Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 06:07 PM EDT

PDB ID	:	4K5Y
Title	:	Crystal structure of human corticotropin-releasing factor receptor 1 (CRF1R) in complex with the antagonist CP-376395
Authors	:	Hollenstein, K.; Kean, J.; Bortolato, A.; Cheng, R.K.Y.; Dore, A.S.; Jazayeri, A.; Cooke, R.M.; Weir, M.; Marshall, F.H.
Deposited on	:	2013-04-15
Resolution	:	2.98 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:

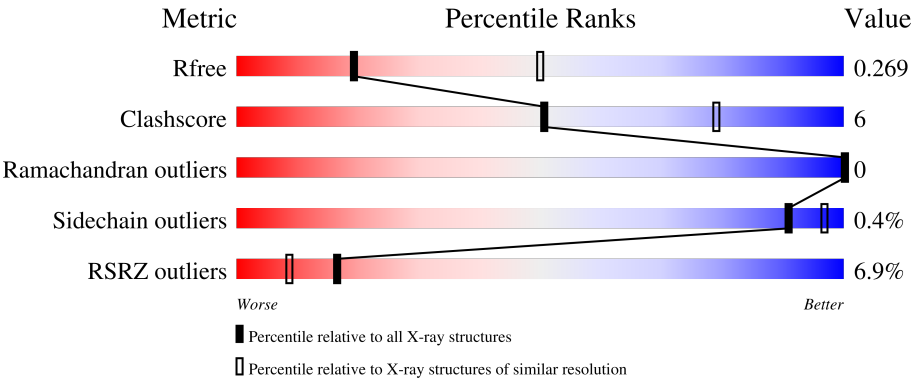
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	441	7% 79% 13% 8%
1	B	441	3% 78% 12% 10%
1	C	441	6% 50% 6% 44%

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
5	SO4	A	504	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8823 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 Corticotropin-releasing factor receptor 1, T4-Lysozyme chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3278	2145	562	554	17			
1	B	396	Total	C	N	O	S	0	0	0
			3194	2091	547	539	17			
1	C	248	Total	C	N	O	S	0	0	0
			2005	1341	330	321	13			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	initiating methionine	UNP P34998
A	120	ALA	VAL	engineered mutation	UNP P34998
A	144	ALA	LEU	engineered mutation	UNP P34998
A	156	ALA	TRP	engineered mutation	UNP P34998
A	160	ALA	SER	engineered mutation	UNP P34998
A	1040	SER	ASN	engineered mutation	UNP P00720
A	1041	VAL	ALA	engineered mutation	UNP P00720
A	1054	SER	CYS	engineered mutation	UNP P00720
A	1097	SER	CYS	engineered mutation	UNP P00720
A	1151	ALA	THR	engineered mutation	UNP P00720
A	228	ALA	LYS	engineered mutation	UNP P34998
A	260	ALA	PHE	engineered mutation	UNP P34998
A	277	ALA	ILE	engineered mutation	UNP P34998
A	309	ALA	TYR	engineered mutation	UNP P34998
A	330	ALA	PHE	engineered mutation	UNP P34998
A	349	ALA	SER	engineered mutation	UNP P34998
A	363	ALA	TYR	engineered mutation	UNP P34998
A	374	ALA	-	expression tag	UNP P34998
A	375	ALA	-	expression tag	UNP P34998
A	376	ALA	-	expression tag	UNP P34998
A	377	HIS	-	expression tag	UNP P34998
A	378	HIS	-	expression tag	UNP P34998

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Chain	Residue	Modelled	Actual	Comment	Reference
A	379	HIS	-	expression tag	UNP P34998
A	380	HIS	-	expression tag	UNP P34998
A	381	HIS	-	expression tag	UNP P34998
A	382	HIS	-	expression tag	UNP P34998
A	383	HIS	-	expression tag	UNP P34998
A	384	HIS	-	expression tag	UNP P34998
A	385	HIS	-	expression tag	UNP P34998
A	386	HIS	-	expression tag	UNP P34998
B	103	MET	-	initiating methionine	UNP P34998
B	120	ALA	VAL	engineered mutation	UNP P34998
B	144	ALA	LEU	engineered mutation	UNP P34998
B	156	ALA	TRP	engineered mutation	UNP P34998
B	160	ALA	SER	engineered mutation	UNP P34998
B	1040	SER	ASN	engineered mutation	UNP P00720
B	1041	VAL	ALA	engineered mutation	UNP P00720
B	1054	SER	CYS	engineered mutation	UNP P00720
B	1097	SER	CYS	engineered mutation	UNP P00720
B	1151	ALA	THR	engineered mutation	UNP P00720
B	228	ALA	LYS	engineered mutation	UNP P34998
B	260	ALA	PHE	engineered mutation	UNP P34998
B	277	ALA	ILE	engineered mutation	UNP P34998
B	309	ALA	TYR	engineered mutation	UNP P34998
B	330	ALA	PHE	engineered mutation	UNP P34998
B	349	ALA	SER	engineered mutation	UNP P34998
B	363	ALA	TYR	engineered mutation	UNP P34998
B	374	ALA	-	expression tag	UNP P34998
B	375	ALA	-	expression tag	UNP P34998
B	376	ALA	-	expression tag	UNP P34998
B	377	HIS	-	expression tag	UNP P34998
B	388	HIS	-	expression tag	UNP P34998
B	389	HIS	-	expression tag	UNP P34998
B	390	HIS	-	expression tag	UNP P34998
B	391	HIS	-	expression tag	UNP P34998
B	392	HIS	-	expression tag	UNP P34998
B	393	HIS	-	expression tag	UNP P34998
B	394	HIS	-	expression tag	UNP P34998
B	395	HIS	-	expression tag	UNP P34998
B	396	HIS	-	expression tag	UNP P34998
C	103	MET	-	initiating methionine	UNP P34998
C	120	ALA	VAL	engineered mutation	UNP P34998
C	144	ALA	LEU	engineered mutation	UNP P34998
C	156	ALA	TRP	engineered mutation	UNP P34998

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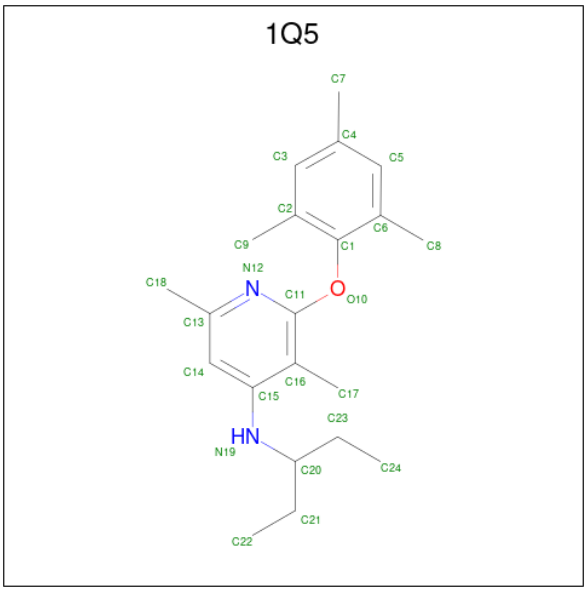
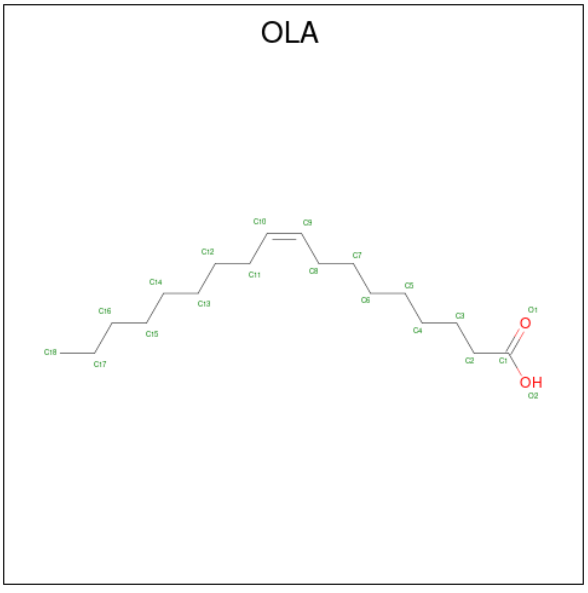
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	ALA	SER	engineered mutation	UNP P34998
C	1040	SER	ASN	engineered mutation	UNP P00720
C	1041	VAL	ALA	engineered mutation	UNP P00720
C	1054	SER	CYS	engineered mutation	UNP P00720
C	1097	SER	CYS	engineered mutation	UNP P00720
C	1151	ALA	THR	engineered mutation	UNP P00720
C	228	ALA	LYS	engineered mutation	UNP P34998
C	260	ALA	PHE	engineered mutation	UNP P34998
C	277	ALA	ILE	engineered mutation	UNP P34998
C	309	ALA	TYR	engineered mutation	UNP P34998
C	330	ALA	PHE	engineered mutation	UNP P34998
C	349	ALA	SER	engineered mutation	UNP P34998
C	363	ALA	TYR	engineered mutation	UNP P34998
C	374	ALA	-	expression tag	UNP P34998
C	375	ALA	-	expression tag	UNP P34998
C	376	ALA	-	expression tag	UNP P34998
C	377	HIS	-	expression tag	UNP P34998
C	378	HIS	-	expression tag	UNP P34998
C	379	HIS	-	expression tag	UNP P34998
C	380	HIS	-	expression tag	UNP P34998
C	381	HIS	-	expression tag	UNP P34998
C	382	HIS	-	expression tag	UNP P34998
C	383	HIS	-	expression tag	UNP P34998
C	384	HIS	-	expression tag	UNP P34998
C	385	HIS	-	expression tag	UNP P34998
C	386	HIS	-	expression tag	UNP P34998

- Molecule 2 is 3,6-dimethyl-N-(pentan-3-yl)-2-(2,4,6-trimethylphenoxy)pyridin-4-amine (three-letter code: 1Q5) (formula: $C_{21}H_{30}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 24 21 2 1	0	0
2	B	1	Total C N O 24 21 2 1	0	0
2	C	1	Total C N O 24 21 2 1	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 13 13	0	0

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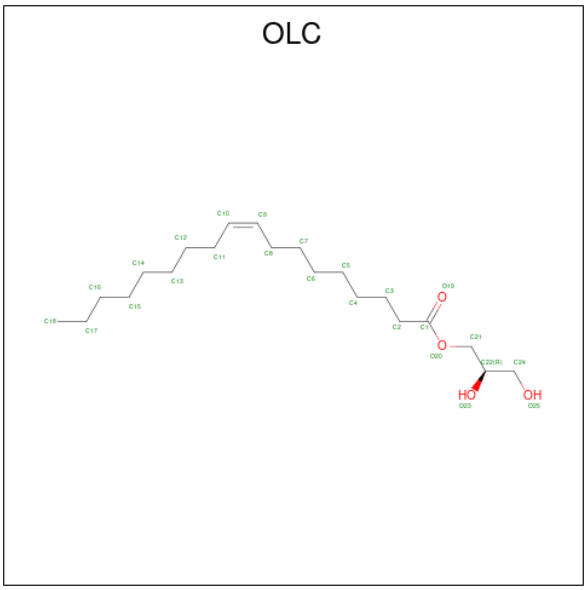
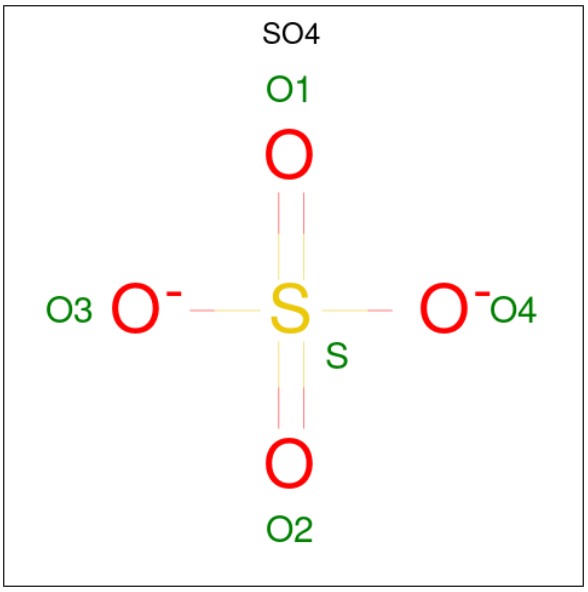
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 20 18 2	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



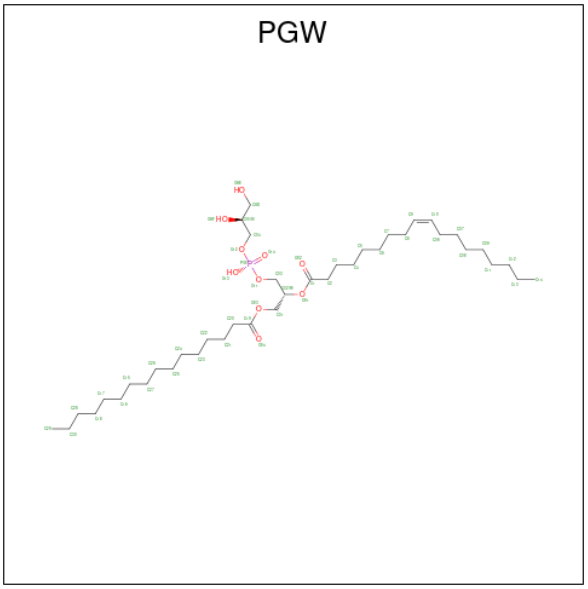
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	B	1	Total C O 25 21 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



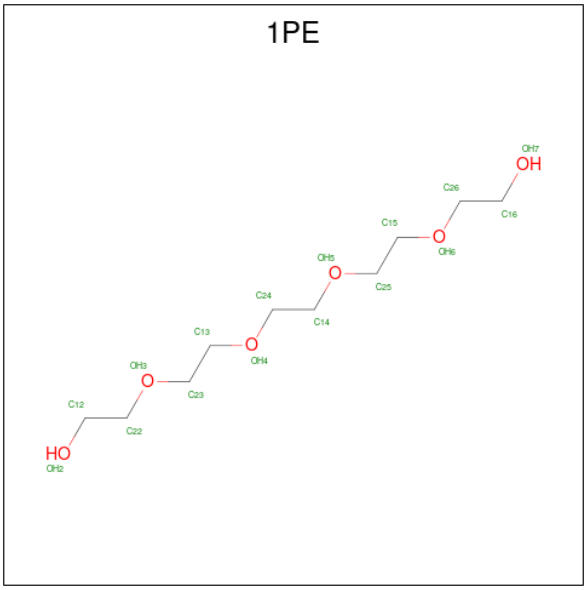
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O P 39 30 8 1	0	0
6	B	1	Total C O P 46 37 8 1	0	0
6	B	1	Total C O 37 32 5	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 16 10 6	0	0

- Molecule 8 is water.

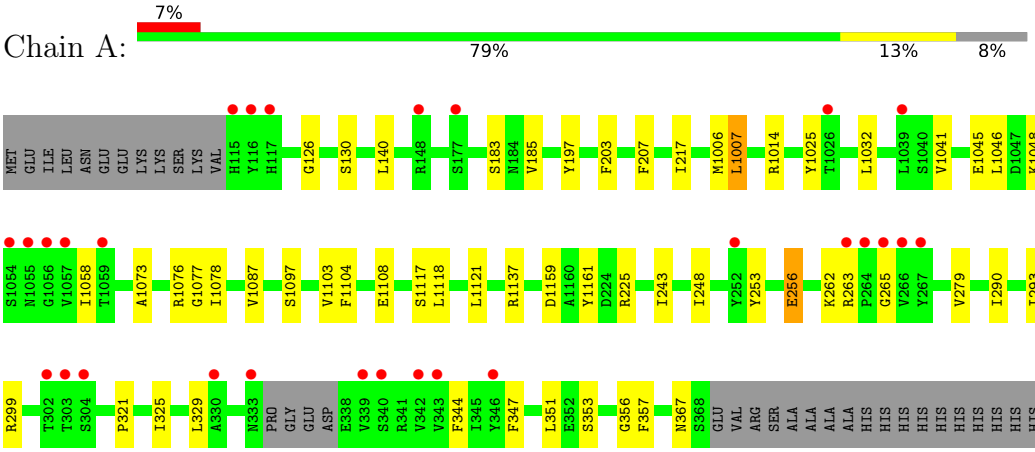
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	4	Total O 4 4	0	0
8	B	4	Total O 4 4	0	0

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.

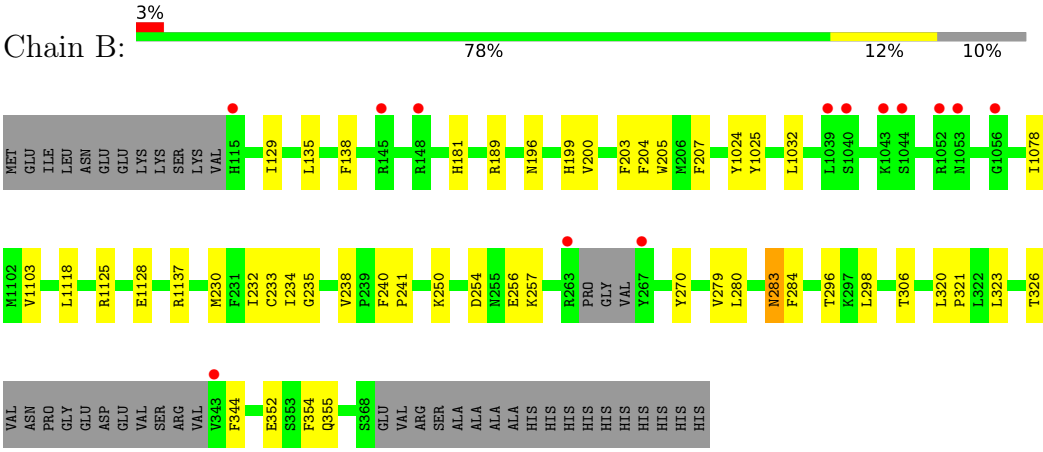
• Molecule 1: Corticotropin-releasing factor receptor 1, T4-Lysozyme chimeric construct

Chain A:



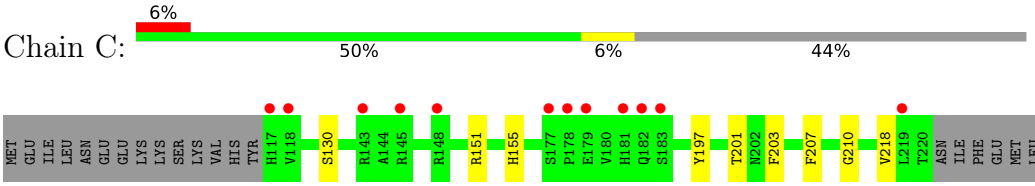
• Molecule 1: Corticotropin-releasing factor receptor 1, T4-Lysozyme chimeric construct

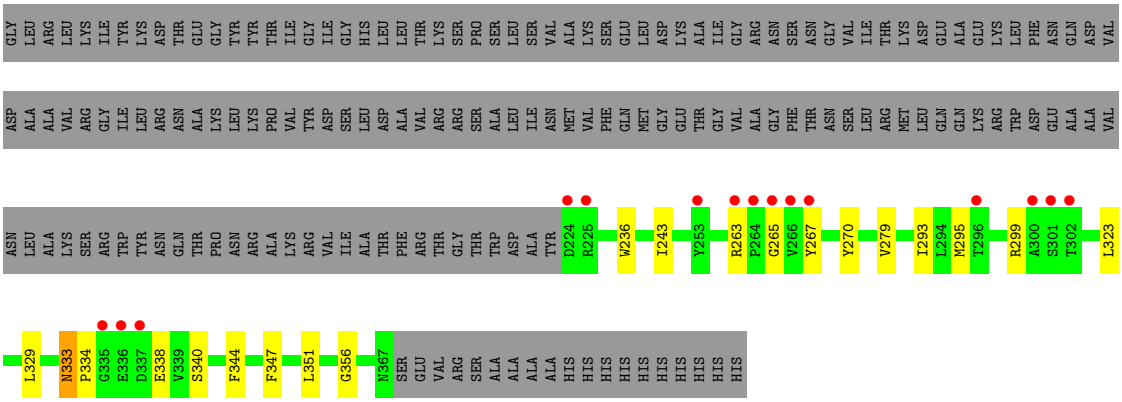
Chain B:



• Molecule 1: Corticotropin-releasing factor receptor 1, T4-Lysozyme chimeric construct

Chain C:




GLY LEU ARG LEU LYS ILE TYR LYS ASP THR GLU GLY TYR TYR THR ILE GLY ILE GLY HIS LEU LEU THR LYS SER PRO SER LEU SER VAL ALA LYS SER GLU LEU ASP LYS ALA ILE GLY ARG ASN SER ASN GLY VAL ILE THR LYS ASP GLU ALA GLU LYS LEU PHE ASN GLN ASP VAL
ASP ALA ALA VAL ARG GLY ILE LEU ARG ASN ALA LYS LEU LYS PRO VAL TYR ASP SER LEU ASP ALA VAL ARG ARG SER ALA LEU ILE ASN MET VAL PHE GLN MET GLY GLU THR GLY VAL ALA GLY PHE THR ASN SER LEU ARG MET LEU GLN GLN LYS ARG TRP ASP GLU ALA ALA VAL
ASN LEU ALA LYS SER ARG TRP TYR ASN GLN THR PRO ASN ARG ALA LYS ARG VAL ILE ALA THR PHE ARG THR GLY THR TRP ASP ALA TYR D224 R225 W236 I243 Y253 R263 P264 G265 V266 Y267 Y270 V279 I293 L294 M295 T296 R299 A300 S301 T302 L323
L329 N333 P334 G335 E336 D337 E338 V339 S340 F344 F347 L351 G356 N367 SER GLU VAL ARG SER ALA ALA ALA ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.56Å 123.97Å 166.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.98 34.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	85.7 (34.14-2.98) 85.7 (34.15-2.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.242 , 0.265 0.245 , 0.269	Depositor DCC
R_{free} test set	1586 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8823	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: 1PE, PGW, OLA, 1Q5, OLC, SO4

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	0.62	0/3358	0.68	3/4556 (0.1%)
1	B	0.65	0/3271	0.65	1/4435 (0.0%)
1	C	0.60	0/2063	0.69	0/2810
All	All	0.63	0/8692	0.67	4/11801 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	LYS	N-CA-C	-7.98	89.46	111.00
1	B	296	THR	N-CA-C	6.72	129.15	111.00
1	A	1048	LYS	CD-CE-NZ	-6.53	96.68	111.70
1	A	1007	LEU	CB-CG-CD2	-5.55	101.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLU	Mainchain

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	3278	0	3333	40	1
1	B	3194	0	3247	40	1
1	C	2005	0	2038	19	1
2	A	24	0	30	2	0
2	B	24	0	30	5	0
2	C	24	0	30	3	0
3	A	13	0	23	1	0
3	C	20	0	33	1	0
4	A	50	0	80	4	0
4	B	25	0	40	2	0
5	A	5	0	0	1	1
5	B	15	0	0	0	1
6	B	122	0	174	10	0
7	B	16	0	22	0	0
8	A	4	0	0	0	0
8	B	4	0	0	1	0
All	All	8823	0	9080	102	3

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 6.

All (102) 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:C:338:GLU:HB2	1:C:340:SER:H	1.44	0.82
1:B:329:LEU:HB3	1:B:344:PHE:HE1	1.48	0.77
1:A:1006:MET:HG2	1:A:1007:LEU:HD12	1.69	0.75
1:A:263:ARG:O	1:A:265:GLY:HA3	1.87	0.74
1:C:263:ARG:O	1:C:265:GLY:HA3	1.92	0.70
1:A:367:ASN:ND2	4:A:502:OLC:O25	2.28	0.67
1:B:1024:TYR:HB3	1:B:1032:LEU:HD11	1.77	0.66
1:B:232:ILE:HD11	6:B:502:PGW:H01A	1.77	0.66
1:A:197:TYR:HA	1:A:243:ILE:HG13	1.78	0.65
1:A:357:PHE:HE1	4:A:502:OLC:H11A	1.63	0.63
1:B:1087:VAL:HG21	1:B:1118:LEU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1025:TYR:O	1:B:1032:LEU:HD12	2.00	0.61
1:A:126:GLY:HA3	1:A:353:SER:HB2	1.82	0.61
1:B:320:LEU:HD22	2:B:401:1Q5:H14	1.84	0.60
1:A:140:LEU:HD13	4:A:502:OLC:H22	1.85	0.58
1:A:1041:VAL:O	1:A:1045:GLU:HG2	2.04	0.58
1:B:323:LEU:HD22	1:B:355:GLN:HG2	1.86	0.58
1:A:347:PHE:CE2	1:A:351:LEU:HD11	2.39	0.57
1:C:218:VAL:HG22	1:C:293:ILE:HD12	1.86	0.55
1:B:203:PHE:CE1	2:B:401:1Q5:H24	2.42	0.55
1:C:334:PRO:HD3	1:C:344:PHE:CZ	2.42	0.55
1:A:203:PHE:CE1	2:A:401:1Q5:H24	2.42	0.54
1:B:199:HIS:HE1	6:B:504:PGW:H02	1.72	0.54
1:B:250:LYS:O	1:B:254:ASP:O	2.26	0.53
1:B:320:LEU:HB3	1:B:321:PRO:HD3	1.90	0.53
1:A:248:ILE:HD12	4:B:501:OLC:H8A	1.92	0.52
1:A:248:ILE:HG23	1:B:230:MET:HE1	1.93	0.51
1:B:135:LEU:HD22	6:B:502:PGW:H11A	1.93	0.51
6:B:504:PGW:H2	6:B:504:PGW:H24	1.93	0.50
1:A:1014:ARG:HH11	1:B:256:GLU:CG	2.24	0.49
1:C:197:TYR:HB2	1:C:243:ILE:HG13	1.94	0.49
1:C:323:LEU:HD12	2:C:401:1Q5:H7	1.93	0.49
1:A:256:GLU:OE2	1:A:263:ARG:HG3	2.12	0.49
1:A:217:ILE:HD12	1:A:290:ILE:HG23	1.95	0.48
1:C:203:PHE:CE1	2:C:401:1Q5:H24	2.48	0.48
1:B:283:ASN:ND2	2:B:401:1Q5:H1	2.29	0.48
1:B:280:LEU:HD23	6:B:504:PGW:H06A	1.95	0.48
1:A:1006:MET:HE1	1:A:1097:SER:HB3	1.95	0.48
1:A:1014:ARG:NH1	1:B:254:ASP:OD1	2.47	0.48
1:C:267:TYR:HB3	1:C:270:TYR:CD1	2.49	0.48
1:A:1118:LEU:HD23	1:A:1121:LEU:HD12	1.94	0.48
1:A:1007:LEU:CD2	1:A:1104:PHE:HD2	2.27	0.48
1:C:207:PHE:HB2	1:C:279:VAL:CG1	2.43	0.48
1:A:1087:VAL:HG21	1:A:1118:LEU:HB3	1.96	0.47
1:B:234:ILE:HD11	4:B:501:OLC:H4A	1.95	0.47
1:B:329:LEU:HB3	1:B:344:PHE:CE1	2.38	0.47
1:A:1078:ILE:HD11	1:A:1103:VAL:HG21	1.97	0.47
1:A:207:PHE:HB2	1:A:279:VAL:CG1	2.45	0.47
1:A:1073:ALA:HA	1:A:1076:ARG:HE	1.79	0.47
1:B:283:ASN:HD22	2:B:401:1Q5:H1	1.80	0.47
1:B:204:PHE:O	1:B:207:PHE:HB3	2.15	0.47
1:C:334:PRO:HD3	1:C:344:PHE:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ASN:O	1:B:200:VAL:HG23	2.16	0.46
1:B:326:THR:HG21	1:B:352:GLU:HG3	1.98	0.46
1:A:1117:SER:N	5:A:504:SO4:O3	2.44	0.46
4:A:503:OLC:H3	1:B:189:ARG:NH2	2.31	0.46
1:C:333:ASN:HD22	1:C:333:ASN:C	2.16	0.46
1:C:201:THR:HG21	1:C:236:TRP:CZ3	2.51	0.45
1:A:321:PRO:O	1:A:325:ILE:HG22	2.17	0.45
1:C:210:GLY:HA2	2:C:401:1Q5:H9	1.97	0.45
3:C:501:OLA:H112	3:C:501:OLA:H82	1.75	0.45
6:B:502:PGW:H22A	6:B:502:PGW:H6	1.99	0.45
1:A:1006:MET:HG3	1:A:1161:TYR:CZ	2.52	0.45
1:A:256:GLU:CD	1:A:263:ARG:HE	2.19	0.45
1:B:207:PHE:HB2	1:B:279:VAL:CG1	2.47	0.45
1:A:183:SER:OG	1:A:185:VAL:HG23	2.17	0.44
1:B:284:PHE:CE1	1:B:320:LEU:HD21	2.53	0.44
1:B:205:TRP:CE2	1:B:235:GLY:HA3	2.53	0.44
1:A:1025:TYR:O	1:A:1032:LEU:HD12	2.18	0.44
1:A:293:ILE:HA	1:A:296:THR:OG1	2.18	0.44
1:A:1117:SER:O	1:A:1121:LEU:HG	2.18	0.44
1:A:325:ILE:HG23	1:A:351:LEU:HD13	1.99	0.44
1:A:1159:ASP:O	1:A:225:ARG:HG3	2.17	0.43
1:A:1077:GLY:HA3	1:A:1108:GLU:OE2	2.18	0.43
1:A:329:LEU:HD22	1:A:344:PHE:HE1	1.84	0.43
1:C:130:SER:HB3	1:C:356:GLY:HA3	2.00	0.43
1:A:325:ILE:HD13	1:A:347:PHE:HE2	1.82	0.43
3:A:501:OLA:H112	3:A:501:OLA:H82	1.84	0.42
1:B:270:TYR:CD2	6:B:504:PGW:H17	2.54	0.42
1:B:129:ILE:HA	6:B:503:PGW:H18A	2.01	0.42
1:B:138:PHE:CE2	6:B:502:PGW:H08	2.55	0.42
1:B:284:PHE:CZ	1:B:320:LEU:HD21	2.55	0.42
2:B:401:1Q5:H8	2:B:401:1Q5:H4	1.78	0.42
1:B:1101:ASN:OD1	8:B:602:HOH:O	2.22	0.42
1:B:199:HIS:CE1	6:B:504:PGW:H02	2.54	0.42
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.89	0.42
1:A:295:MET:O	1:A:299:ARG:HG3	2.20	0.42
1:B:238:VAL:O	1:B:241:PRO:HD2	2.20	0.42
1:A:1046:LEU:HD21	1:A:1058:ILE:HG23	2.01	0.41
1:C:151:ARG:HG2	1:C:155:HIS:CE1	2.55	0.41
1:C:329:LEU:HD22	1:C:344:PHE:CE2	2.55	0.41
1:A:130:SER:HB3	1:A:356:GLY:HA3	2.02	0.41
1:B:298:LEU:HD13	1:B:306:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:401:1Q5:H8	2:A:401:1Q5:H4	1.77	0.41
1:B:1078:ILE:HD11	1:B:1103:VAL:HG21	2.03	0.41
1:C:295:MET:O	1:C:299:ARG:HB2	2.21	0.41
1:B:1125:ARG:HH11	1:B:1128:GLU:CD	2.24	0.40
1:C:207:PHE:HB2	1:C:279:VAL:HG13	2.03	0.40
1:C:347:PHE:CZ	1:C:351:LEU:HD11	2.56	0.40
1:B:240:PHE:HB3	1:B:241:PRO:HD3	2.03	0.40
1:B:181:HIS:NE2	1:B:257:LYS:HB3	2.36	0.40
1:B:233:CYS:O	1:B:238:VAL:HG23	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:ARG:NH1	5:B:506:SO4:O1[1_655]	2.16	0.04
1:B:1137:ARG:NH1	5:A:504:SO4:O2[1_455]	2.17	0.03
1:C:270:TYR:OH	1:C:338:GLU:OE1[2_556]	2.19	0.01

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	403/441 (91%)	394 (98%)	9 (2%)	0	100	100
1	B	390/441 (88%)	383 (98%)	7 (2%)	0	100	100
1	C	244/441 (55%)	240 (98%)	4 (2%)	0	100	100
All	All	1037/1323 (78%)	1017 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	345/374 (92%)	344 (100%)	1 (0%)	92	97
1	B	335/374 (90%)	333 (99%)	2 (1%)	86	94
1	C	211/374 (56%)	210 (100%)	1 (0%)	88	95
All	All	891/1122 (79%)	887 (100%)	4 (0%)	91	97

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

Mol	Chain	Res	Type
1	A	253	TYR
1	B	283	ASN
1	B	354	PHE
1	C	333	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	367	ASN
1	C	333	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\|>2$
4	OLC	A	502	-	24,24,24	0.80	2 (8%)	25,25,25	0.99	1 (4%)
6	PGW	B	503	-	45,45,50	0.89	3 (6%)	49,50,56	1.18	3 (6%)
2	1Q5	A	401	-	24,25,25	1.59	3 (12%)	31,35,35	1.96	9 (29%)
6	PGW	B	504	-	36,36,50	0.92	3 (8%)	38,38,56	1.23	2 (5%)
2	1Q5	B	401	-	24,25,25	1.57	3 (12%)	31,35,35	1.82	7 (22%)
5	SO4	B	507	-	4,4,4	0.15	0	6,6,6	0.14	0
4	OLC	A	503	-	24,24,24	0.83	2 (8%)	25,25,25	0.98	2 (8%)
7	1PE	B	505	-	15,15,15	0.52	0	14,14,14	0.86	0
5	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.10	0
4	OLC	B	501	-	24,24,24	0.80	2 (8%)	25,25,25	0.98	1 (4%)
3	OLA	A	501	-	12,12,19	0.31	0	11,11,19	0.67	0
5	SO4	B	508	-	4,4,4	0.15	0	6,6,6	0.07	0
2	1Q5	C	401	-	24,25,25	1.56	3 (12%)	31,35,35	1.79	7 (22%)
3	OLA	C	501	-	19,19,19	0.50	0	19,19,19	1.03	0
5	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.06	0
6	PGW	B	502	-	38,38,50	0.97	3 (7%)	42,43,56	1.25	3 (7%)

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
4	OLC	A	502	-	-	9/24/24/24	-
6	PGW	B	503	-	-	17/47/47/55	-
2	1Q5	A	401	-	-	2/12/12/12	0/2/2/2
6	PGW	B	504	-	-	18/38/38/55	-
2	1Q5	B	401	-	-	3/12/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	A	503	-	-	17/24/24/24	-
7	1PE	B	505	-	-	6/13/13/13	-
4	OLC	B	501	-	-	9/24/24/24	-
3	OLA	A	501	-	-	4/10/10/17	-
2	1Q5	C	401	-	-	3/12/12/12	0/2/2/2
3	OLA	C	501	-	-	9/17/17/17	-
6	PGW	B	502	-	-	14/40/40/55	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1Q5	C1-C6	4.40	1.47	1.40
2	B	401	1Q5	C1-C6	4.39	1.47	1.40
2	C	401	1Q5	C1-C6	4.30	1.47	1.40
2	A	401	1Q5	C1-C2	4.11	1.47	1.40
2	C	401	1Q5	C1-C2	3.98	1.47	1.40
2	B	401	1Q5	C1-C2	3.96	1.47	1.40
2	A	401	1Q5	C15-C16	3.93	1.46	1.40
2	B	401	1Q5	C15-C16	3.92	1.46	1.40
2	C	401	1Q5	C15-C16	3.86	1.46	1.40
6	B	503	PGW	O01-C1	-3.16	1.25	1.34
6	B	504	PGW	O01-C1	-3.10	1.25	1.34
6	B	502	PGW	O01-C1	-2.95	1.26	1.34
6	B	503	PGW	O03-C19	-2.64	1.25	1.33
4	B	501	OLC	O20-C1	-2.62	1.25	1.33
4	A	502	OLC	O20-C1	-2.52	1.25	1.33
6	B	504	PGW	O03-C19	-2.50	1.26	1.33
6	B	502	PGW	O03-C19	-2.47	1.26	1.33
4	A	503	OLC	O20-C21	2.45	1.50	1.45
4	A	503	OLC	O20-C1	-2.44	1.26	1.33
6	B	504	PGW	O03-C01	2.31	1.50	1.45
4	A	502	OLC	O20-C21	2.29	1.50	1.45
6	B	502	PGW	O03-C01	2.25	1.50	1.45
4	B	501	OLC	O20-C21	2.21	1.50	1.45
6	B	503	PGW	O03-C01	2.06	1.49	1.45

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	1Q5	C1-O10-C11	5.37	122.38	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	1Q5	C1-O10-C11	4.27	121.26	116.88
6	B	503	PGW	O01-C1-C2	4.16	120.47	111.50
6	B	504	PGW	O01-C1-C2	4.14	120.43	111.50
2	C	401	1Q5	C1-O10-C11	3.95	120.92	116.88
2	A	401	1Q5	C16-C11-N12	-3.92	120.02	125.36
2	B	401	1Q5	C16-C11-N12	-3.86	120.11	125.36
2	C	401	1Q5	C16-C11-N12	-3.84	120.13	125.36
6	B	502	PGW	O01-C1-C2	3.84	119.78	111.50
2	B	401	1Q5	C3-C4-C5	3.53	122.30	118.09
2	C	401	1Q5	C3-C4-C5	3.53	122.30	118.09
2	A	401	1Q5	C3-C4-C5	3.45	122.20	118.09
2	B	401	1Q5	C11-N12-C13	3.36	121.61	116.89
2	C	401	1Q5	C11-N12-C13	3.28	121.49	116.89
2	A	401	1Q5	C11-N12-C13	3.20	121.39	116.89
2	A	401	1Q5	C14-C15-C16	-3.06	117.60	121.32
2	C	401	1Q5	C14-C15-C16	-2.98	117.69	121.32
2	A	401	1Q5	C15-N19-C20	-2.96	119.61	124.69
2	B	401	1Q5	C14-C15-C16	-2.94	117.75	121.32
2	B	401	1Q5	C15-N19-C20	-2.69	120.07	124.69
6	B	502	PGW	O03-C19-C20	2.62	120.13	111.91
4	A	502	OLC	O20-C1-C2	2.48	119.70	111.91
2	C	401	1Q5	C15-N19-C20	-2.48	120.43	124.69
4	A	503	OLC	O20-C1-C2	2.36	119.33	111.91
4	B	501	OLC	O20-C1-C2	2.35	119.30	111.91
6	B	503	PGW	O03-C19-C20	2.34	119.26	111.91
6	B	504	PGW	O03-C19-C20	2.30	119.13	111.91
2	A	401	1Q5	C18-C13-C14	-2.30	118.30	121.81
2	A	401	1Q5	C7-C4-C3	-2.17	117.73	120.94
2	B	401	1Q5	C7-C4-C3	-2.07	117.87	120.94
2	A	401	1Q5	C2-C1-C6	-2.07	117.70	122.11
4	A	503	OLC	O20-C1-O19	-2.02	118.48	123.59
6	B	502	PGW	O03-C01-C02	2.02	114.31	108.43
2	C	401	1Q5	C7-C4-C3	-2.01	117.96	120.94
6	B	503	PGW	O01-C1-O02	-2.00	118.86	123.70

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	1Q5	C23-C20-C21-C22
2	B	401	1Q5	N19-C20-C21-C22
2	C	401	1Q5	N19-C20-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	501	OLA	C6-C7-C8-C9
4	A	503	OLC	C21-C22-C24-O25
4	A	503	OLC	O23-C22-C24-O25
4	A	503	OLC	O20-C21-C22-C24
4	A	503	OLC	O20-C21-C22-O23
4	B	501	OLC	O20-C21-C22-C24
4	B	501	OLC	O20-C21-C22-O23
4	B	501	OLC	O19-C1-O20-C21
6	B	502	PGW	C2-C1-O01-C02
6	B	503	PGW	C03-O11-P-O12
6	B	503	PGW	C03-O11-P-O13
6	B	503	PGW	C03-O11-P-O14
6	B	503	PGW	O02-C1-O01-C02
6	B	504	PGW	C2-C1-O01-C02
4	B	501	OLC	C2-C1-O20-C21
4	A	503	OLC	O19-C1-O20-C21
6	B	502	PGW	O04-C19-O03-C01
6	B	502	PGW	O02-C1-O01-C02
6	B	504	PGW	O02-C1-O01-C02
6	B	502	PGW	C20-C19-O03-C01
6	B	503	PGW	C2-C1-O01-C02
4	A	503	OLC	C2-C1-O20-C21
7	B	505	1PE	OH6-C15-C25-OH5
6	B	504	PGW	C1-C2-C3-C4
3	C	501	OLA	C1-C2-C3-C4
6	B	502	PGW	C1-C2-C3-C4
7	B	505	1PE	OH5-C14-C24-OH4
7	B	505	1PE	OH7-C16-C26-OH6
4	A	502	OLC	C12-C13-C14-C15
4	A	502	OLC	C14-C15-C16-C17
6	B	503	PGW	C1-C2-C3-C4
6	B	503	PGW	C27-C15-C16-C17
6	B	504	PGW	C21-C22-C23-C24
4	A	503	OLC	C3-C4-C5-C6
4	B	501	OLC	C21-C22-C24-O25
6	B	503	PGW	C5-C6-C7-C8
4	A	502	OLC	C5-C6-C7-C8
6	B	504	PGW	C06-C07-C08-C09
6	B	503	PGW	C15-C16-C17-C18
6	B	504	PGW	C27-C15-C16-C17
4	A	502	OLC	C1-C2-C3-C4
6	B	504	PGW	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
7	B	505	1PE	OH4-C13-C23-OH3
6	B	504	PGW	C20-C19-O03-C01
3	A	501	OLA	C11-C12-C13-C14
6	B	504	PGW	C10-C06-C07-C08
3	C	501	OLA	C13-C14-C15-C16
6	B	502	PGW	C4-C5-C6-C7
4	A	503	OLC	C10-C11-C12-C13
6	B	502	PGW	O03-C01-C02-C03
6	B	503	PGW	C20-C21-C22-C23
4	A	502	OLC	C11-C10-C9-C8
4	B	501	OLC	C14-C15-C16-C17
6	B	504	PGW	C15-C16-C17-C18
4	B	501	OLC	O23-C22-C24-O25
3	C	501	OLA	C12-C13-C14-C15
6	B	503	PGW	C20-C19-O03-C01
6	B	503	PGW	C22-C23-C24-C25
3	C	501	OLA	C4-C5-C6-C7
4	A	502	OLC	C11-C12-C13-C14
2	C	401	1Q5	C21-C20-C23-C24
3	C	501	OLA	C3-C4-C5-C6
6	B	503	PGW	C01-C02-C03-O11
4	A	503	OLC	C11-C12-C13-C14
6	B	504	PGW	C3-C4-C5-C6
6	B	504	PGW	C07-C08-C09-C11
6	B	503	PGW	O01-C02-C03-O11
6	B	502	PGW	O03-C01-C02-O01
6	B	504	PGW	O03-C01-C02-O01
6	B	503	PGW	C06-C07-C08-C09
4	A	503	OLC	C13-C14-C15-C16
6	B	502	PGW	C6-C7-C8-C9
4	A	503	OLC	C15-C16-C17-C18
6	B	504	PGW	C22-C23-C24-C25
6	B	504	PGW	C23-C24-C25-C26
7	B	505	1PE	OH2-C12-C22-OH3
6	B	502	PGW	C11-C12-C13-C14
4	A	502	OLC	C15-C16-C17-C18
7	B	505	1PE	C25-C15-OH6-C26
6	B	504	PGW	O03-C01-C02-C03
3	A	501	OLA	C15-C16-C17-C18
2	A	401	1Q5	N19-C20-C23-C24
2	A	401	1Q5	N19-C20-C21-C22
2	B	401	1Q5	N19-C20-C23-C24

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Mol	Chain	Res	Type	Atoms
6	B	502	PGW	O01-C1-C2-C3
4	A	502	OLC	C2-C3-C4-C5
4	A	503	OLC	C4-C5-C6-C7
6	B	502	PGW	C5-C6-C7-C8
4	A	503	OLC	C11-C10-C9-C8
3	C	501	OLA	C11-C12-C13-C14
4	A	503	OLC	C2-C3-C4-C5
6	B	502	PGW	C06-C10-C9-C8
3	C	501	OLA	O1-C1-C2-C3
3	C	501	OLA	C2-C3-C4-C5
6	B	504	PGW	C5-C6-C7-C8
4	A	502	OLC	C13-C14-C15-C16
3	C	501	OLA	O2-C1-C2-C3
4	A	503	OLC	C9-C10-C11-C12
6	B	503	PGW	C11-C12-C13-C14
2	C	401	1Q5	N19-C20-C21-C22
4	A	503	OLC	C14-C15-C16-C17
6	B	502	PGW	C7-C8-C9-C10
4	B	501	OLC	C4-C5-C6-C7
3	A	501	OLA	C13-C14-C15-C16
4	A	503	OLC	O19-C1-C2-C3
6	B	504	PGW	C25-C26-C27-C15
4	B	501	OLC	C9-C10-C11-C12
6	B	503	PGW	O03-C19-C20-C21

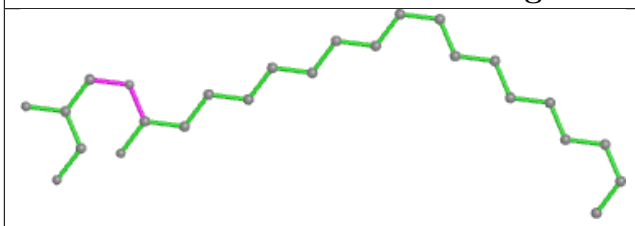
There are no ring outliers.

13 monomers are involved in 31 short contacts:

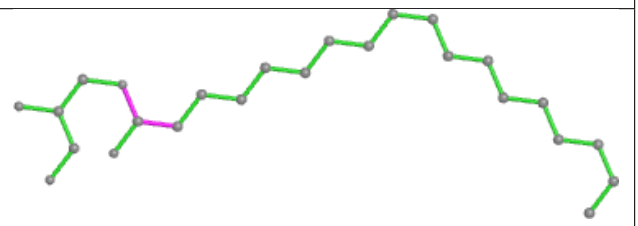
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	OLC	3	0
6	B	503	PGW	1	0
2	A	401	1Q5	2	0
6	B	504	PGW	5	0
2	B	401	1Q5	5	0
4	A	503	OLC	1	0
5	A	504	SO4	1	1
4	B	501	OLC	2	0
3	A	501	OLA	1	0
2	C	401	1Q5	3	0
3	C	501	OLA	1	0
5	B	506	SO4	0	1
6	B	502	PGW	4	0

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.

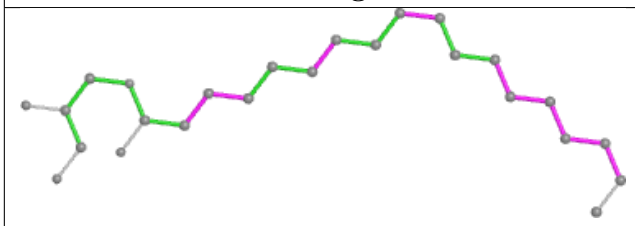
Ligand OLC A 502



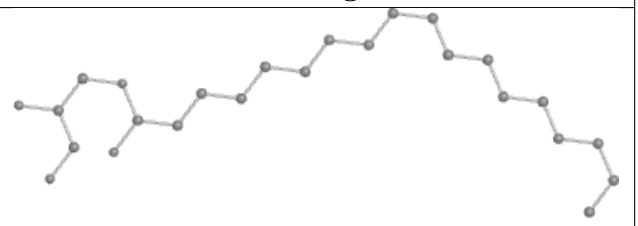
Bond lengths



Bond angles

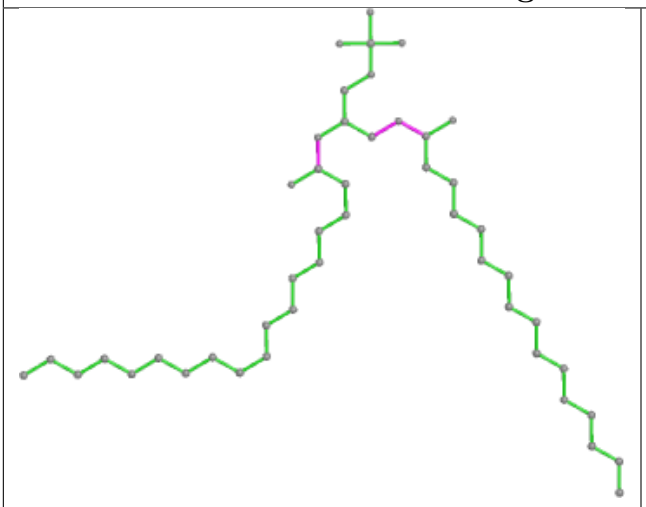


Torsions

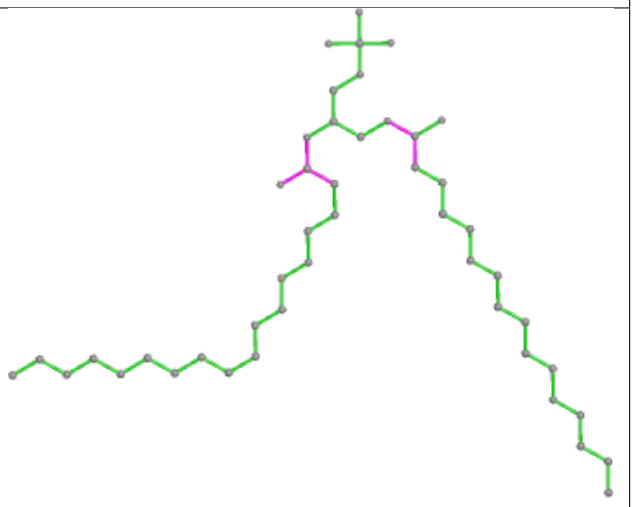


Rings

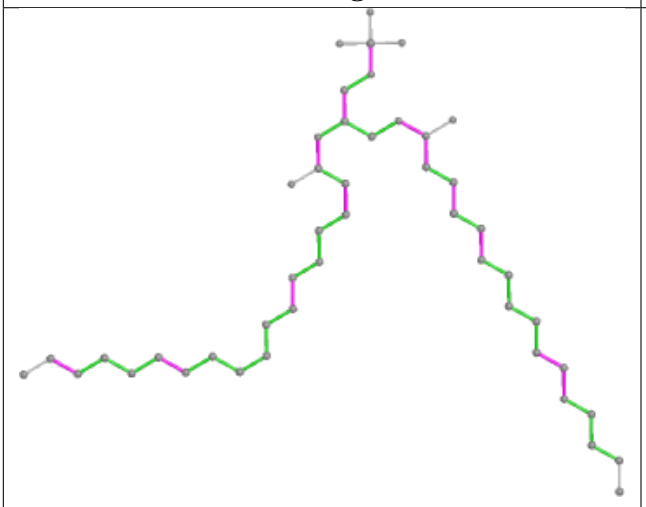
Ligand PGW B 503



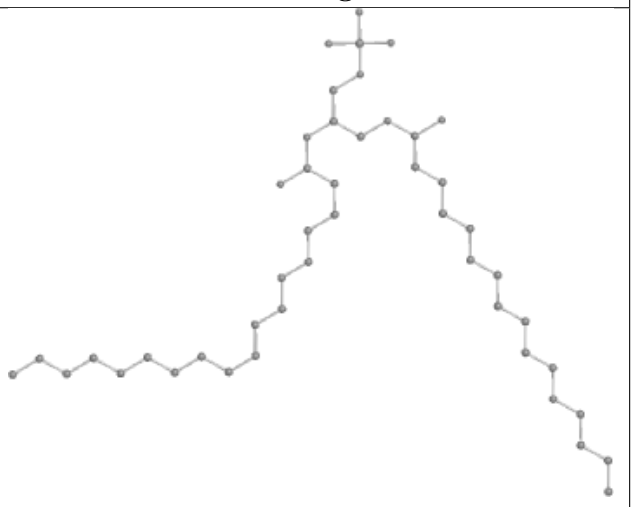
Bond lengths



Bond angles

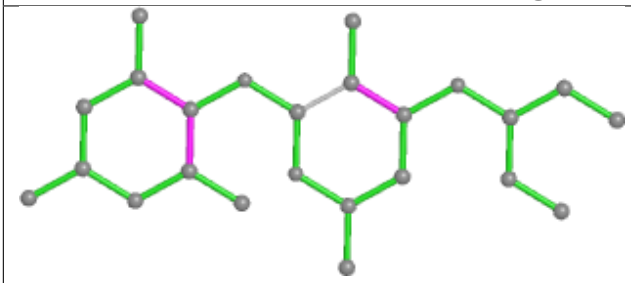


Torsions

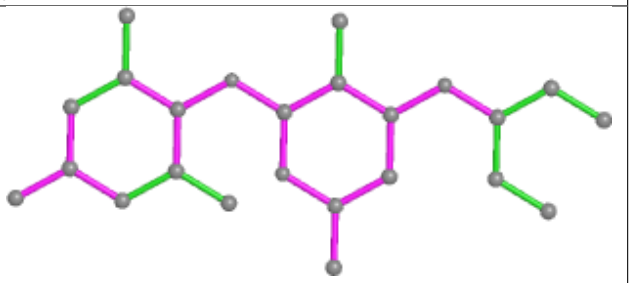


Rings

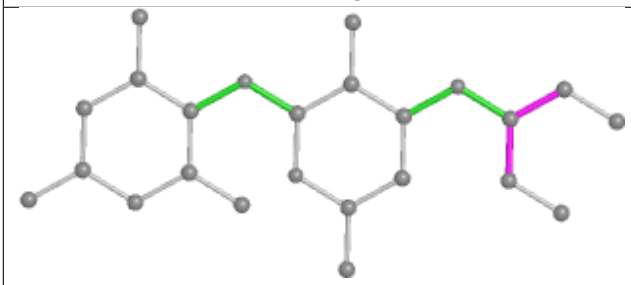
Ligand 1Q5 A 401



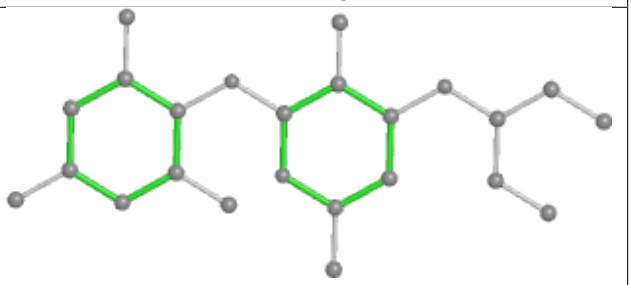
Bond lengths



Bond angles

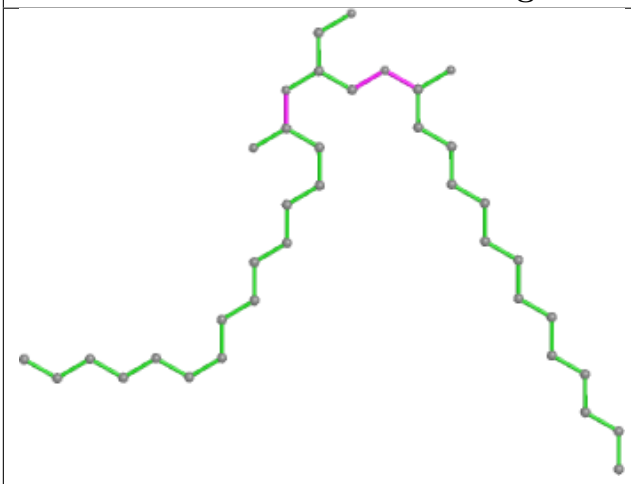


Torsions

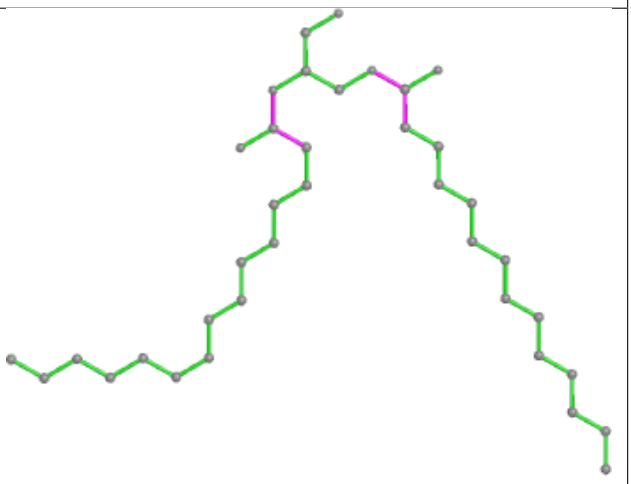


Rings

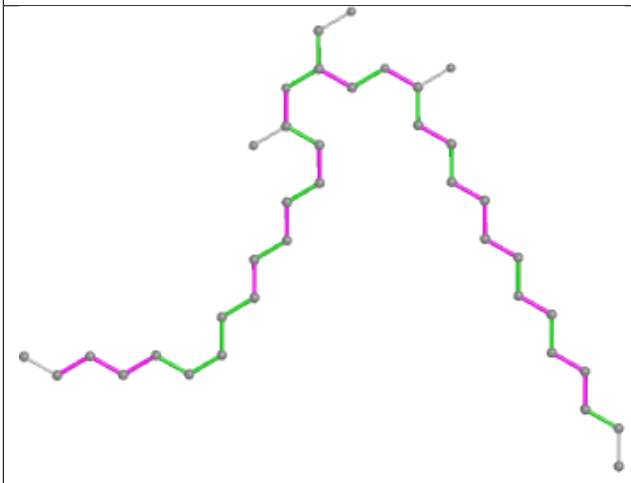
Ligand PGW B 504



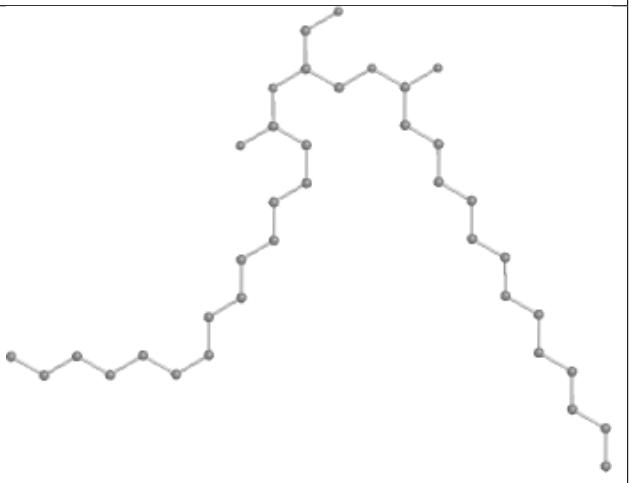
Bond lengths



Bond angles

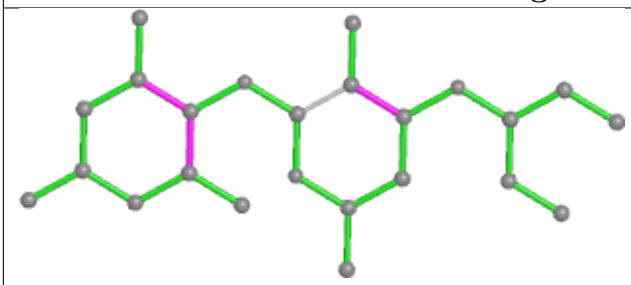


Torsions

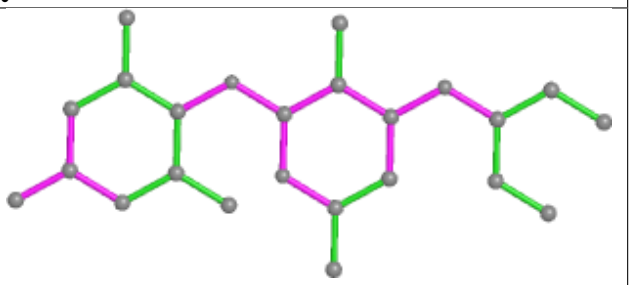


Rings

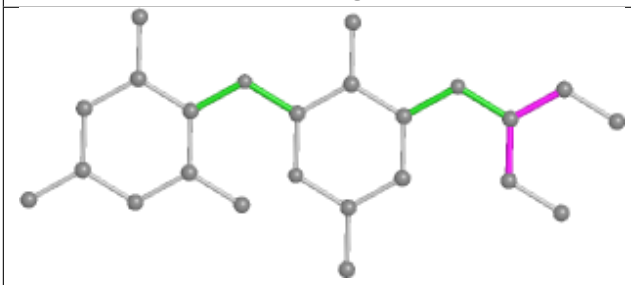
Ligand 1Q5 B 401



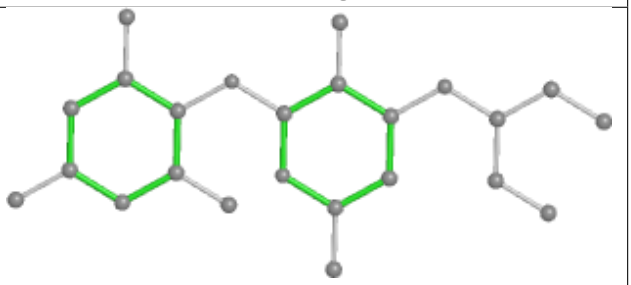
Bond lengths



Bond angles

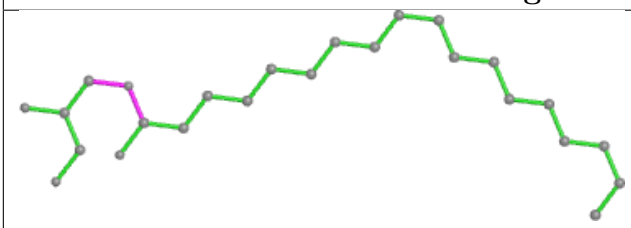


Torsions

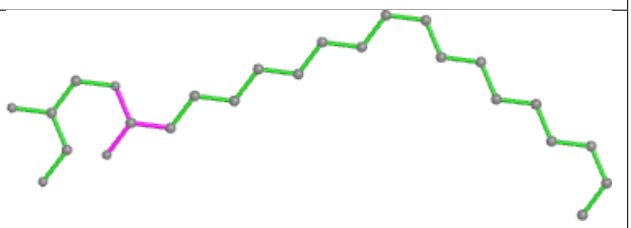


Rings

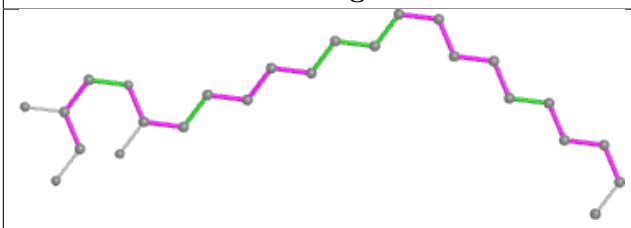
Ligand OLC A 503



Bond lengths



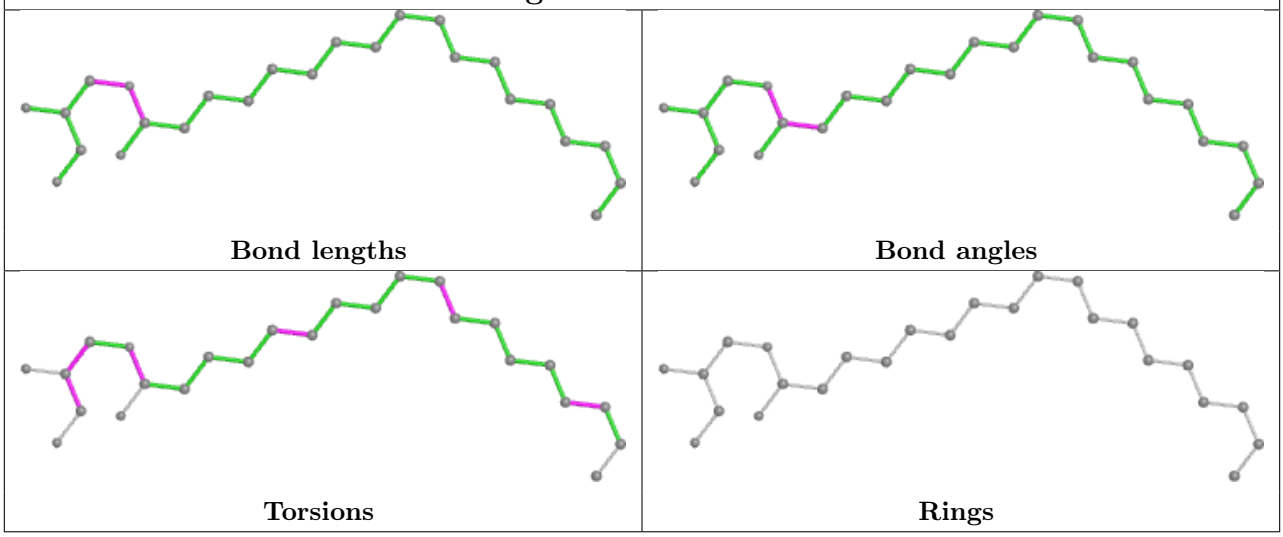
Bond angles



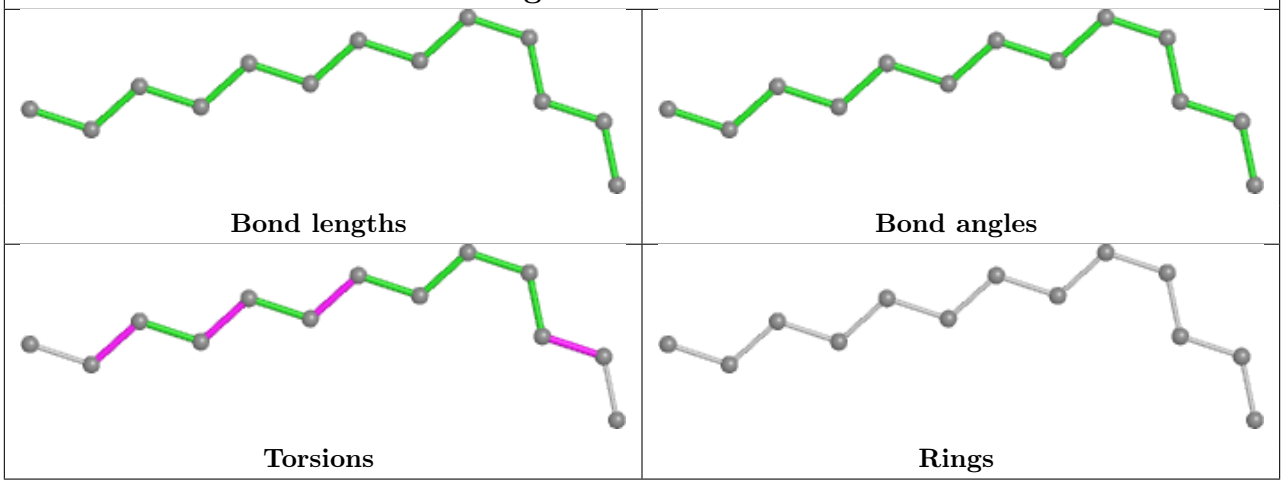
Torsions

Rings

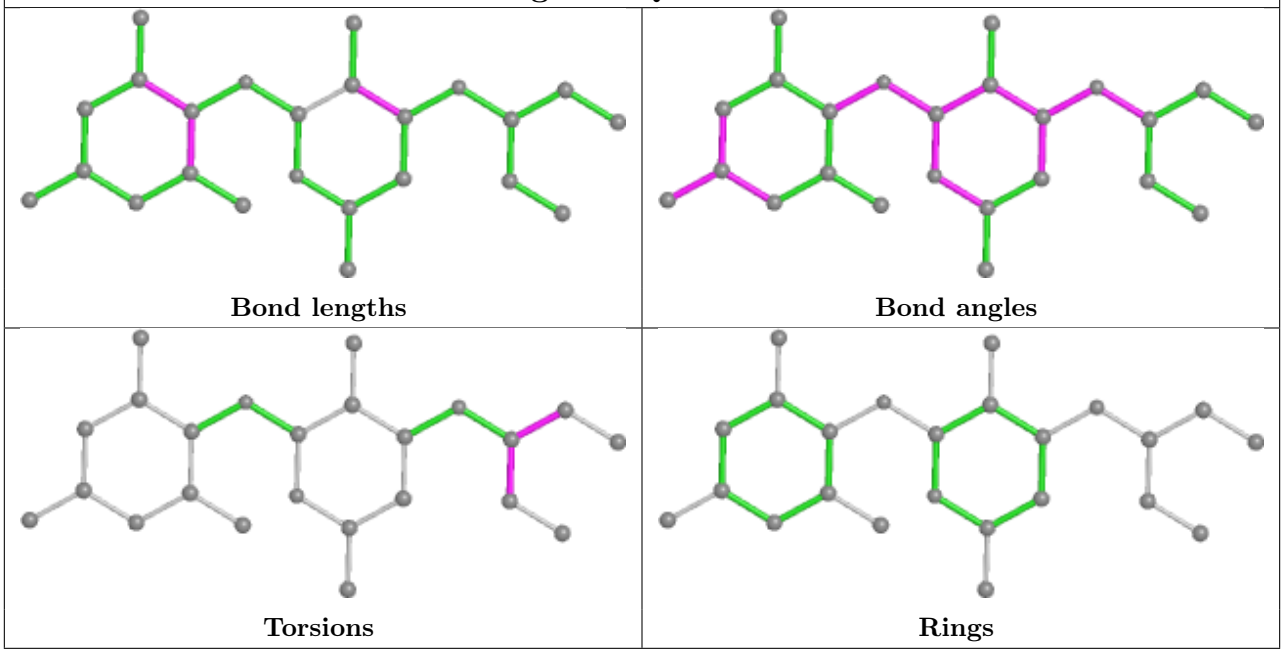
Ligand OLC B 501



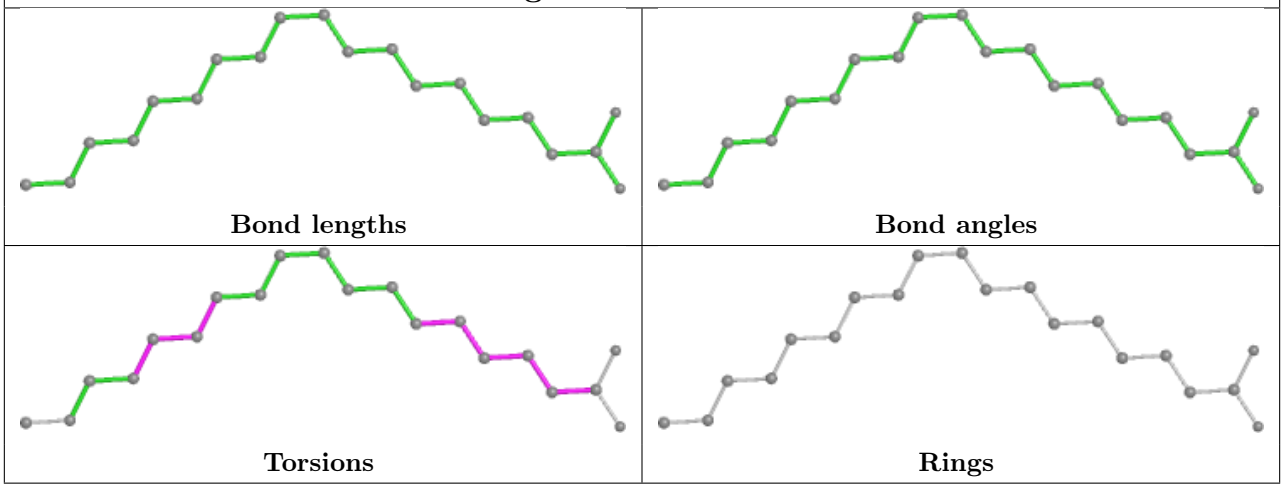
Ligand OLA A 501



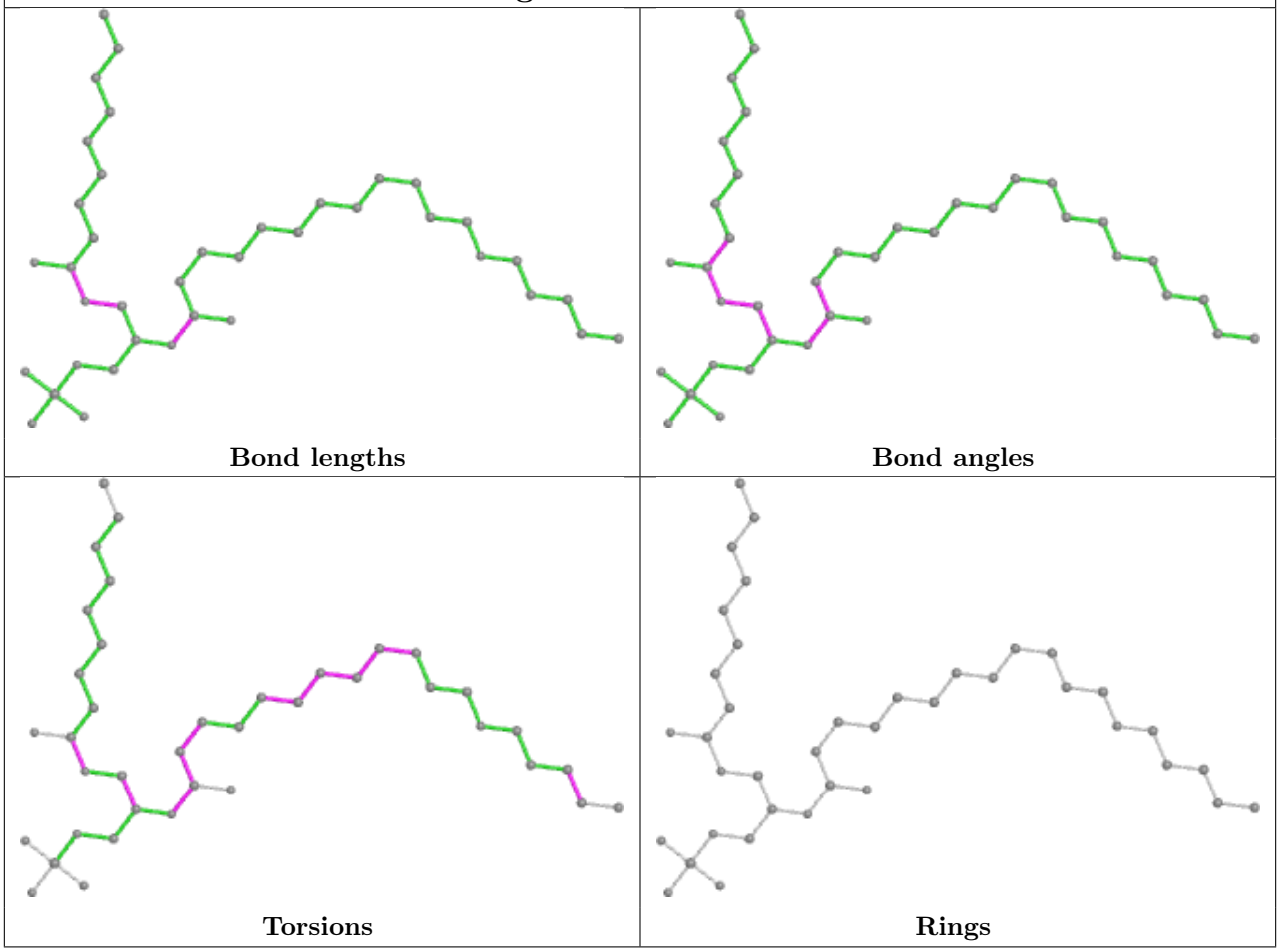
Ligand 1Q5 C 401



Ligand OLA C 501



Ligand PGW B 502



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, 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	407/441 (92%)	0.24	33 (8%) 12 6	32, 56, 112, 131	0
1	B	396/441 (89%)	0.02	13 (3%) 46 28	28, 50, 92, 116	0
1	C	248/441 (56%)	0.37	27 (10%) 5 3	37, 66, 115, 139	0
All	All	1051/1323 (79%)	0.19	73 (6%) 16 9	28, 55, 109, 139	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	PRO	6.5
1	A	116	TYR	6.3
1	A	1054	SER	5.4
1	C	300	ALA	5.1
1	C	117	HIS	5.0
1	C	336	GLU	4.8
1	C	266	VAL	4.7
1	A	1053	ASN	4.6
1	C	148	ARG	4.3
1	A	1052	ARG	4.3
1	A	342	VAL	4.1
1	C	225	ARG	4.1
1	A	333	ASN	4.0
1	A	265	GLY	3.9
1	A	302	THR	3.8
1	C	253	TYR	3.7
1	A	115	HIS	3.6
1	C	118	VAL	3.6
1	A	1055	ASN	3.6
1	C	267	TYR	3.6
1	A	340	SER	3.4
1	C	301	SER	3.4
1	B	115	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	3.4
1	B	267	TYR	3.3
1	C	296	THR	3.3
1	B	1039	LEU	3.3
1	A	263	ARG	3.3
1	C	302	THR	3.2
1	B	1044	SER	3.2
1	C	265	GLY	3.2
1	B	1043	LYS	3.2
1	A	264	PRO	3.1
1	C	181	HIS	3.1
1	A	296	THR	3.1
1	A	295	MET	3.0
1	C	178	PRO	3.0
1	C	219	LEU	3.0
1	A	343	VAL	3.0
1	B	148	ARG	3.0
1	B	145	ARG	3.0
1	A	346	TYR	3.0
1	A	1056	GLY	2.9
1	A	1057	VAL	2.8
1	C	179	GLU	2.8
1	B	1052	ARG	2.8
1	A	303	THR	2.7
1	C	182	GLN	2.7
1	B	1040	SER	2.7
1	C	183	SER	2.7
1	A	339	VAL	2.7
1	A	267	TYR	2.6
1	A	1051	GLY	2.6
1	B	263	ARG	2.6
1	C	335	GLY	2.6
1	A	330	ALA	2.6
1	C	177	SER	2.5
1	B	1053	ASN	2.5
1	C	224	ASP	2.5
1	B	1056	GLY	2.5
1	C	145	ARG	2.5
1	A	117	HIS	2.5
1	A	177	SER	2.4
1	A	266	VAL	2.4
1	C	337	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1039	LEU	2.2
1	A	148	ARG	2.2
1	A	304	SER	2.2
1	A	1026	THR	2.2
1	C	143	ARG	2.1
1	C	263	ARG	2.1
1	A	1059	THR	2.1
1	A	252	TYR	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
6	PGW	B	504	37/51	0.83	0.26	41,54,75,81	0
6	PGW	B	502	39/51	0.84	0.31	31,53,90,114	0
4	OLC	A	503	25/25	0.84	0.22	28,50,67,70	0
6	PGW	B	503	46/51	0.85	0.26	29,49,93,111	0
4	OLC	B	501	25/25	0.87	0.27	25,58,79,83	0
4	OLC	A	502	25/25	0.89	0.19	41,53,77,82	0
3	OLA	C	501	20/20	0.89	0.22	35,47,79,79	0
7	1PE	B	505	16/16	0.91	0.30	45,56,64,66	0
3	OLA	A	501	13/20	0.92	0.20	28,39,47,47	0
5	SO4	B	508	5/5	0.93	0.17	69,80,92,103	0
2	1Q5	C	401	24/24	0.94	0.21	47,52,58,69	0
2	1Q5	B	401	24/24	0.95	0.19	35,47,52,54	0
2	1Q5	A	401	24/24	0.96	0.20	43,52,58,60	0
5	SO4	B	506	5/5	0.97	0.12	62,64,72,76	0
5	SO4	A	504	5/5	0.97	0.10	61,62,73,74	0

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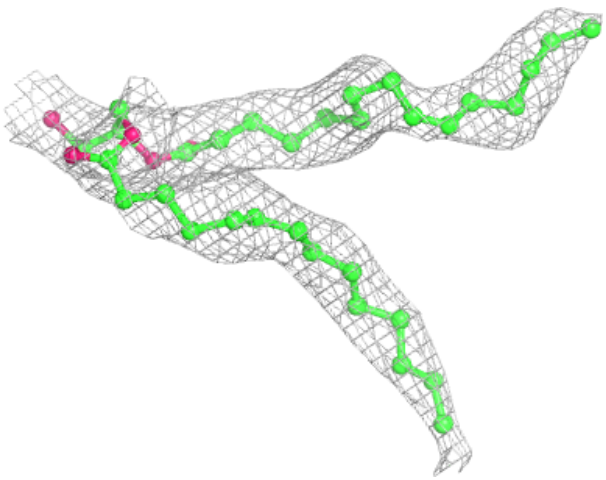
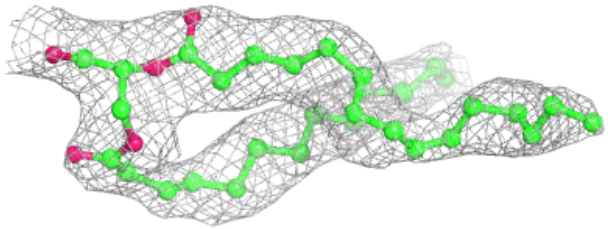
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	507	5/5	0.99	0.18	40,48,54,55	0

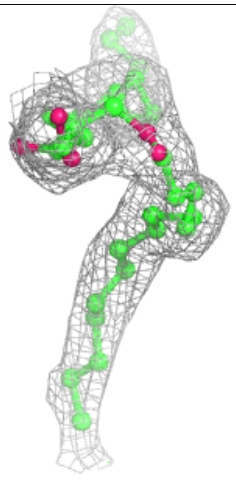
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW B 504:

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

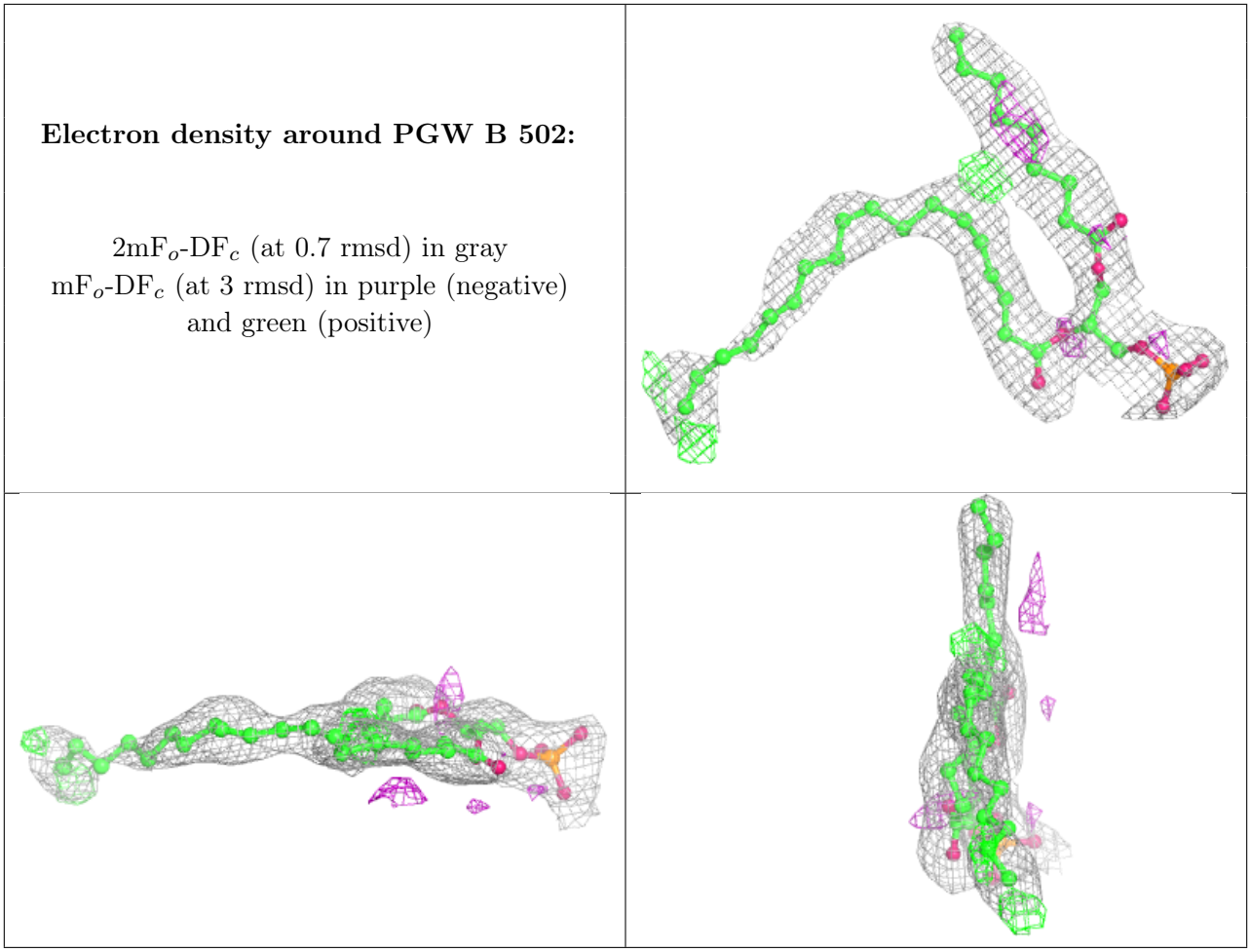






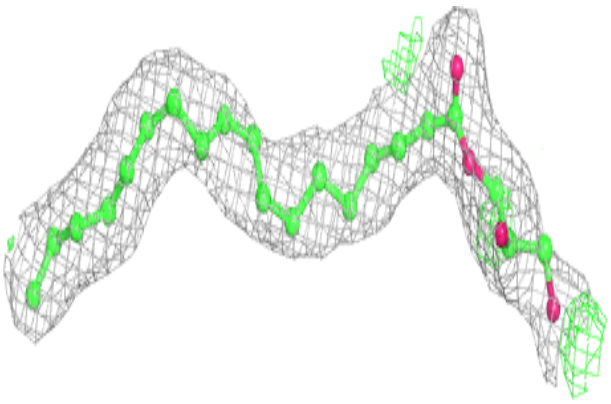
Electron density around PGW B 502:

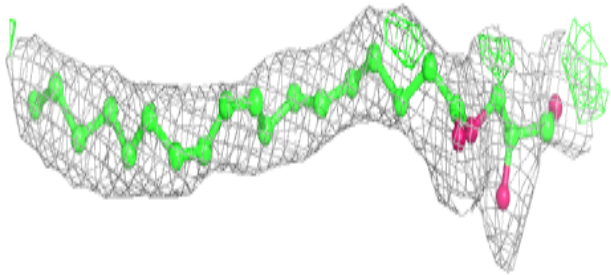
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

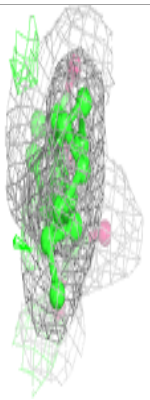


Electron density around OLC A 503:

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

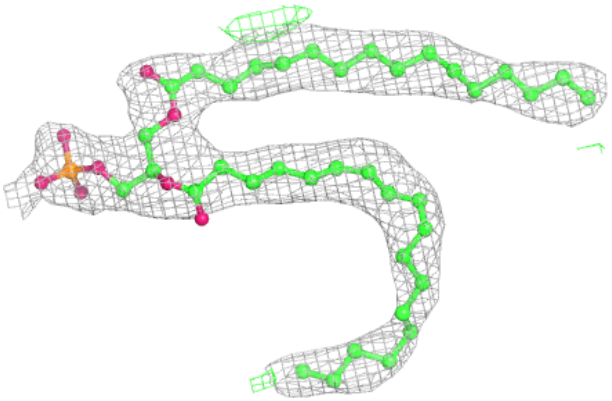


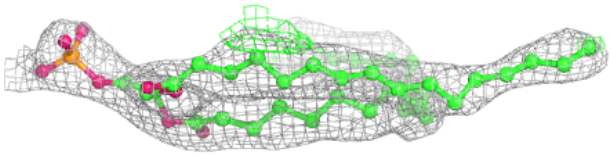


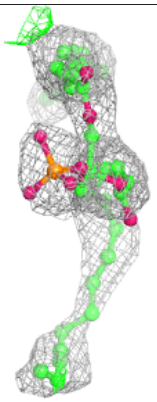


Electron density around PGW B 503:

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

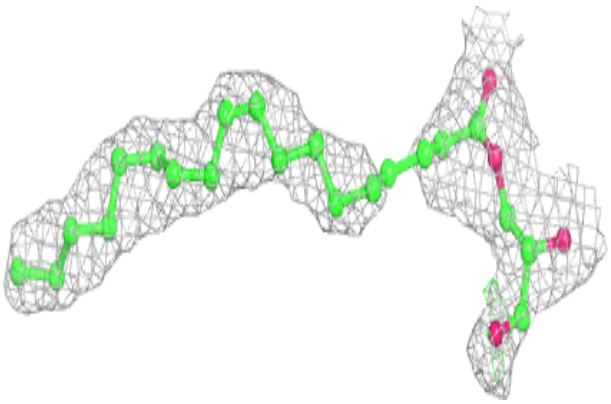


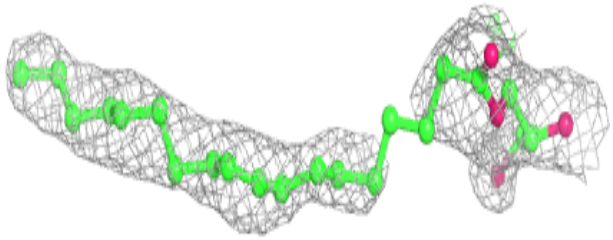


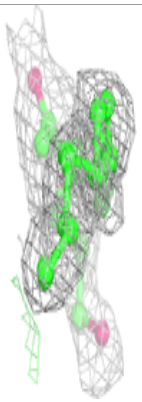


Electron density around OLC B 501:

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

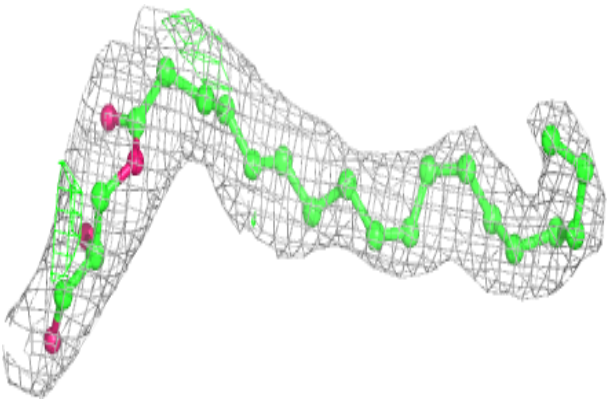


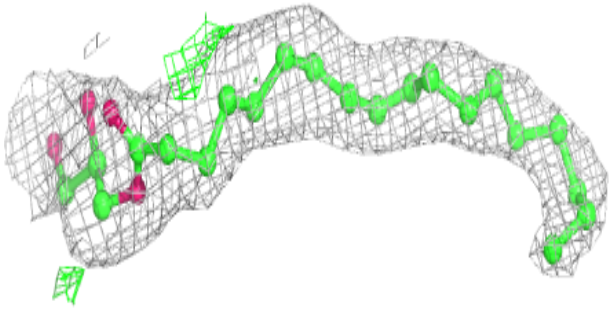


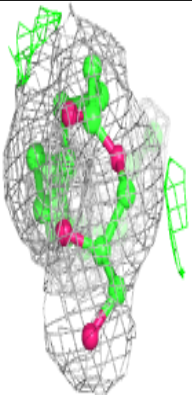


Electron density around OLC A 502:

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

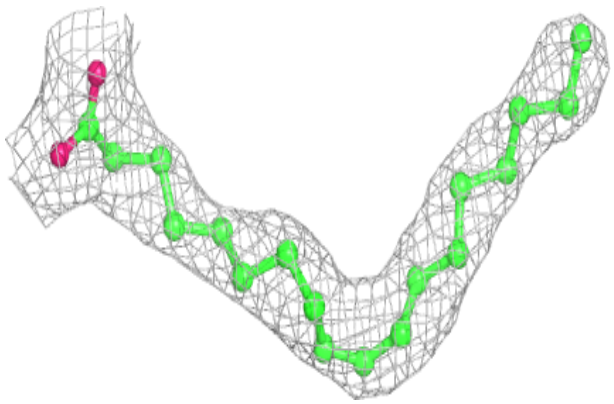


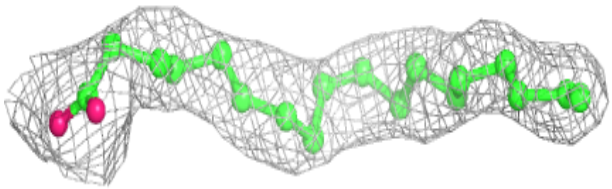


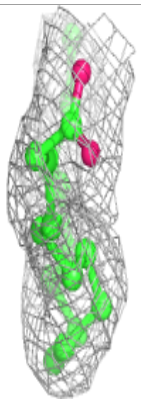


Electron density around OLA C 501:

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

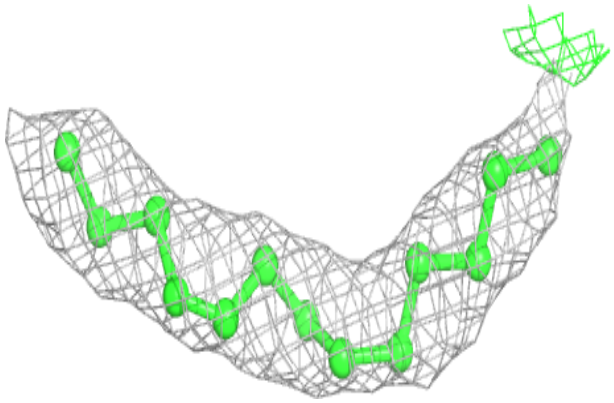


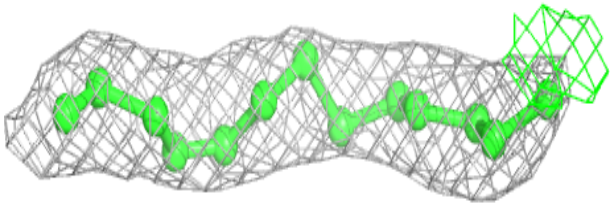


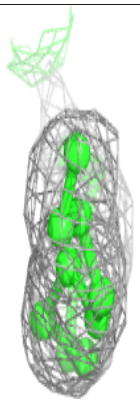


Electron density around OLA A 501:

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

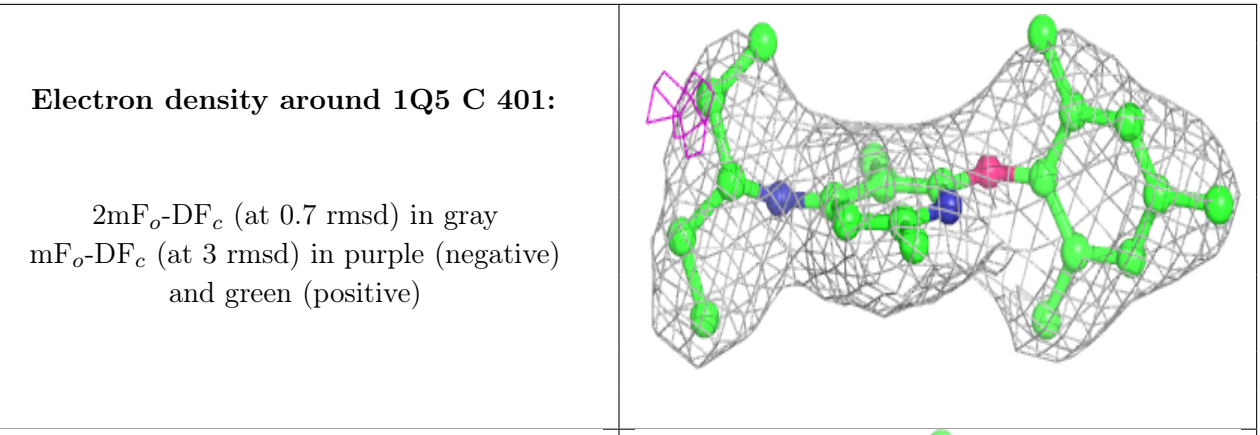






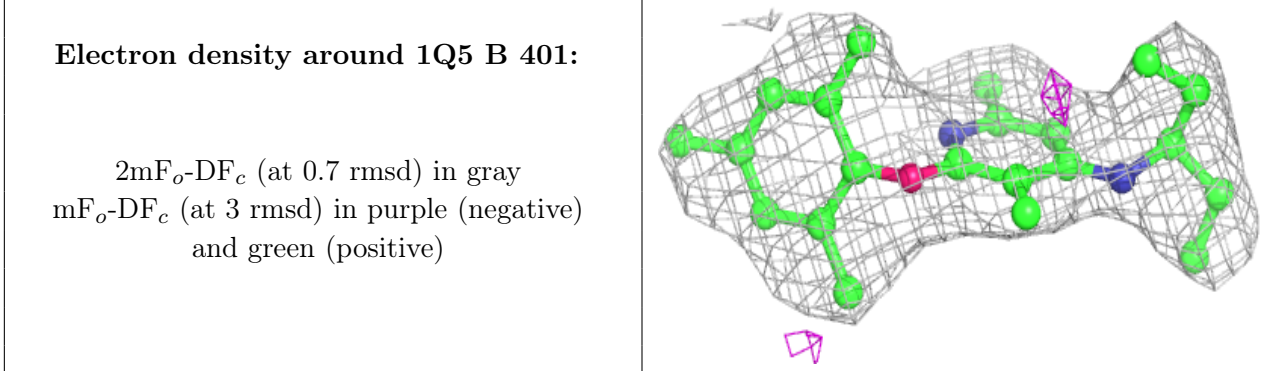
Electron density around 1Q5 C 401:

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



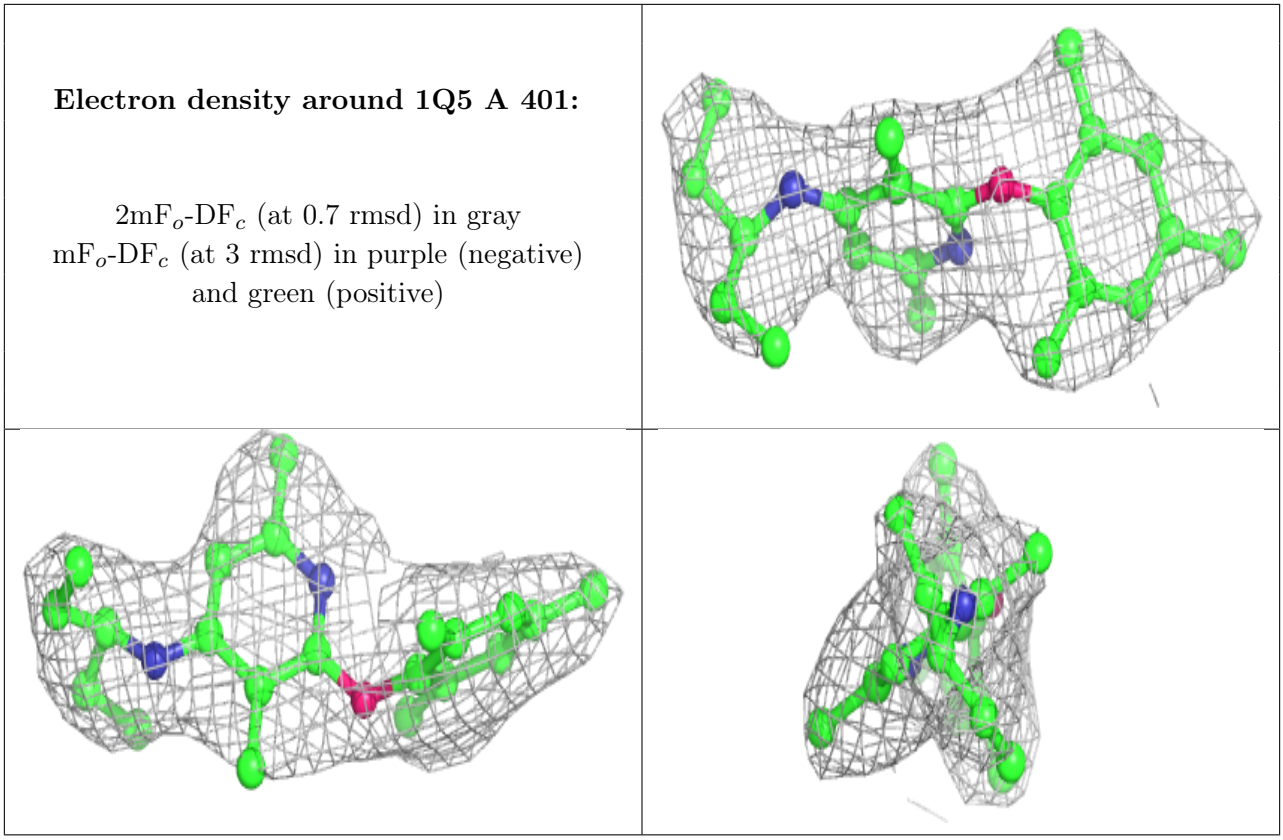
Electron density around 1Q5 B 401:

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



Electron density around 1Q5 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.