



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:28 AM UTC

PDB ID : 1QHJ / pdb_00001qhj
Title : X-RAY STRUCTURE OF BACTERIORHODOPSIN GROWN IN LIPIDIC CUBIC PHASES
Authors : Belrhali, H.; Nollert, P.; Royant, A.; Menzel, C.; Rosenbusch, J.P.; Landau, E.M.; Pebay-Peyroula, E.
Deposited on : 1999-05-04
Resolution : 1.90 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

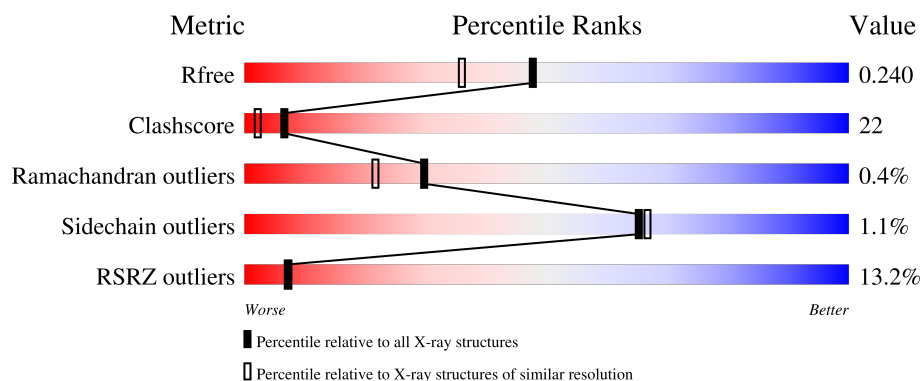
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	248	12% 63% 28% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PH1	A	502	X	-	-	-
3	PH1	A	503	X	-	-	-
3	PH1	A	506	X	-	-	-
3	PH1	A	507	X	-	-	-
3	PH1	A	508	X	-	-	-

2 Entry composition [i](#)

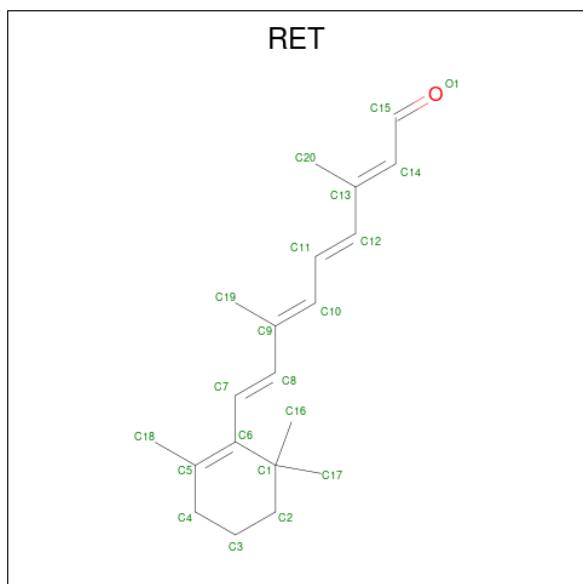
There are 4 unique types of molecules in this entry. The entry contains 2203 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (BACTERIORHODOPSIN).

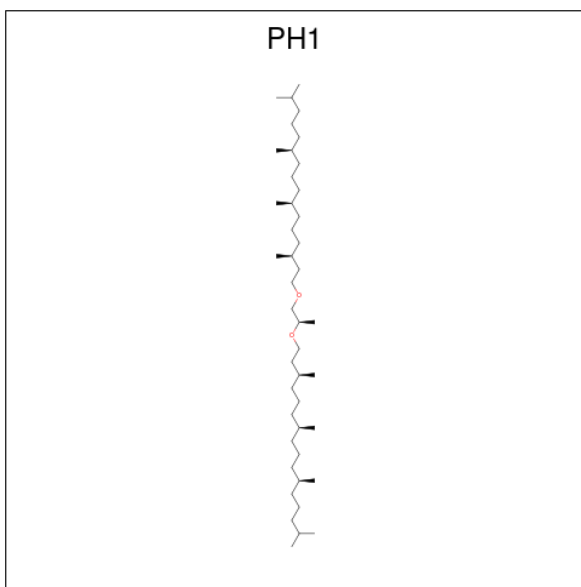
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1752	1178	266	300	8			

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



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

- Molecule 3 is 1,2-[DI-2,6,10,14-TETRAMETHYL-HEXADECAN-16-OXY]-PROPANE (CCD ID: PH1) (formula: C₄₃H₈₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		
3	A	1	Total	C	O	0	0
			45	43	2		

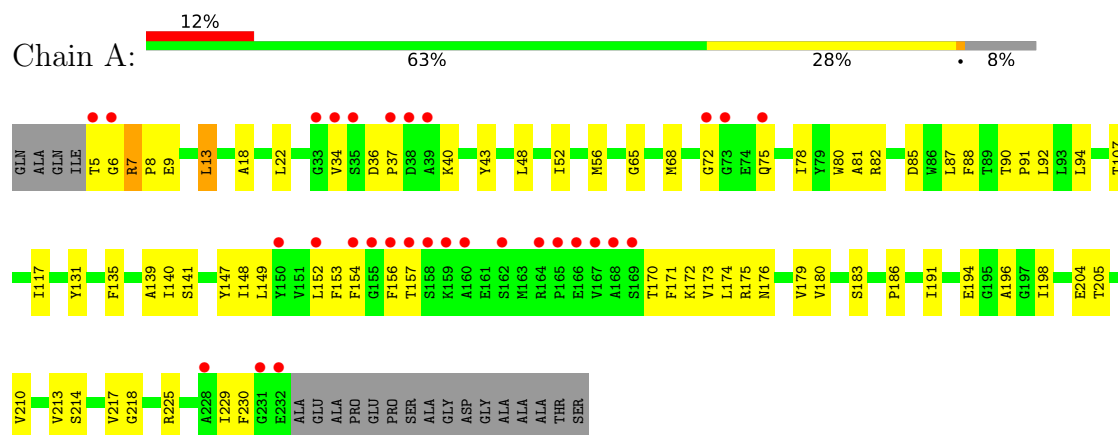
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

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: PROTEIN (BACTERIORHODOPSIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.80Å 60.80Å 110.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.00 – 1.90 38.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.00-1.90) 98.6 (38.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.91Å)	Xtriage
Refinement program	CNS 5.0	Depositor
R, R_{free}	0.224 , 0.245 0.216 , 0.240	Depositor DCC
R_{free} test set	869 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2203	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RET, PH1

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	0.36	0/1800	0.78	1/2461 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	GLY	N-CA-C	-5.47	106.48	114.90

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	1752	0	1796	85	0
2	A	20	0	27	2	0
3	A	405	0	791	68	0
4	A	26	0	0	2	0
All	All	2203	0	2614	104	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 22.

All (104) 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:196:ALA:HB2	3:A:502:PH1:H343	1.44	0.97
1:A:139:ALA:HB2	3:A:502:PH1:H141	1.55	0.86
1:A:92:LEU:HD21	3:A:500:PH1:H201	1.59	0.84
1:A:198:ILE:HD13	3:A:503:PH1:H12	1.60	0.83
3:A:502:PH1:H342	3:A:503:PH1:H352	1.69	0.75
3:A:500:PH1:C47	3:A:500:PH1:H441	2.17	0.74
1:A:180:VAL:HG21	3:A:505:PH1:H442	1.71	0.70
1:A:154:PHE:HZ	3:A:507:PH1:H51	1.56	0.69
1:A:172:LYS:HD3	3:A:505:PH1:H312	1.73	0.69
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.29	0.68
1:A:87:LEU:HD23	3:A:500:PH1:H502	1.76	0.68
1:A:196:ALA:HB3	4:A:410:HOH:O	1.93	0.68
3:A:500:PH1:H441	3:A:500:PH1:H471	1.75	0.67
1:A:92:LEU:HD11	3:A:500:PH1:H203	1.77	0.67
1:A:183:SER:HB2	3:A:505:PH1:H121	1.77	0.67
1:A:48:LEU:HD21	3:A:500:PH1:H161	1.77	0.66
1:A:213:VAL:HG12	3:A:508:PH1:H203	1.76	0.65
1:A:154:PHE:HE1	3:A:507:PH1:H21	1.63	0.64
1:A:80:TRP:CE3	3:A:500:PH1:H442	2.34	0.63
1:A:6:GLY:HA2	1:A:9:GLU:OE2	1.98	0.62
1:A:175:ARG:HH21	1:A:176:ASN:HD21	1.45	0.62
1:A:175:ARG:NH2	3:A:505:PH1:H512	2.14	0.62
1:A:191:ILE:HA	4:A:410:HOH:O	1.99	0.61
1:A:198:ILE:CD1	3:A:503:PH1:H12	2.30	0.60
1:A:196:ALA:HB2	3:A:502:PH1:C34	2.26	0.59
1:A:186:PRO:HB3	2:A:300:RET:H183	1.84	0.59
3:A:502:PH1:H533	3:A:503:PH1:H311	1.84	0.59
1:A:180:VAL:O	3:A:505:PH1:H142	2.03	0.58
1:A:37:PRO:O	1:A:40:LYS:HB2	2.04	0.57
1:A:140:ILE:HG13	3:A:501:PH1:H503	1.87	0.57
1:A:87:LEU:HD23	3:A:500:PH1:C50	2.36	0.56
1:A:140:ILE:HG23	3:A:506:PH1:H191	1.87	0.56
1:A:154:PHE:CZ	3:A:507:PH1:H51	2.40	0.56
1:A:92:LEU:CD2	3:A:500:PH1:H201	2.36	0.55
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.42	0.54
1:A:218:GLY:N	3:A:508:PH1:H202	2.23	0.54
1:A:5:THR:OG1	1:A:6:GLY:N	2.38	0.53
1:A:214:SER:HB3	3:A:508:PH1:H38	1.89	0.53
1:A:34:VAL:HG21	1:A:43:TYR:CE2	2.44	0.53
1:A:7:ARG:HB2	1:A:8:PRO:HD3	1.90	0.53
1:A:148:ILE:O	1:A:152:LEU:HD13	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:PH1:C17	3:A:500:PH1:H141	2.39	0.53
1:A:214:SER:OG	3:A:508:PH1:H422	2.09	0.52
1:A:7:ARG:CB	1:A:8:PRO:HD3	2.40	0.52
1:A:140:ILE:CG2	3:A:506:PH1:H191	2.41	0.51
1:A:78:ILE:HD12	1:A:194:GLU:HG3	1.93	0.51
1:A:131:TYR:OH	3:A:502:PH1:H312	2.10	0.51
3:A:500:PH1:C47	3:A:500:PH1:C44	2.84	0.50
1:A:147:TYR:CD1	3:A:506:PH1:H142	2.47	0.50
3:A:501:PH1:H512	3:A:501:PH1:H371	1.94	0.50
3:A:502:PH1:H311	3:A:503:PH1:H322	1.94	0.49
1:A:52:ILE:HD11	3:A:500:PH1:H152	1.95	0.48
1:A:68:MET:HE3	1:A:75:GLN:HG3	1.95	0.48
1:A:175:ARG:HH21	3:A:505:PH1:H512	1.77	0.47
1:A:217:VAL:HG11	3:A:508:PH1:H142	1.97	0.47
3:A:504:PH1:H202	3:A:506:PH1:H472	1.96	0.47
1:A:157:THR:HA	1:A:171:PHE:HE2	1.80	0.46
3:A:500:PH1:C44	3:A:500:PH1:H472	2.45	0.46
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.97	0.46
1:A:107:THR:HG23	3:A:506:PH1:H512	1.96	0.46
3:A:506:PH1:H343	3:A:506:PH1:H42	1.97	0.46
1:A:90:THR:N	1:A:91:PRO:HD2	2.31	0.46
3:A:502:PH1:H21	3:A:502:PH1:H61	1.82	0.46
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.79	0.46
3:A:501:PH1:H143	3:A:504:PH1:H8	1.97	0.46
3:A:507:PH1:H421	3:A:507:PH1:H143	1.98	0.46
1:A:183:SER:OG	3:A:507:PH1:H493	2.16	0.46
1:A:147:TYR:CE2	3:A:506:PH1:H102	2.51	0.46
1:A:156:PHE:HB3	1:A:171:PHE:HZ	1.80	0.46
1:A:56:MET:HE2	1:A:56:MET:HA	1.99	0.45
1:A:92:LEU:HD21	3:A:500:PH1:C20	2.39	0.45
1:A:36:ASP:O	1:A:40:LYS:HG3	2.17	0.44
1:A:80:TRP:CZ3	3:A:500:PH1:H442	2.51	0.44
1:A:180:VAL:HA	3:A:505:PH1:H122	1.98	0.44
1:A:210:VAL:HG13	3:A:508:PH1:H442	1.99	0.44
1:A:229:ILE:HG13	1:A:230:PHE:CD1	2.53	0.44
1:A:141:SER:HB3	2:A:300:RET:H41	2.00	0.44
1:A:210:VAL:CG1	3:A:508:PH1:H442	2.47	0.43
3:A:500:PH1:H351	3:A:500:PH1:H311	1.67	0.43
1:A:198:ILE:HD11	3:A:503:PH1:H321	1.99	0.43
3:A:500:PH1:H141	3:A:500:PH1:H171	2.00	0.43
1:A:135:PHE:CZ	3:A:502:PH1:H33	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:OE1	1:A:204:GLU:OE2	2.36	0.43
1:A:88:PHE:CE2	3:A:500:PH1:H501	2.53	0.43
1:A:147:TYR:HA	3:A:506:PH1:H451	2.01	0.43
1:A:180:VAL:HG13	3:A:505:PH1:H143	2.00	0.43
1:A:7:ARG:HD2	1:A:7:ARG:HA	1.95	0.42
1:A:13:LEU:HD13	1:A:205:THR:CG2	2.49	0.42
1:A:82:ARG:O	1:A:85:ASP:HB3	2.19	0.42
3:A:508:PH1:H351	3:A:508:PH1:H312	1.82	0.42
1:A:149:LEU:HD22	1:A:179:VAL:HG22	2.00	0.42
1:A:173:VAL:HG13	1:A:174:LEU:N	2.33	0.42
1:A:175:ARG:HE	1:A:176:ASN:ND2	2.16	0.42
1:A:153:PHE:CZ	1:A:179:VAL:HG21	2.54	0.42
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.85	0.41
1:A:117:ILE:HG21	3:A:506:PH1:C20	2.50	0.41
1:A:170:THR:O	1:A:173:VAL:HG12	2.19	0.41
3:A:503:PH1:H391	3:A:503:PH1:H412	1.77	0.41
1:A:140:ILE:HG23	3:A:506:PH1:C19	2.51	0.40
1:A:149:LEU:HD13	3:A:507:PH1:H471	2.03	0.40
1:A:18:ALA:O	1:A:22:LEU:HG	2.21	0.40
1:A:154:PHE:CE1	3:A:507:PH1:H21	2.49	0.40
1:A:85:ASP:OD1	1:A:85:ASP:C	2.64	0.40
3:A:502:PH1:H93	3:A:502:PH1:H351	2.02	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	226/248 (91%)	216 (96%)	9 (4%)	1 (0%)	30 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG

5.3.2 Protein sidechains [i](#)

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	180/194 (93%)	178 (99%)	2 (1%)	65 67

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	105	GLN
1	A	176	ASN
1	A	202	ASN

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

10 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
3	PH1	A	501	-	44,44,44	1.85	5 (11%)	50,52,52	1.42	6 (12%)
3	PH1	A	504	-	44,44,44	1.96	5 (11%)	50,52,52	1.33	5 (10%)
3	PH1	A	506	-	44,44,44	1.78	5 (11%)	50,52,52	1.39	6 (12%)
3	PH1	A	500	-	44,44,44	2.27	4 (9%)	50,52,52	1.25	5 (10%)
3	PH1	A	505	-	44,44,44	1.88	5 (11%)	50,52,52	1.55	5 (10%)
3	PH1	A	508	-	44,44,44	2.33	4 (9%)	50,52,52	1.25	5 (10%)
3	PH1	A	503	-	44,44,44	1.98	4 (9%)	50,52,52	1.46	5 (10%)
2	RET	A	300	1	20,20,21	1.68	5 (25%)	27,27,28	2.94	11 (40%)
3	PH1	A	502	-	44,44,44	1.67	5 (11%)	50,52,52	1.50	5 (10%)
3	PH1	A	507	-	44,44,44	1.86	5 (11%)	50,52,52	1.49	7 (14%)

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	A	300	1	-	0/13/30/31	0/1/1/1
3	PH1	A	501	-	-	19/49/49/49	-
3	PH1	A	506	-	1/1/9/9	10/49/49/49	-
3	PH1	A	504	-	-	14/49/49/49	-
3	PH1	A	500	-	-	28/49/49/49	-
3	PH1	A	505	-	-	13/49/49/49	-
3	PH1	A	508	-	1/1/9/9	8/49/49/49	-
3	PH1	A	503	-	2/2/9/9	12/49/49/49	-
3	PH1	A	502	-	2/2/9/9	18/49/49/49	-
3	PH1	A	507	-	1/1/9/9	13/49/49/49	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	PH1	O31-C52	-11.92	1.25	1.44
3	A	500	PH1	O31-C52	-11.50	1.26	1.44
3	A	503	PH1	O31-C52	-9.31	1.29	1.44
3	A	504	PH1	O31-C52	-9.09	1.29	1.44
3	A	507	PH1	O31-C52	-8.95	1.30	1.44
3	A	501	PH1	O31-C52	-8.92	1.30	1.44
3	A	506	PH1	O31-C52	-7.83	1.31	1.44
3	A	505	PH1	O31-C52	-7.70	1.32	1.44
3	A	502	PH1	O31-C52	-6.97	1.33	1.44
3	A	508	PH1	O31-C31	-6.57	1.25	1.43
3	A	500	PH1	O1-C51	-6.40	1.26	1.42
3	A	500	PH1	O31-C31	-6.07	1.26	1.43
3	A	505	PH1	O1-C51	-5.96	1.27	1.42
3	A	503	PH1	O31-C31	-5.62	1.27	1.43
3	A	508	PH1	O1-C51	-5.61	1.28	1.42
3	A	504	PH1	O1-C51	-5.47	1.28	1.42
3	A	502	PH1	O1-C51	-5.37	1.28	1.42
3	A	504	PH1	O31-C31	-5.25	1.28	1.43
3	A	503	PH1	O1-C51	-5.17	1.29	1.42
3	A	505	PH1	O31-C31	-5.07	1.29	1.43
3	A	506	PH1	O1-C51	-4.82	1.30	1.42
3	A	501	PH1	O1-C51	-4.69	1.30	1.42
3	A	507	PH1	O31-C31	-4.66	1.30	1.43
3	A	506	PH1	O31-C31	-4.60	1.30	1.43
3	A	502	PH1	O31-C31	-4.16	1.31	1.43
3	A	501	PH1	O31-C31	-4.15	1.31	1.43
3	A	507	PH1	O1-C51	-4.02	1.32	1.42
3	A	508	PH1	O1-C1	-3.97	1.24	1.42
3	A	505	PH1	O1-C1	-3.85	1.25	1.42
3	A	500	PH1	O1-C1	-3.74	1.25	1.42
3	A	506	PH1	C51-C52	3.62	1.58	1.50
2	A	300	RET	C1-C6	3.50	1.58	1.53
3	A	504	PH1	O1-C1	-3.40	1.27	1.42
3	A	502	PH1	O1-C1	-3.36	1.27	1.42
3	A	503	PH1	O1-C1	-3.33	1.27	1.42
2	A	300	RET	C15-C14	-3.29	1.37	1.49
2	A	300	RET	C5-C6	3.19	1.39	1.34
3	A	501	PH1	C51-C52	3.18	1.57	1.50
3	A	501	PH1	O1-C1	-3.04	1.28	1.42
3	A	507	PH1	C51-C52	3.03	1.57	1.50
2	A	300	RET	C14-C13	3.03	1.35	1.33
3	A	504	PH1	C51-C52	2.91	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	PH1	C51-C52	2.73	1.56	1.50
3	A	506	PH1	O1-C1	-2.63	1.30	1.42
3	A	502	PH1	C51-C52	2.47	1.56	1.50
3	A	507	PH1	O1-C1	-2.28	1.32	1.42
2	A	300	RET	C4-C5	2.06	1.54	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	PH1	O31-C31-C32	7.33	124.15	108.77
3	A	501	PH1	O31-C31-C32	6.80	123.06	108.77
3	A	502	PH1	O31-C31-C32	6.70	122.84	108.77
3	A	507	PH1	O31-C31-C32	6.52	122.46	108.77
2	A	300	RET	C8-C9-C10	-6.11	109.40	119.01
3	A	506	PH1	O31-C31-C32	5.94	121.24	108.77
3	A	503	PH1	O31-C31-C32	5.83	121.02	108.77
2	A	300	RET	C18-C5-C6	5.81	130.82	124.48
3	A	500	PH1	O31-C31-C32	5.64	120.60	108.77
2	A	300	RET	C8-C7-C6	5.43	141.52	127.00
3	A	504	PH1	O31-C31-C32	5.21	119.72	108.77
3	A	508	PH1	O31-C31-C32	5.08	119.44	108.77
2	A	300	RET	C16-C1-C6	5.02	118.11	110.24
2	A	300	RET	C7-C8-C9	5.00	133.64	126.23
3	A	503	PH1	O31-C52-C51	4.19	122.42	108.90
2	A	300	RET	C19-C9-C10	4.15	129.53	122.82
3	A	504	PH1	O31-C52-C51	4.14	122.25	108.90
3	A	502	PH1	O31-C52-C51	4.10	122.11	108.90
3	A	501	PH1	O1-C51-C52	3.93	124.99	110.87
3	A	507	PH1	O1-C51-C52	3.91	124.90	110.87
3	A	505	PH1	O1-C51-C52	3.83	124.64	110.87
3	A	506	PH1	O1-C51-C52	3.79	124.47	110.87
2	A	300	RET	C18-C5-C4	-3.78	105.54	113.60
3	A	506	PH1	O31-C52-C51	3.76	121.03	108.90
3	A	505	PH1	C31-O31-C52	3.58	125.09	115.49
3	A	504	PH1	O1-C51-C52	3.58	123.74	110.87
3	A	502	PH1	C31-O31-C52	3.49	124.85	115.49
3	A	505	PH1	O31-C52-C51	3.49	120.14	108.90
3	A	507	PH1	C31-O31-C52	3.48	124.80	115.49
2	A	300	RET	C12-C13-C14	-3.47	109.34	118.55
3	A	508	PH1	O1-C51-C52	3.44	123.22	110.87
2	A	300	RET	C20-C13-C12	3.39	123.27	118.09
3	A	503	PH1	O31-C52-C53	3.29	122.13	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PH1	O1-C51-C52	3.22	122.43	110.87
3	A	508	PH1	O31-C52-C51	3.20	119.23	108.90
3	A	500	PH1	O31-C52-C51	3.15	119.05	108.90
3	A	500	PH1	O1-C51-C52	3.14	122.15	110.87
3	A	502	PH1	O31-C52-C53	3.13	121.57	110.22
3	A	503	PH1	O1-C51-C52	3.11	122.04	110.87
3	A	501	PH1	O31-C52-C51	3.00	118.58	108.90
3	A	506	PH1	O31-C52-C53	2.82	120.44	110.22
3	A	504	PH1	C31-O31-C52	2.72	122.77	115.49
3	A	507	PH1	O31-C52-C53	2.67	119.91	110.22
3	A	503	PH1	C31-O31-C52	2.63	122.52	115.49
3	A	508	PH1	C31-O31-C52	2.56	122.34	115.49
3	A	507	PH1	O31-C52-C51	2.49	116.92	108.90
3	A	500	PH1	O31-C52-C53	2.47	119.17	110.22
3	A	504	PH1	O31-C52-C53	2.46	119.16	110.22
3	A	506	PH1	C31-O31-C52	2.42	121.96	115.49
3	A	500	PH1	C31-O31-C52	2.38	121.85	115.49
3	A	507	PH1	C1-O1-C51	2.34	123.88	113.58
2	A	300	RET	C16-C1-C2	-2.34	99.98	108.95
2	A	300	RET	C1-C6-C7	2.27	121.80	115.65
3	A	505	PH1	O1-C1-C2	2.26	124.59	110.29
3	A	508	PH1	O31-C52-C53	2.26	118.41	110.22
3	A	507	PH1	O1-C1-C2	2.24	124.46	110.29
3	A	501	PH1	O31-C52-C53	2.21	118.24	110.22
3	A	501	PH1	C1-O1-C51	2.19	123.21	113.58
3	A	506	PH1	C1-O1-C51	2.12	122.92	113.58
3	A	501	PH1	C31-O31-C52	2.12	121.16	115.49

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	502	PH1	C52
3	A	502	PH1	C43
3	A	503	PH1	C52
3	A	503	PH1	C38
3	A	506	PH1	C33
3	A	507	PH1	C52
3	A	508	PH1	C52

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	PH1	C53-C52-O31-C31
3	A	500	PH1	C31-C32-C33-C34
3	A	500	PH1	C31-C32-C33-C35
3	A	500	PH1	O1-C51-C52-C53
3	A	502	PH1	C31-C32-C33-C34
3	A	502	PH1	O1-C51-C52-C53
3	A	503	PH1	C1-C2-C3-C4
3	A	500	PH1	C43-C45-C46-C47
3	A	500	PH1	C11-C10-C8-C9
3	A	500	PH1	C14-C13-C15-C16
3	A	500	PH1	C41-C42-C43-C44
3	A	501	PH1	C6-C7-C8-C9
3	A	503	PH1	C4-C3-C5-C6
3	A	507	PH1	C52-C51-O1-C1
3	A	504	PH1	C33-C35-C36-C37
3	A	503	PH1	C12-C13-C15-C16
3	A	501	PH1	C40-C41-C42-C43
3	A	508	PH1	C5-C6-C7-C8
3	A	501	PH1	C3-C5-C6-C7
3	A	503	PH1	C8-C10-C11-C12
3	A	503	PH1	C45-C46-C47-C48
3	A	508	PH1	C3-C5-C6-C7
3	A	500	PH1	C5-C6-C7-C8
3	A	501	PH1	C33-C35-C36-C37
3	A	505	PH1	C35-C36-C37-C38
3	A	501	PH1	C8-C10-C11-C12
3	A	504	PH1	C35-C36-C37-C38
3	A	507	PH1	C3-C5-C6-C7
3	A	507	PH1	C5-C6-C7-C8
3	A	505	PH1	C3-C5-C6-C7
3	A	506	PH1	C43-C45-C46-C47
3	A	508	PH1	C38-C40-C41-C42
3	A	502	PH1	C3-C5-C6-C7
3	A	507	PH1	C15-C16-C17-C18
3	A	500	PH1	C15-C16-C17-C18
3	A	501	PH1	C15-C16-C17-C18
3	A	504	PH1	C5-C6-C7-C8
3	A	502	PH1	C34-C33-C35-C36
3	A	502	PH1	C39-C38-C40-C41
3	A	500	PH1	C8-C10-C11-C12
3	A	506	PH1	C5-C6-C7-C8
3	A	502	PH1	C40-C41-C42-C43
3	A	504	PH1	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	501	PH1	C5-C6-C7-C8
3	A	500	PH1	O31-C31-C32-C33
3	A	505	PH1	C10-C11-C12-C13
3	A	505	PH1	C8-C10-C11-C12
3	A	507	PH1	C45-C46-C47-C48
3	A	502	PH1	C35-C36-C37-C38
3	A	506	PH1	C38-C40-C41-C42
3	A	501	PH1	C45-C46-C47-C48
3	A	502	PH1	C43-C45-C46-C47
3	A	505	PH1	C38-C40-C41-C42
3	A	500	PH1	C3-C5-C6-C7
3	A	501	PH1	C38-C40-C41-C42
3	A	507	PH1	C10-C11-C12-C13
3	A	504	PH1	C38-C40-C41-C42
3	A	500	PH1	C35-C36-C37-C38
3	A	500	PH1	C12-C13-C15-C16
3	A	506	PH1	C35-C36-C37-C38
3	A	504	PH1	C32-C31-O31-C52
3	A	502	PH1	C8-C10-C11-C12
3	A	503	PH1	C15-C16-C17-C18
3	A	506	PH1	C15-C16-C17-C18
3	A	500	PH1	C45-C46-C47-C48
3	A	503	PH1	C46-C47-C48-C49
3	A	502	PH1	C52-C51-O1-C1
3	A	505	PH1	C51-C52-O31-C31
3	A	500	PH1	C32-C33-C35-C36
3	A	500	PH1	C37-C38-C40-C41
3	A	501	PH1	C6-C7-C8-C10
3	A	505	PH1	C32-C33-C35-C36
3	A	506	PH1	C10-C11-C12-C13
3	A	501	PH1	O1-C51-C52-C53
3	A	503	PH1	O1-C51-C52-C53
3	A	504	PH1	O1-C51-C52-C53
3	A	500	PH1	O1-C1-C2-C3
3	A	503	PH1	O31-C31-C32-C33
3	A	508	PH1	O1-C1-C2-C3
3	A	502	PH1	O1-C51-C52-O31
3	A	506	PH1	O1-C51-C52-O31
3	A	507	PH1	O1-C51-C52-O31
3	A	506	PH1	C2-C1-O1-C51
3	A	503	PH1	C32-C31-O31-C52
3	A	502	PH1	C46-C47-C48-C50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	508	PH1	C33-C35-C36-C37
3	A	501	PH1	C10-C11-C12-C13
3	A	500	PH1	C33-C35-C36-C37
3	A	507	PH1	C16-C17-C18-C19
3	A	508	PH1	C2-C1-O1-C51
3	A	501	PH1	C43-C45-C46-C47
3	A	500	PH1	C6-C7-C8-C10
3	A	500	PH1	C41-C42-C43-C45
3	A	500	PH1	C39-C38-C40-C41
3	A	500	PH1	C1-C2-C3-C5
3	A	504	PH1	C31-C32-C33-C35
3	A	502	PH1	O1-C1-C2-C3
3	A	507	PH1	O31-C31-C32-C33
3	A	502	PH1	C2-C1-O1-C51
3	A	500	PH1	C34-C33-C35-C36
3	A	505	PH1	C14-C13-C15-C16
3	A	505	PH1	C34-C33-C35-C36
3	A	504	PH1	C52-C51-O1-C1
3	A	504	PH1	C2-C1-O1-C51
3	A	502	PH1	C2-C3-C5-C6
3	A	500	PH1	C10-C11-C12-C13
3	A	503	PH1	C6-C7-C8-C9
3	A	501	PH1	C16-C17-C18-C20
3	A	501	PH1	C32-C33-C35-C36
3	A	501	PH1	C42-C43-C45-C46
3	A	506	PH1	C37-C38-C40-C41
3	A	507	PH1	C36-C37-C38-C40
3	A	508	PH1	C40-C41-C42-C43
3	A	504	PH1	C14-C13-C15-C16
3	A	502	PH1	C32-C31-O31-C52
3	A	506	PH1	C32-C31-O31-C52
3	A	507	PH1	C32-C31-O31-C52
3	A	507	PH1	C2-C1-O1-C51
3	A	502	PH1	C41-C42-C43-C45
3	A	503	PH1	C11-C12-C13-C15
3	A	504	PH1	C32-C33-C35-C36
3	A	505	PH1	C4-C3-C5-C6
3	A	504	PH1	C15-C16-C17-C18
3	A	500	PH1	C13-C15-C16-C17
3	A	501	PH1	C44-C43-C45-C46
3	A	505	PH1	C6-C7-C8-C9
3	A	508	PH1	C32-C31-O31-C52

Continued on next page...

Continued from previous page...

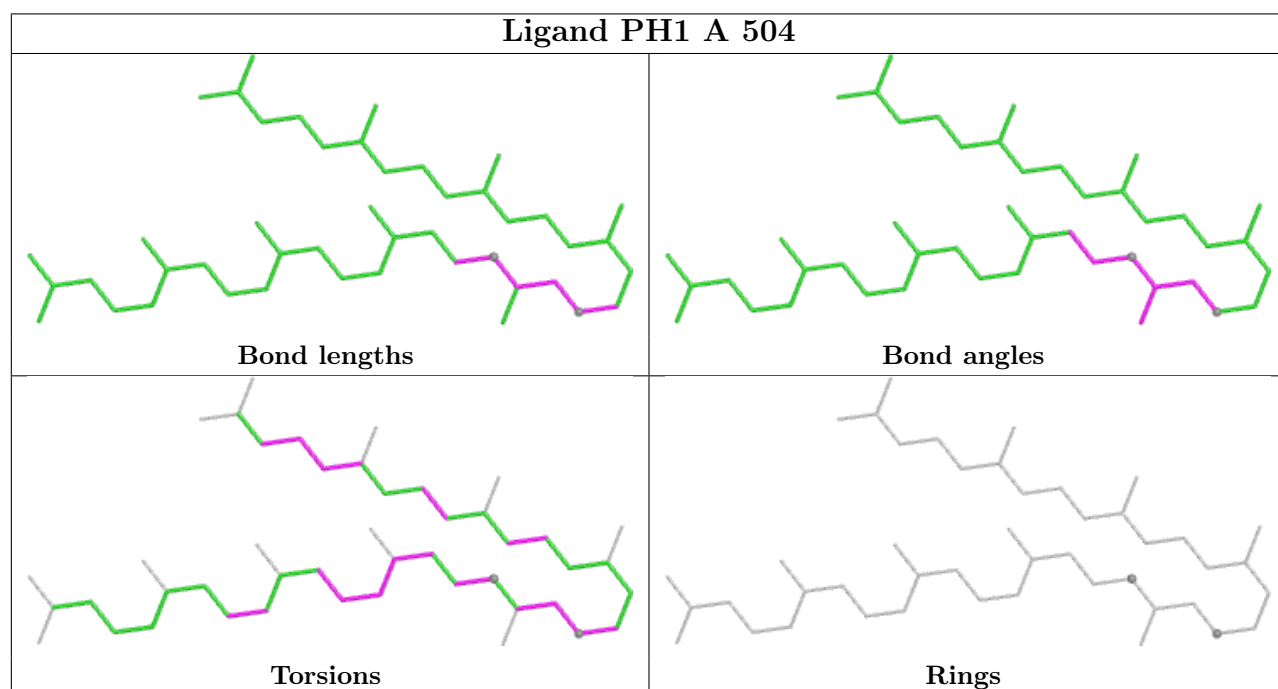
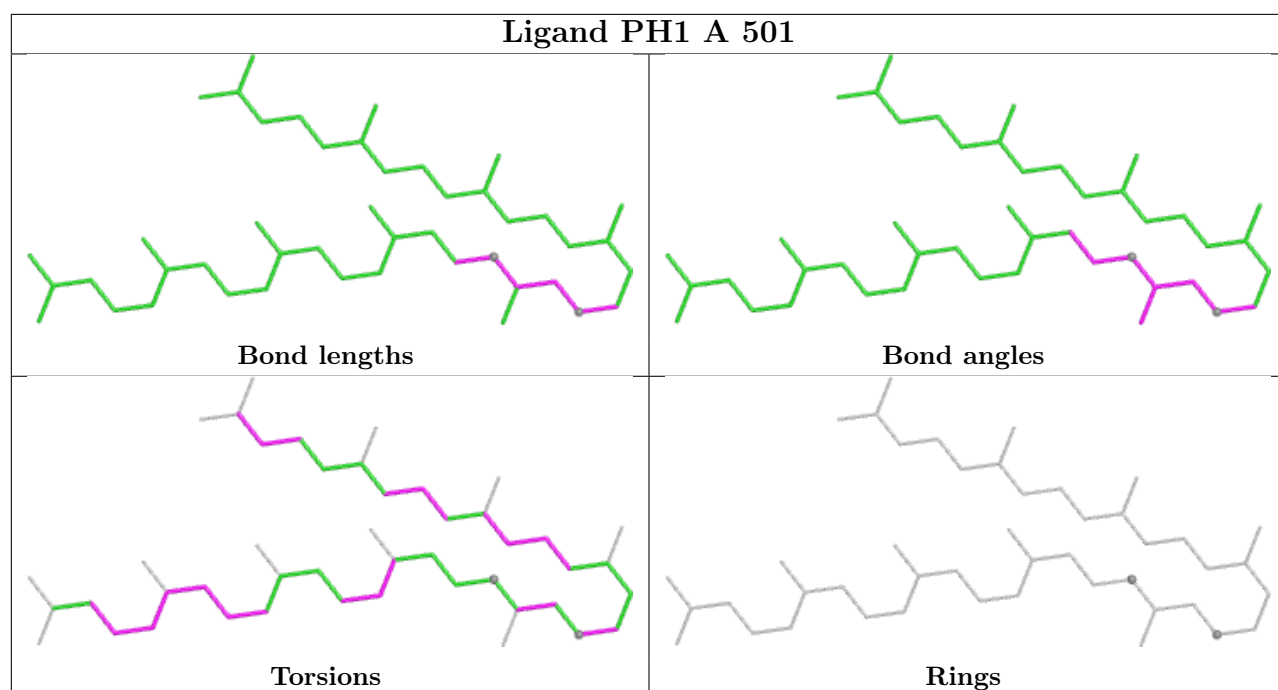
Mol	Chain	Res	Type	Atoms
3	A	501	PH1	C41-C42-C43-C44
3	A	501	PH1	C2-C1-O1-C51
3	A	502	PH1	C36-C37-C38-C40
3	A	505	PH1	C53-C52-O31-C31
3	A	505	PH1	C32-C31-O31-C52
3	A	504	PH1	C8-C10-C11-C12
3	A	500	PH1	C1-C2-C3-C4
3	A	507	PH1	C40-C41-C42-C43

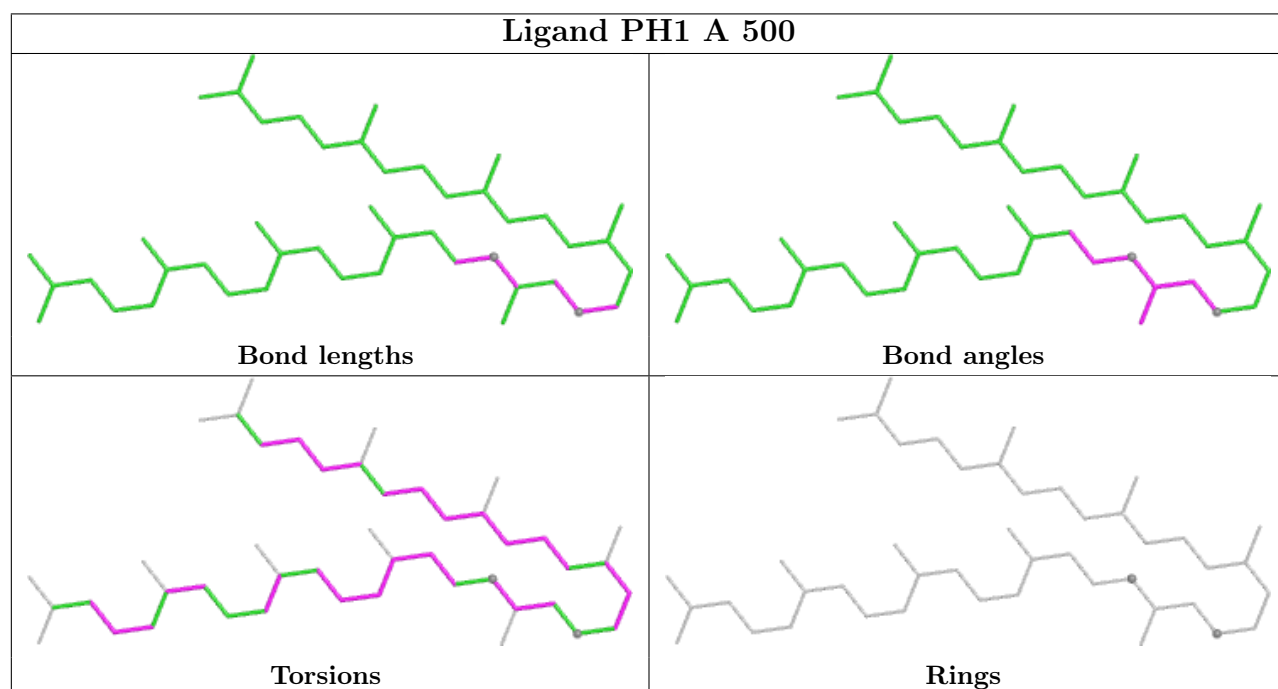
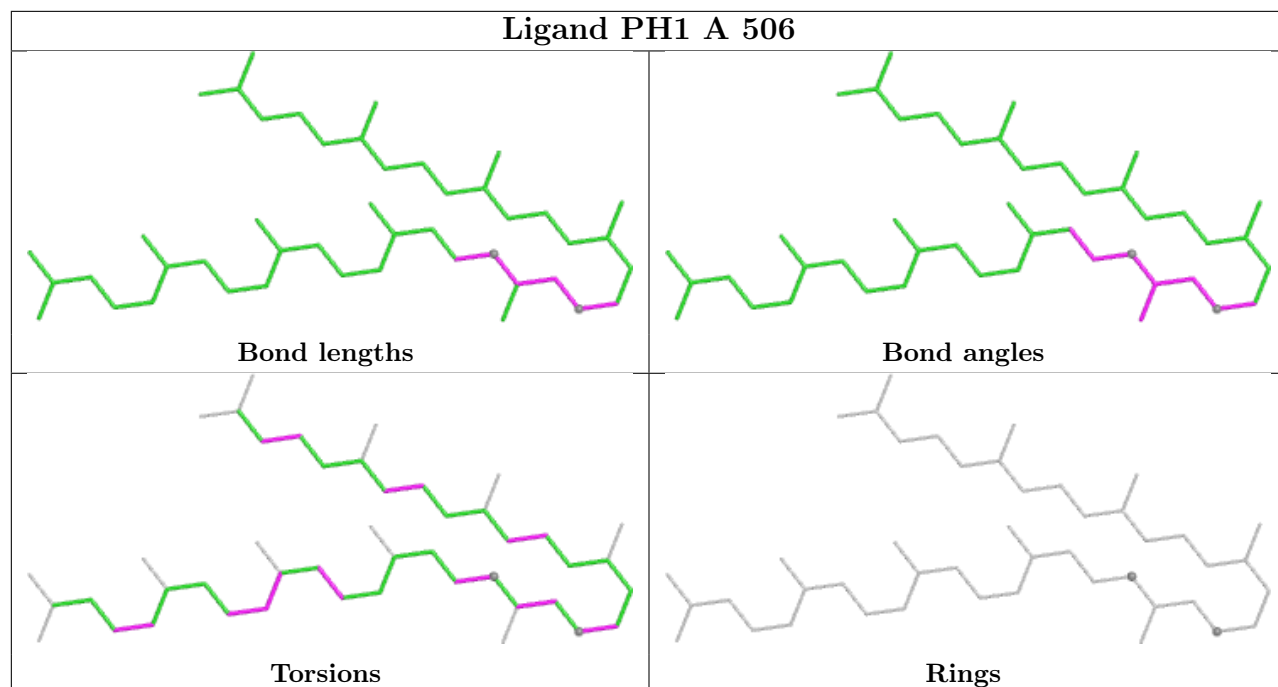
There are no ring outliers.

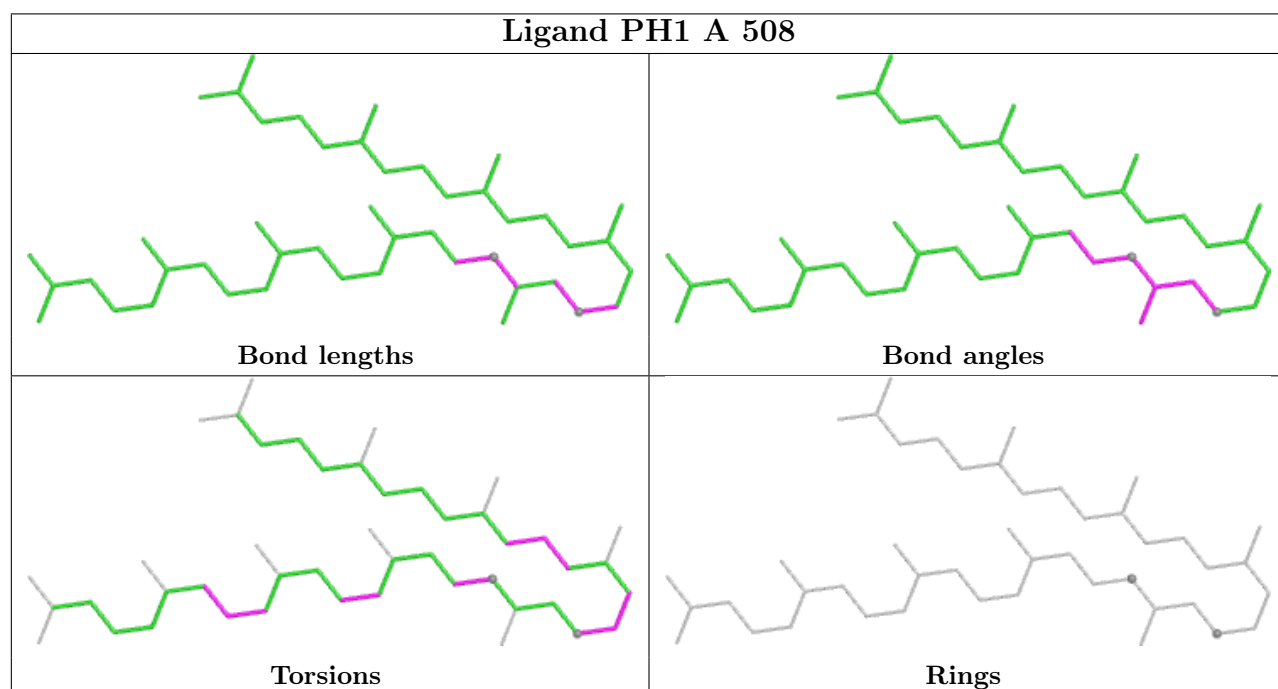
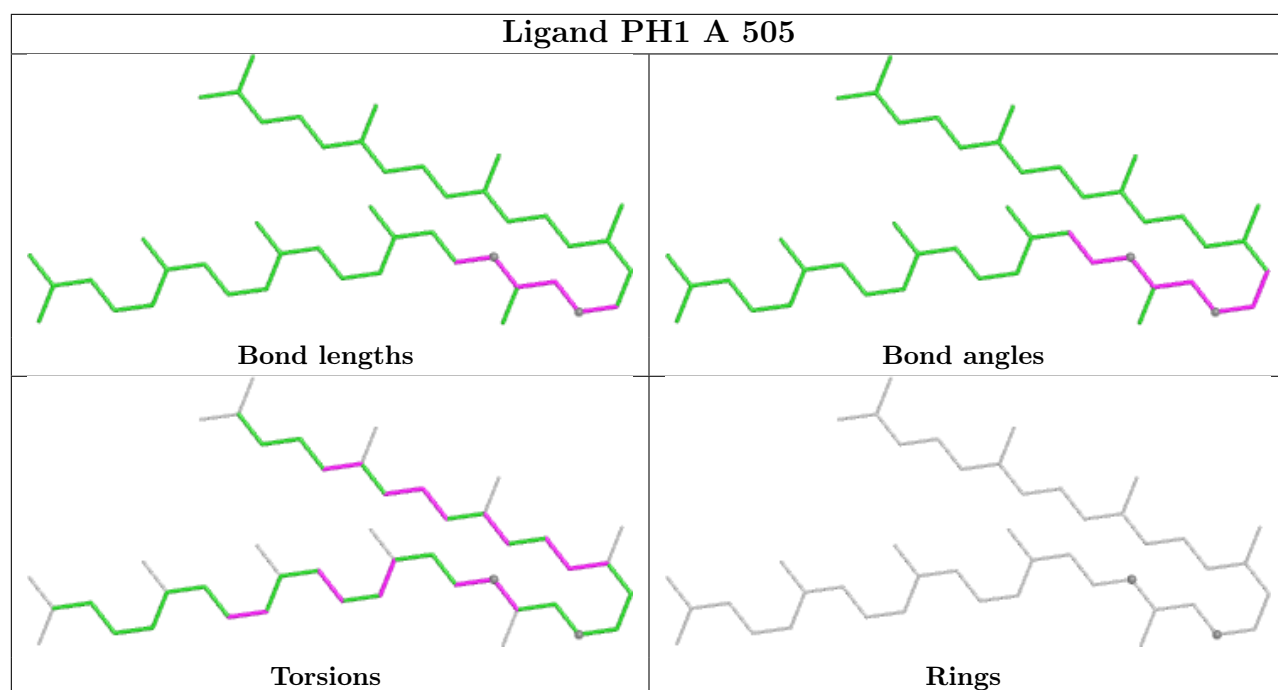
10 monomers are involved in 70 short contacts:

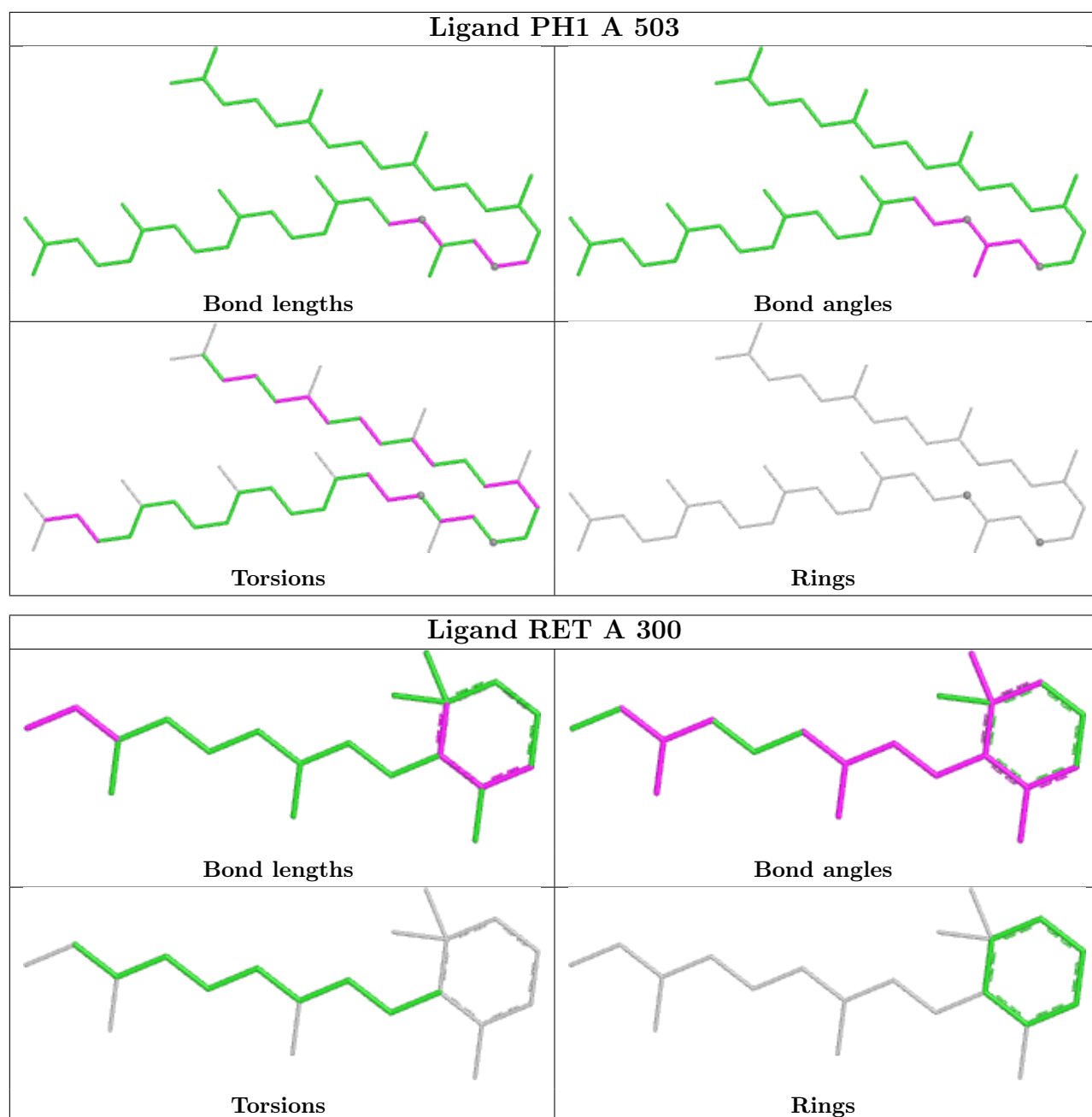
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PH1	3	0
3	A	504	PH1	2	0
3	A	506	PH1	10	0
3	A	500	PH1	18	0
3	A	505	PH1	8	0
3	A	508	PH1	8	0
3	A	503	PH1	7	0
2	A	300	RET	2	0
3	A	502	PH1	10	0
3	A	507	PH1	7	0

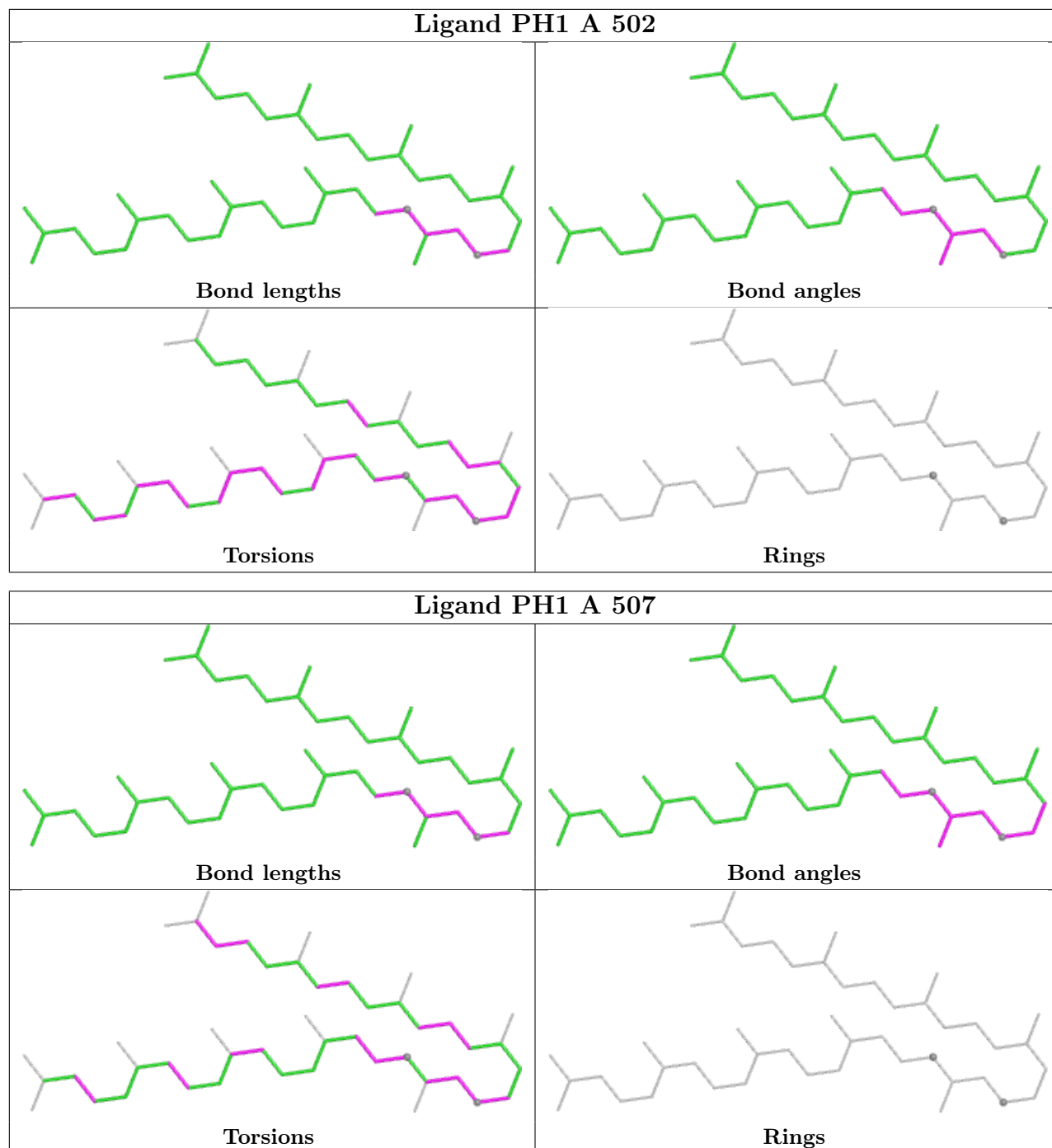
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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, 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	228/248 (91%)	0.76	30 (13%) 7 7	17, 27, 53, 68	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	THR	7.4
1	A	155	GLY	6.1
1	A	160	ALA	5.5
1	A	158	SER	5.3
1	A	156	PHE	5.0
1	A	5	THR	4.4
1	A	72	GLY	4.2
1	A	73	GLY	4.1
1	A	35	SER	3.5
1	A	39	ALA	3.5
1	A	166	GLU	3.3
1	A	38	ASP	3.3
1	A	165	PRO	3.3
1	A	34	VAL	3.1
1	A	162	SER	3.0
1	A	168	ALA	3.0
1	A	232	GLU	3.0
1	A	6	GLY	2.9
1	A	75	GLN	2.8
1	A	169	SER	2.7
1	A	33	GLY	2.7
1	A	150	TYR	2.5
1	A	37	PRO	2.5
1	A	154	PHE	2.4
1	A	159	LYS	2.3
1	A	228	ALA	2.2
1	A	167	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	LEU	2.1
1	A	164	ARG	2.1
1	A	231	GLY	2.0

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](#)

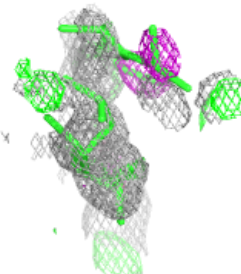
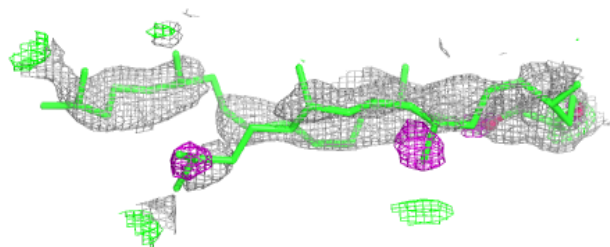
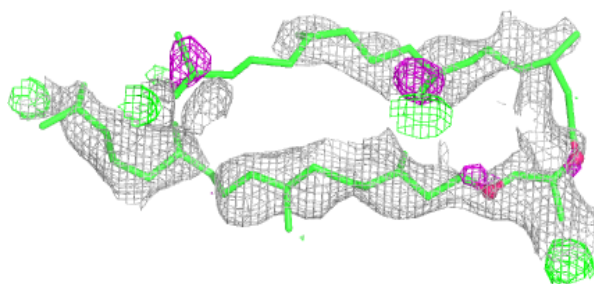
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PH1	A	505	45/45	0.52	0.18	57,57,57,57	0
3	PH1	A	507	45/45	0.56	0.19	57,57,57,57	0
3	PH1	A	503	45/45	0.61	0.16	57,57,57,57	0
3	PH1	A	502	45/45	0.64	0.18	57,57,57,57	0
3	PH1	A	500	45/45	0.65	0.19	57,57,57,57	0
3	PH1	A	504	45/45	0.65	0.15	57,57,57,57	0
3	PH1	A	501	45/45	0.68	0.19	57,57,57,57	0
3	PH1	A	508	45/45	0.69	0.18	57,57,57,57	0
3	PH1	A	506	45/45	0.72	0.16	57,57,57,57	0
2	RET	A	300	20/21	0.89	0.09	20,22,23,23	0

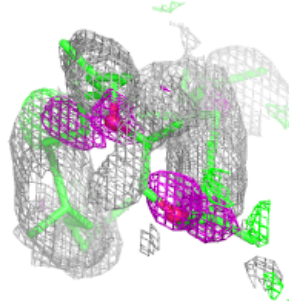
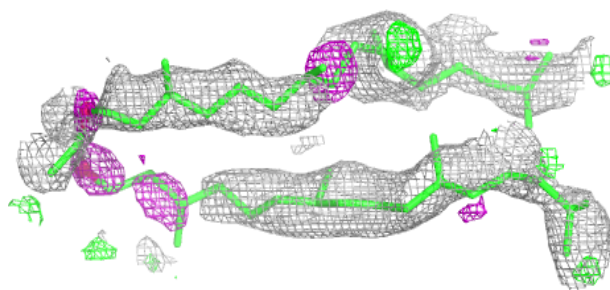
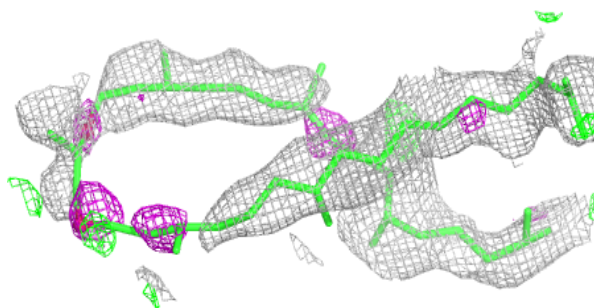
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PH1 A 505:

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

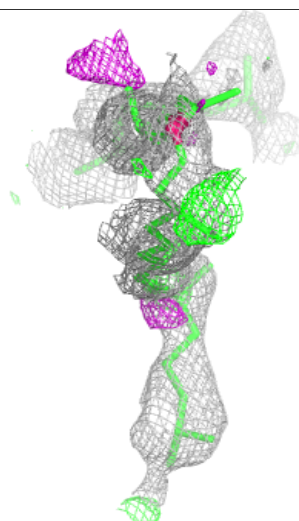
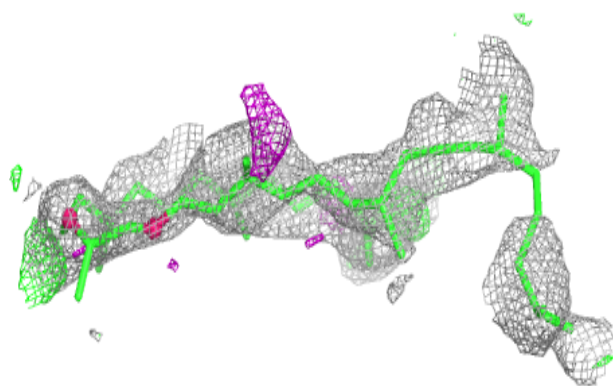
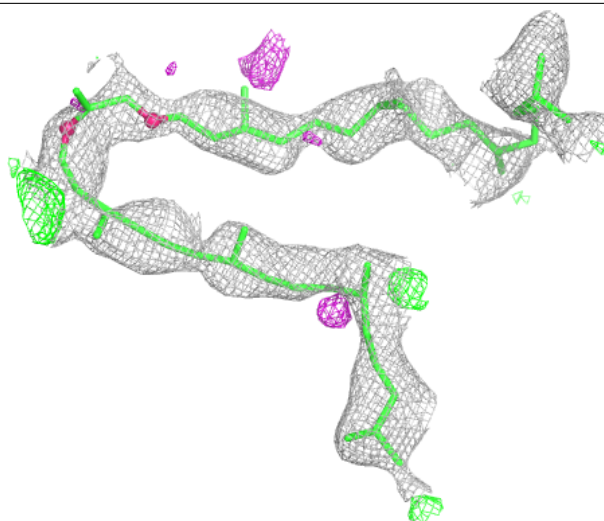
**Electron density around PH1 A 507:**

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



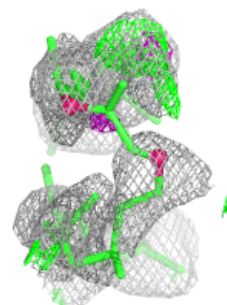
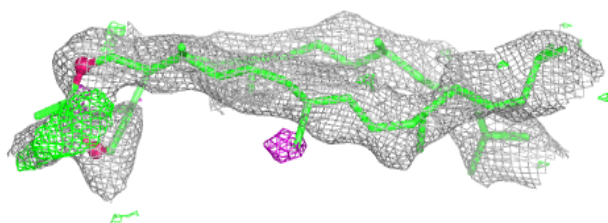
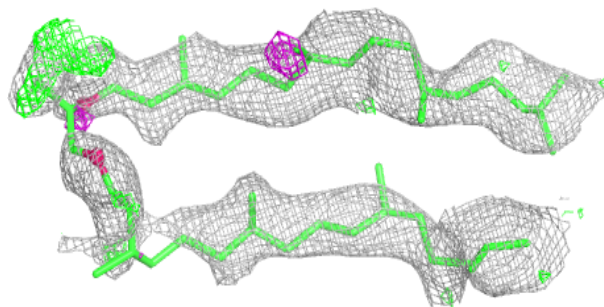
Electron density around PH1 A 503:

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

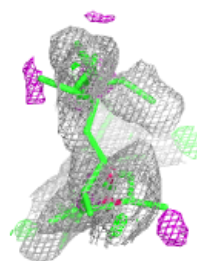
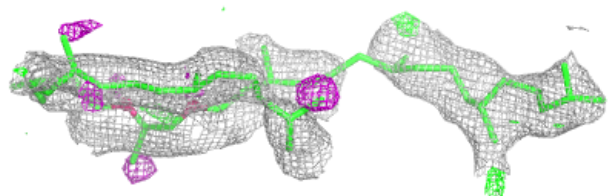
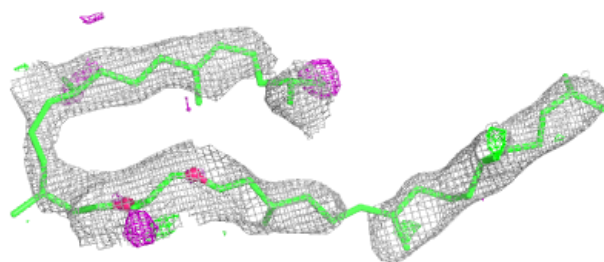


Electron density around PH1 A 502:

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

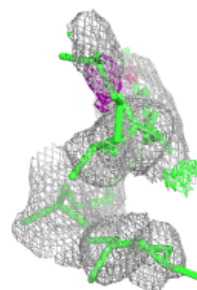
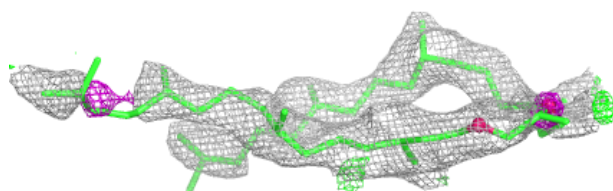
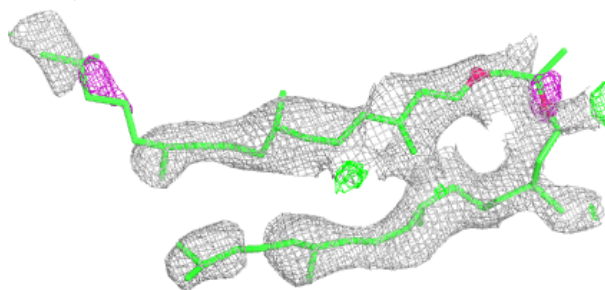
**Electron density around PH1 A 500:**

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

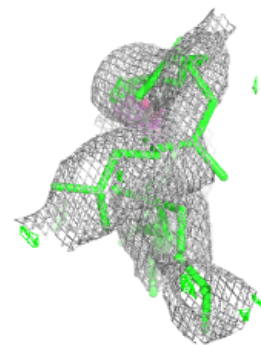
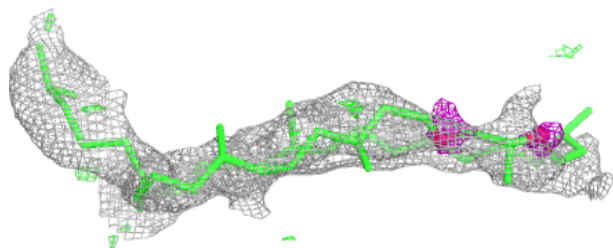
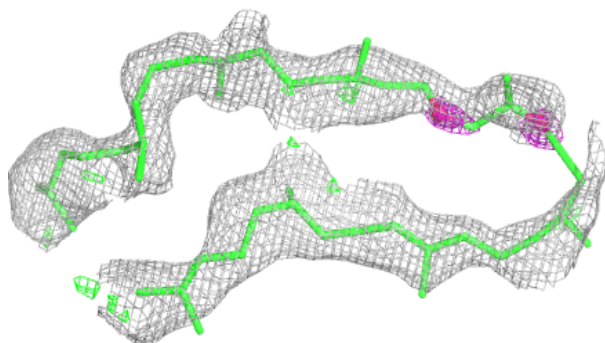


Electron density around PH1 A 504:

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

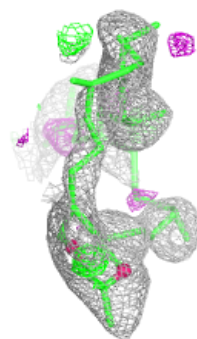
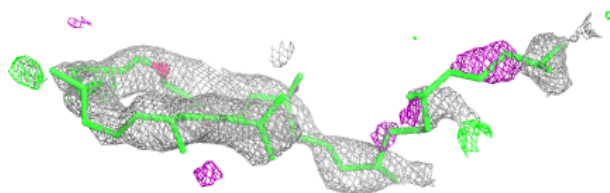
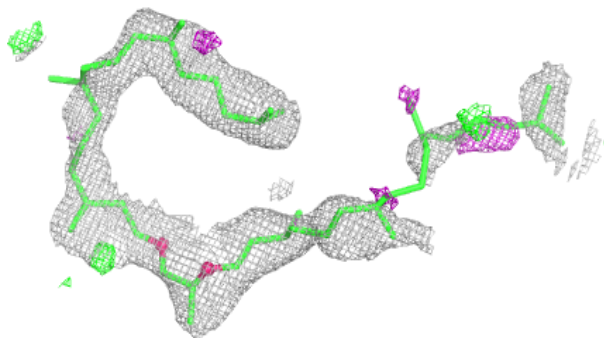
**Electron density around PH1 A 501:**

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



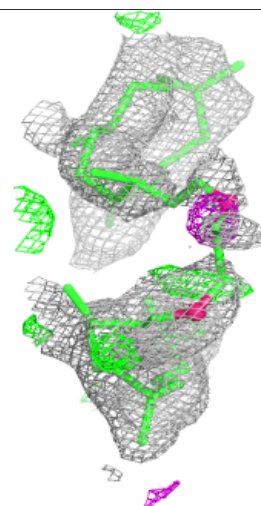
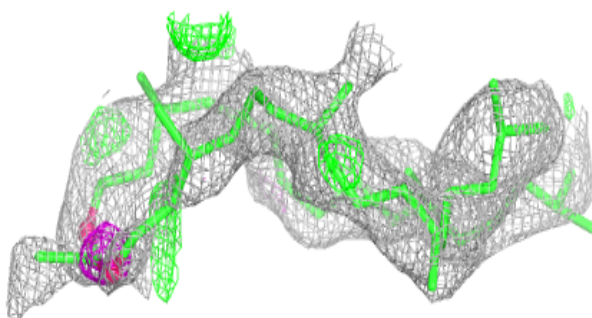
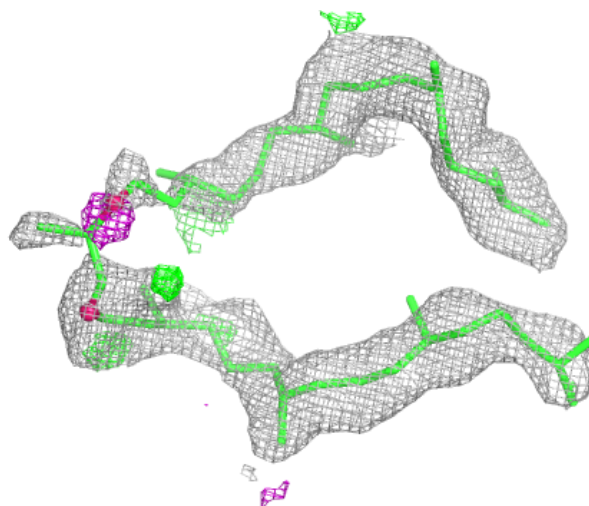
Electron density around PH1 A 508:

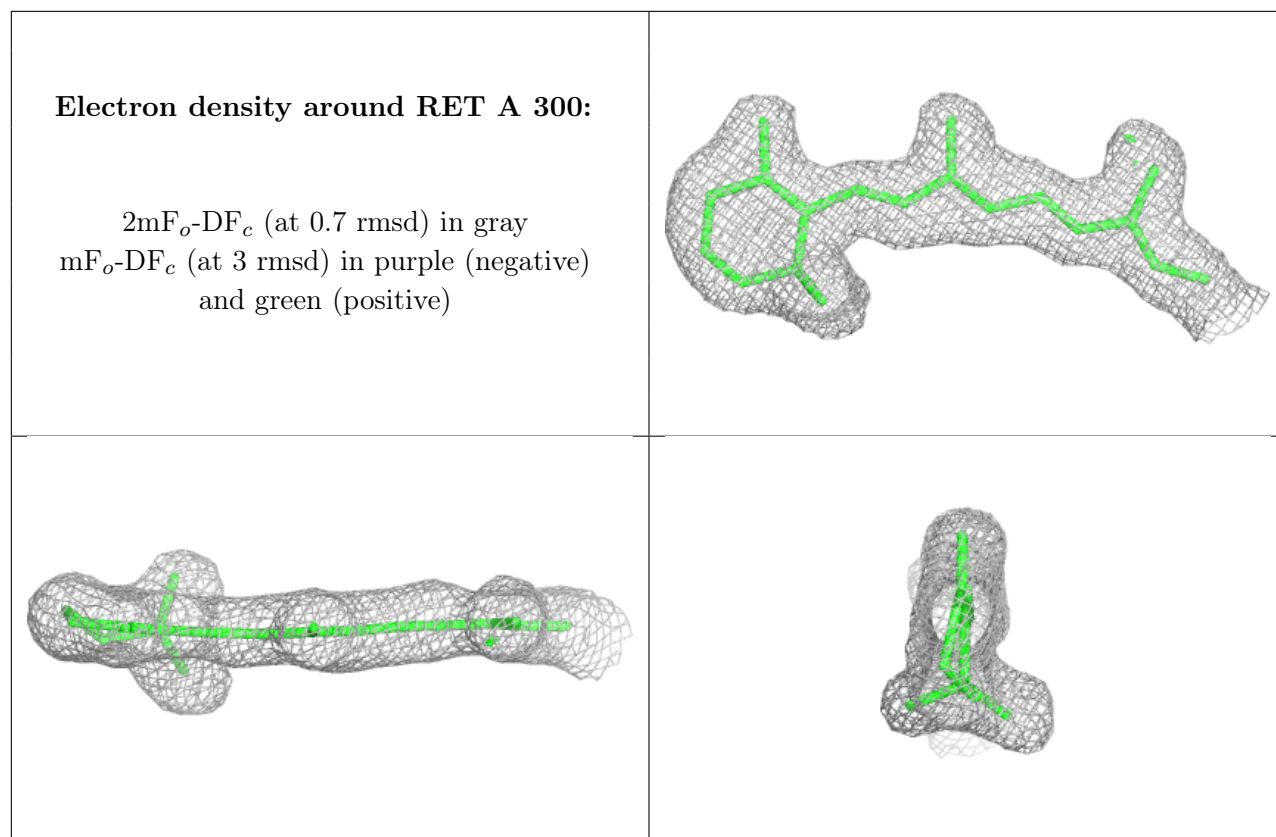
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PH1 A 506:

$2mF_o-DF_c$ (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.