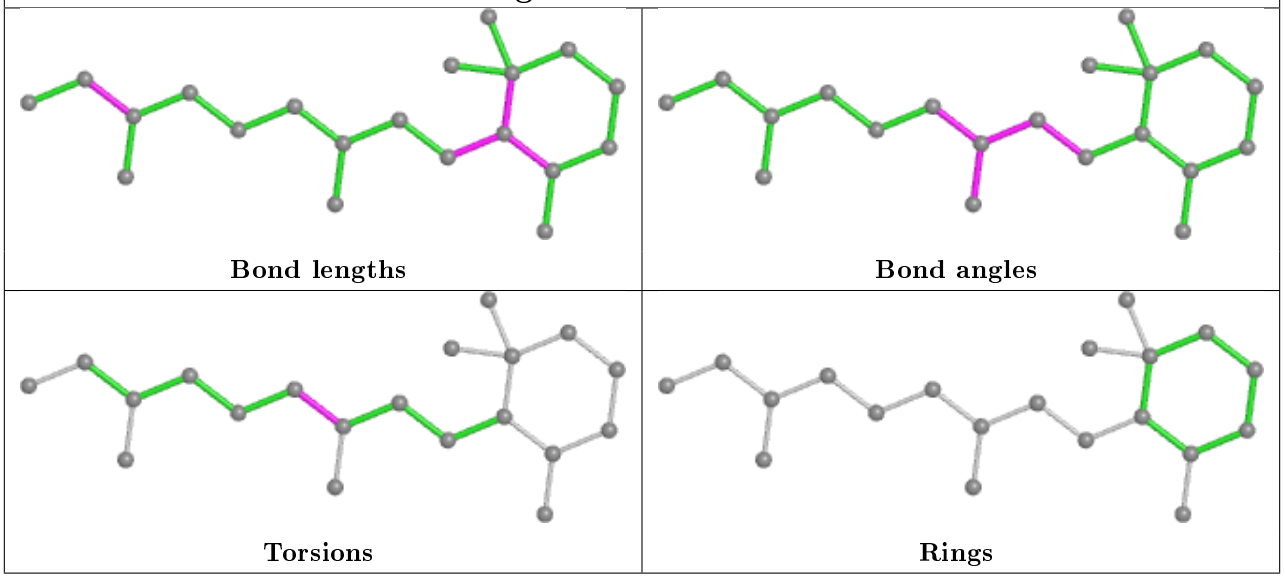
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	PC1	1	0
2	B	1000	RET	1	0
6	B	1005	BOG	3	0

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 then 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.

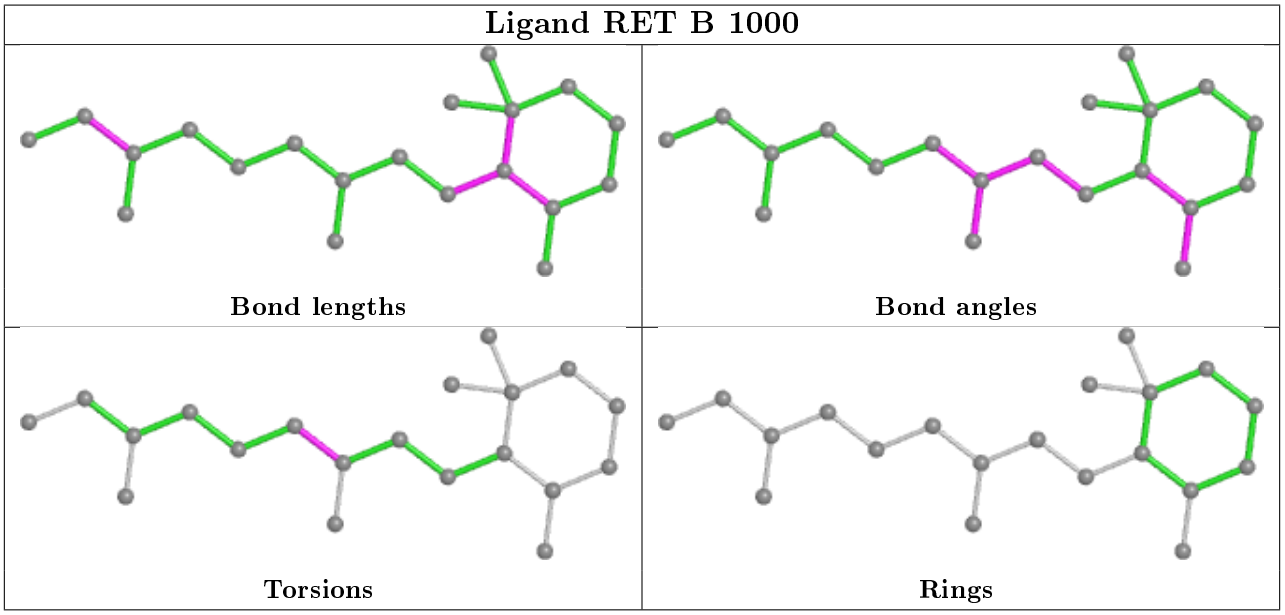
Ligand PC1 B 1004



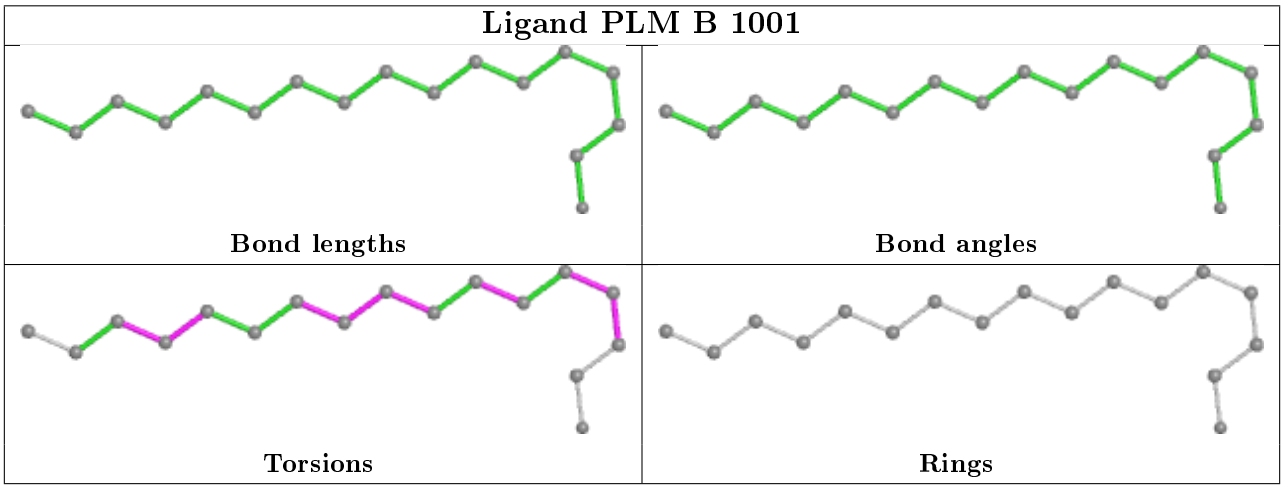
Ligand RET A 1000

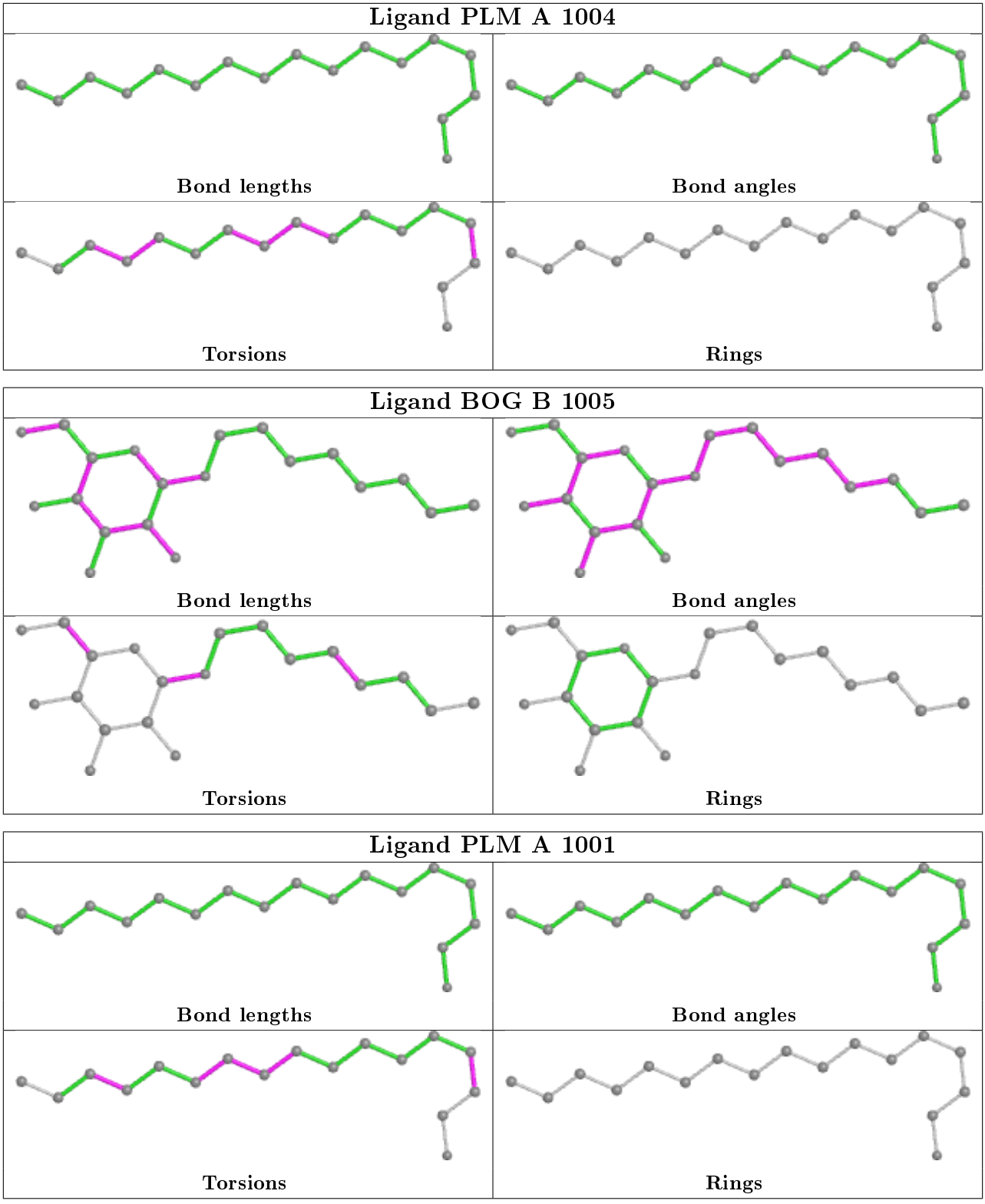


Ligand RET B 1000



Ligand PLM B 1001





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	350/448 (78%)	0.59	35 (10%) 7 5	28, 51, 114, 136	0
1	B	347/448 (77%)	0.50	15 (4%) 35 33	27, 44, 96, 118	0
All	All	697/896 (77%)	0.55	50 (7%) 15 13	27, 48, 105, 136	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	7.2
1	A	237	MET	6.3
1	B	238	ALA	5.7
1	A	240	ARG	5.3
1	A	236	ALA	5.2
1	A	234	MET	5.0
1	A	241	LEU	5.0
1	A	238	ALA	4.8
1	A	246	LEU	4.6
1	B	241	LEU	4.3
1	A	141	MET	3.7
1	B	246	LEU	3.7
1	B	239	LYS	3.7
1	A	245	GLU	3.6
1	A	242	ASN	3.4
1	A	244	LYS	3.4
1	A	354	ILE	3.1
1	A	358	GLU	3.1
1	B	136	VAL	3.0
1	A	229	ASN	3.0
1	B	235	ALA	2.9
1	A	136	VAL	2.8
1	A	249	ALA	2.7
1	A	233	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	2.6
1	A	349	ASP	2.6
1	A	250	GLN	2.6
1	B	230	HIS	2.6
1	A	248	LYS	2.5
1	B	355	PRO	2.5
1	A	348	LYS	2.5
1	B	237	MET	2.4
1	A	230	HIS	2.4
1	B	240	ARG	2.4
1	A	140	PRO	2.4
1	B	247	ARG	2.3
1	A	145	LYS	2.3
1	A	243	ALA	2.2
1	A	352	THR	2.2
1	A	221	PHE	2.2
1	A	346	ASP	2.2
1	A	228	SER	2.2
1	A	232	LYS	2.1
1	A	255	ALA	2.1
1	A	247	ARG	2.1
1	B	229	ASN	2.1
1	B	242	ASN	2.1
1	A	347	ASP	2.1
1	B	251	ALA	2.1
1	B	141	MET	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

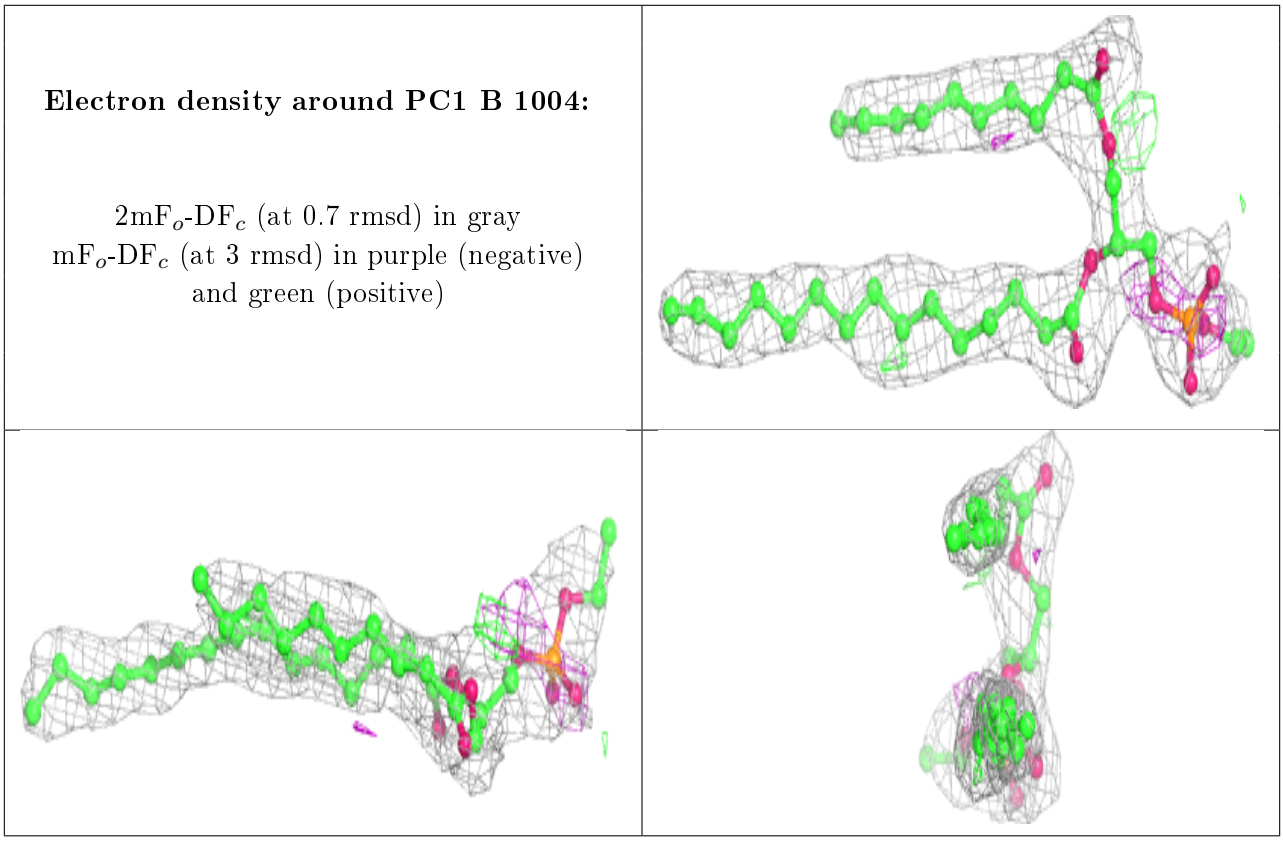
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	PC1	B	1004	39/54	0.83	0.27	41,66,112,113	0
6	BOG	B	1005	20/20	0.83	0.45	71,104,106,106	0
3	PLM	B	1001	17/18	0.84	0.39	45,65,68,69	0
3	PLM	A	1004	17/18	0.88	0.26	67,72,76,76	0
3	PLM	A	1001	17/18	0.91	0.28	49,58,64,65	0
2	RET	A	1000	20/21	0.94	0.32	43,51,57,57	0
4	SO4	B	449	5/5	0.96	0.17	110,110,111,111	0
2	RET	B	1000	20/21	0.96	0.25	30,38,43,44	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.

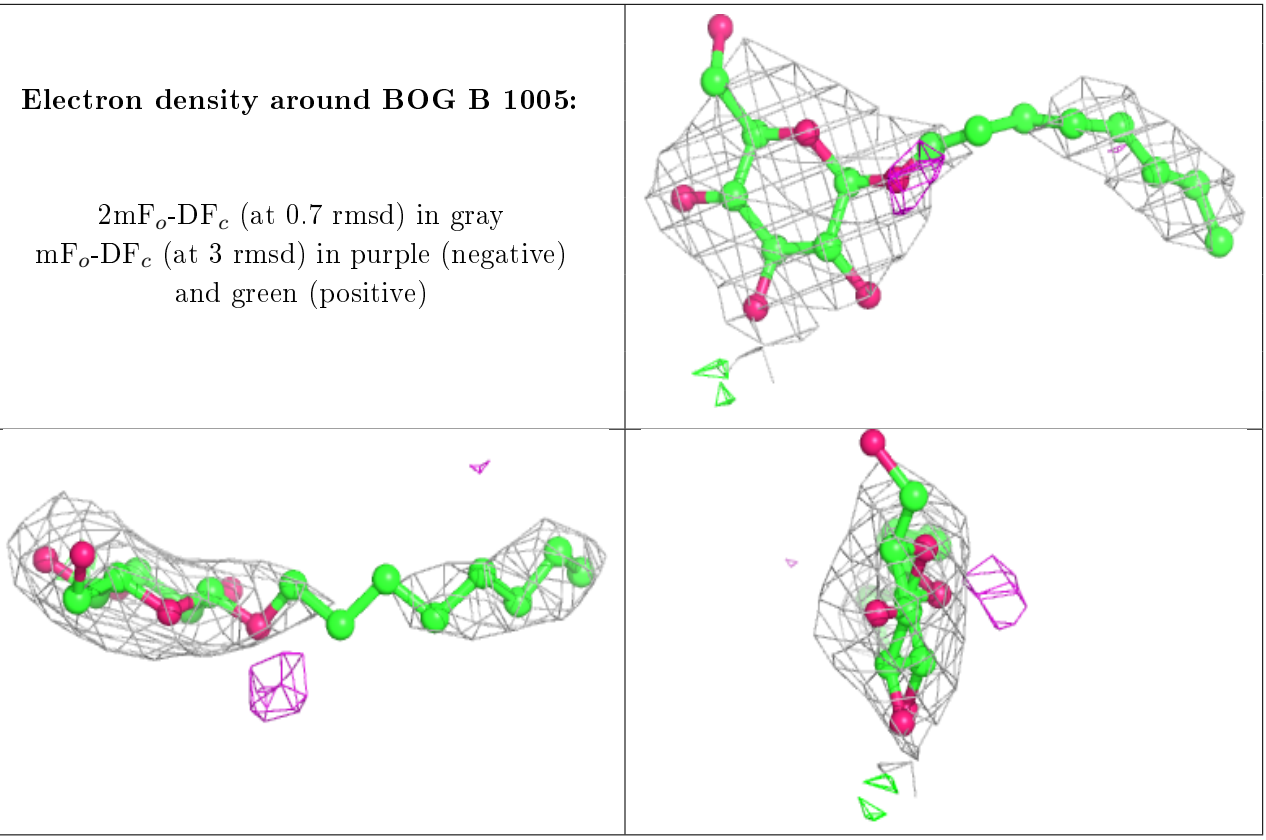
Electron density around PC1 B 1004:

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



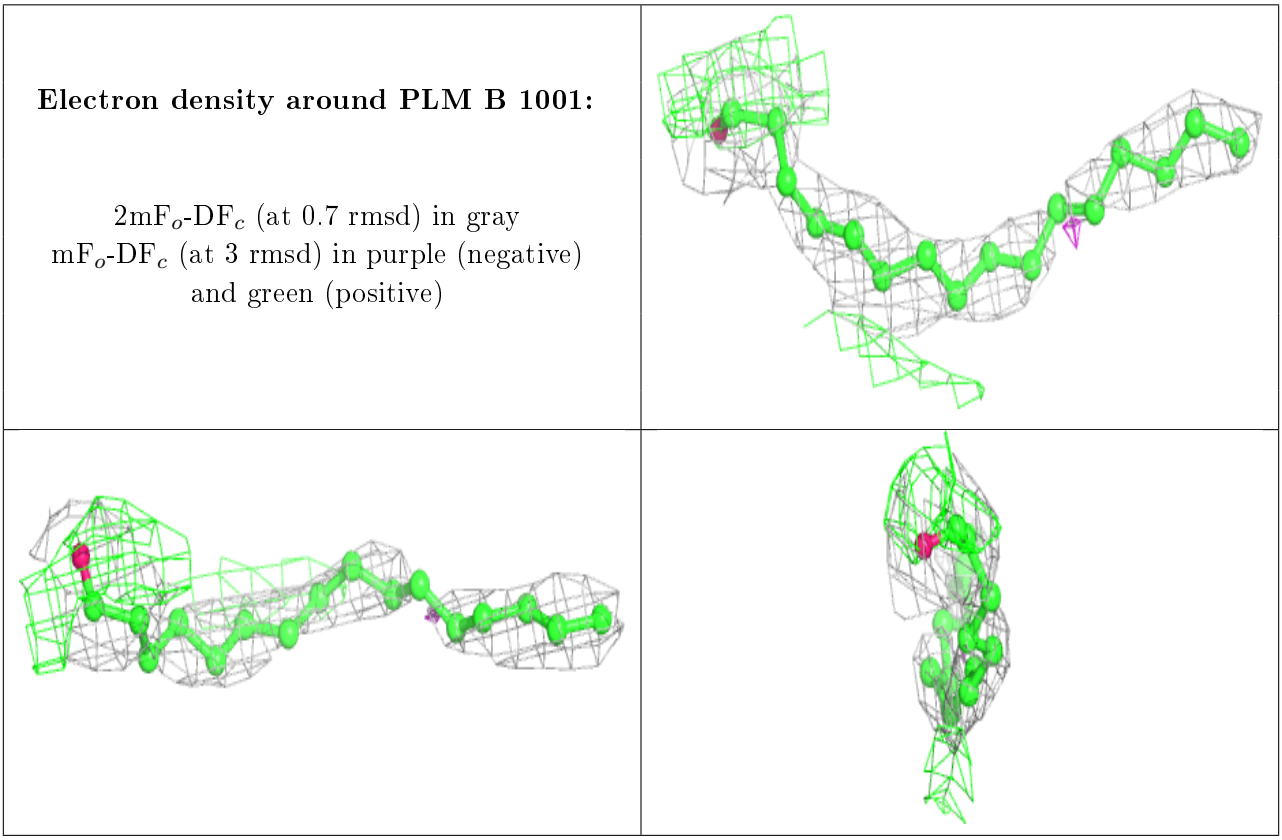
Electron density around BOG B 1005:

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



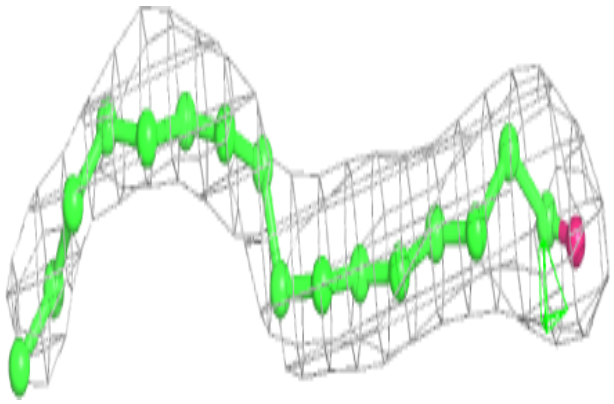
Electron density around PLM B 1001:

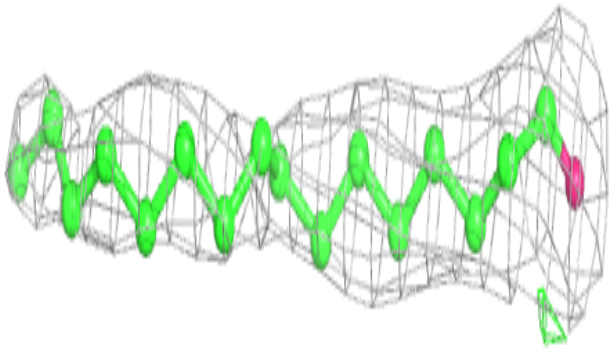
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

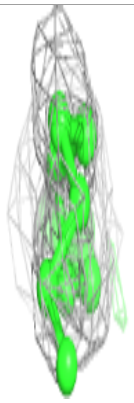


Electron density around PLM A 1004:

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

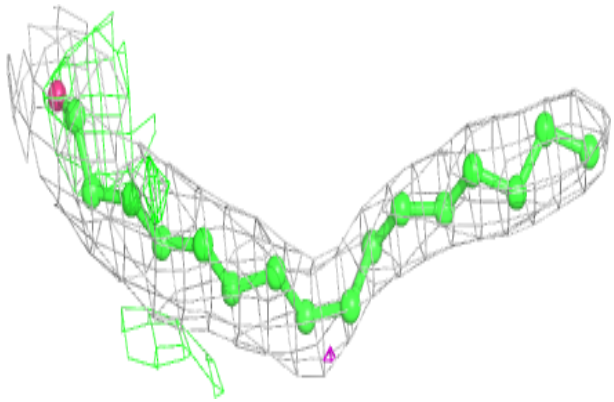


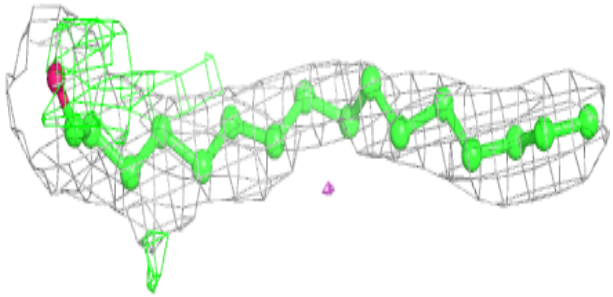


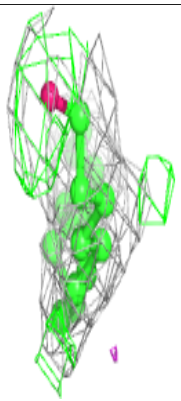


Electron density around PLM A 1001:

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

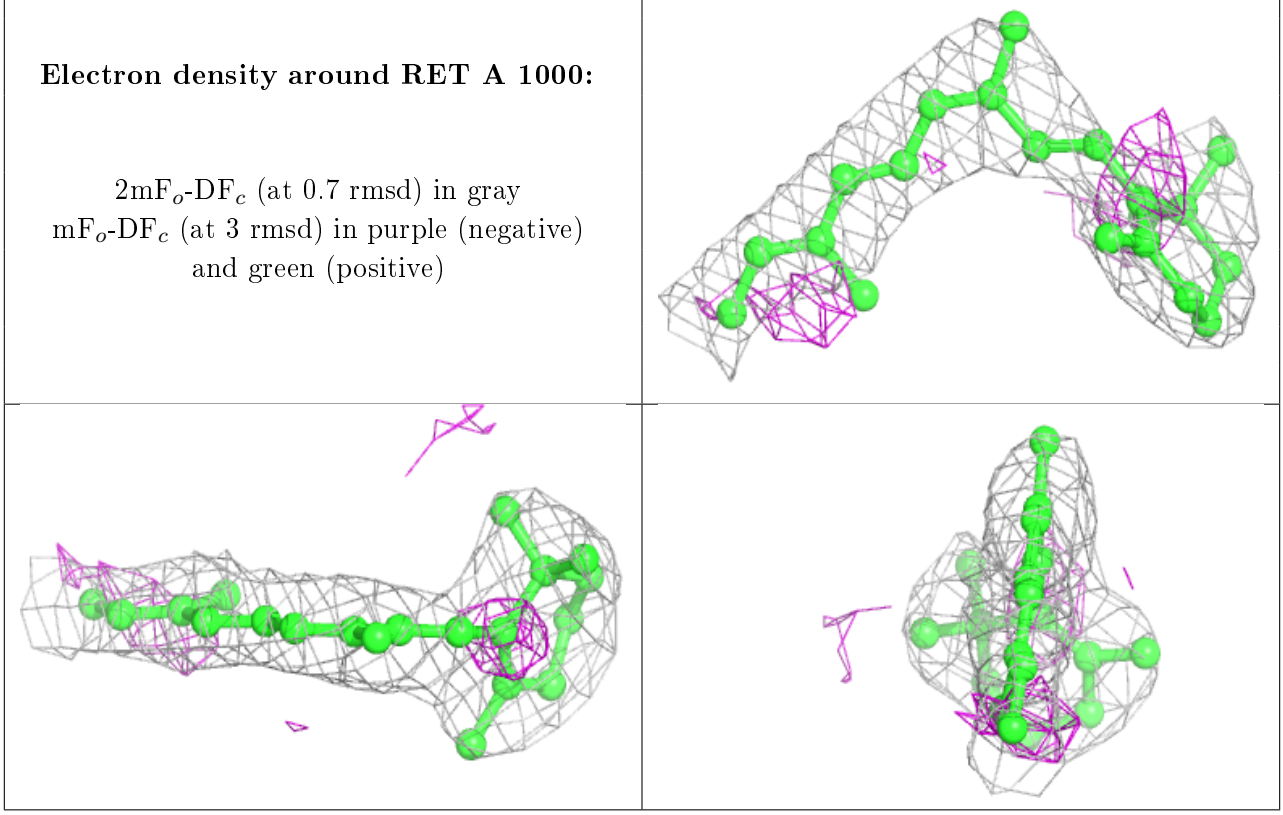






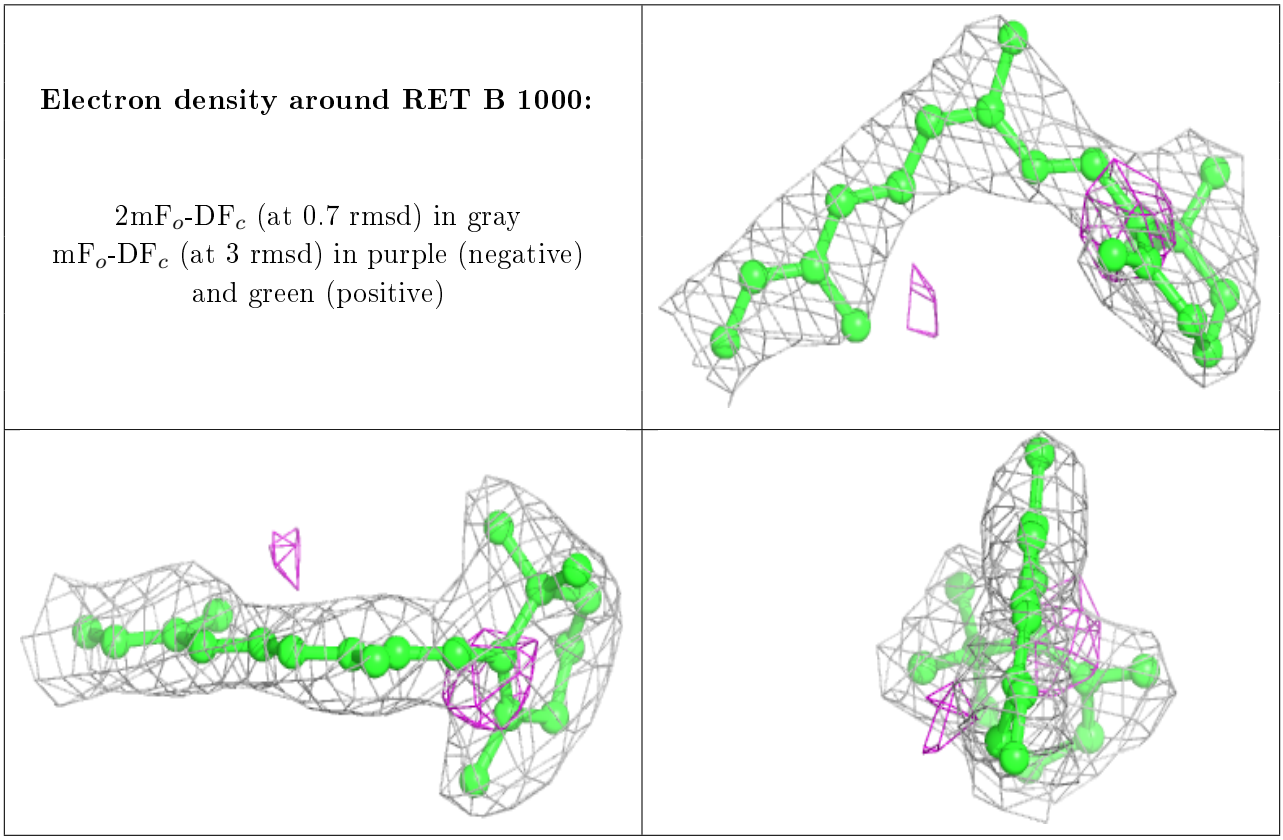
Electron density around RET A 1000:

$2mF_o$-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 1000:

$2mF_o$-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.