Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 11:26 PM JST

PDB ID	:	5Z0B
Title	:	Crystal structure of plasma-derived human serum albumin
Authors	:	Park, J.; Kim, M.-S.; Shin, D.H.
Deposited on	:	2017-12-19
Resolution	:	2.17 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 (i) 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 (i)) were used in the production of this report:

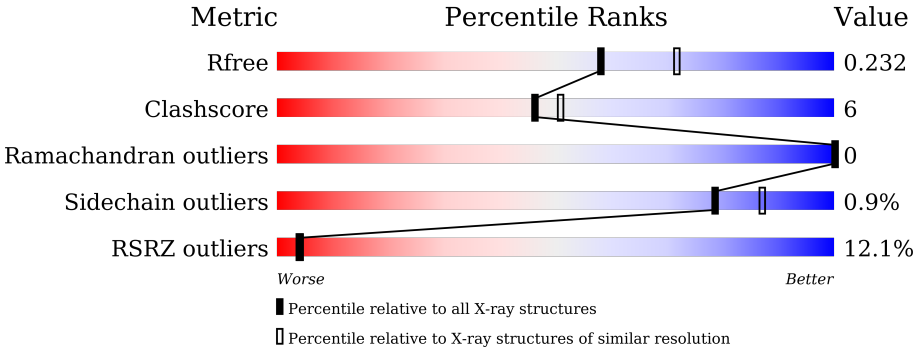
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	585	10% 87% 12% •
1	B	585	12% 88% 11% •
1	C	585	14% 78% 13% 9%

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	OCA	C	604	-	X	-	-
4	PLM	B	604	-	-	X	-
6	SO4	C	609	-	-	X	-

2 Entry composition (i)

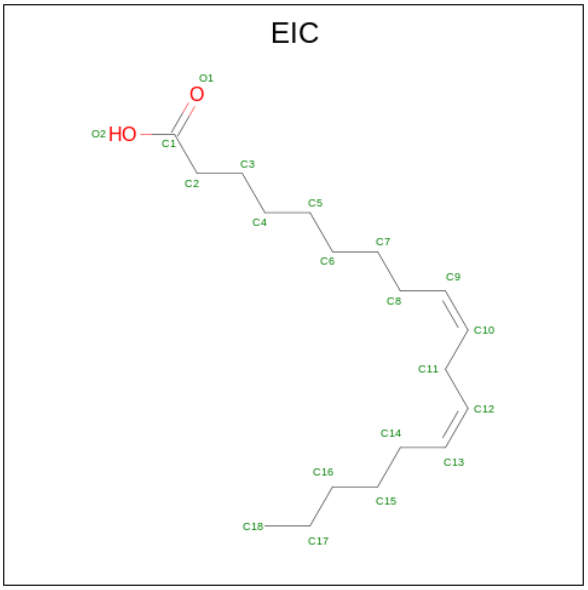
There are 11 unique types of molecules in this entry. The entry contains 14517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

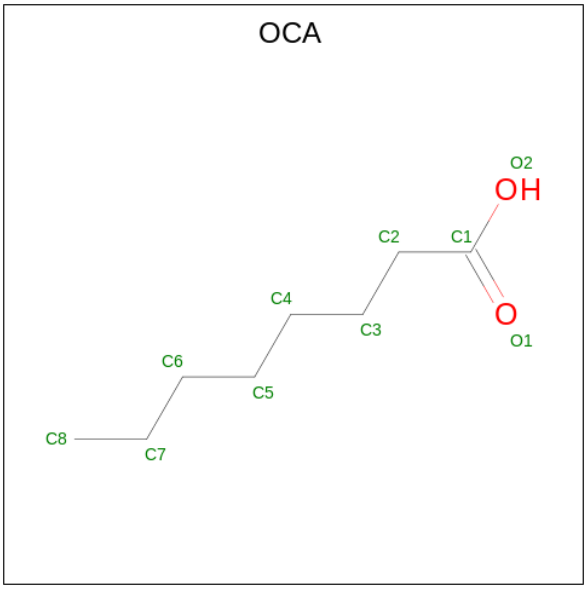
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4621	2917	780	883	41	0	0	0
1	B	581	4629	2922	783	883	41	0	1	0
1	C	532	4272	2697	730	808	37	0	2	0

- Molecule 2 is LINOLEIC ACID (three-letter code: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



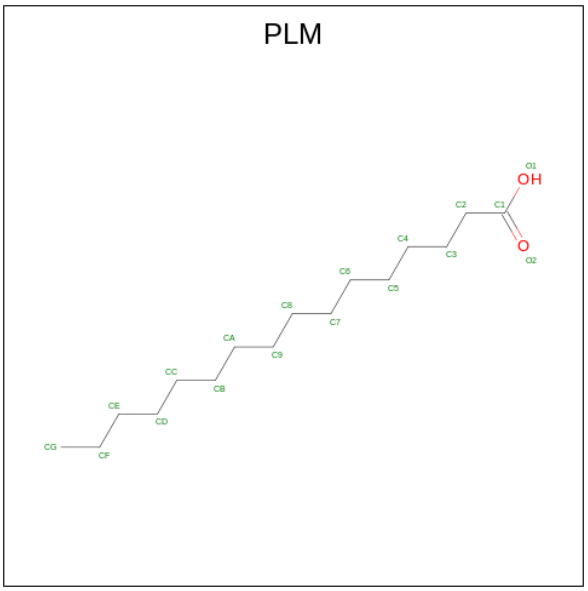
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	20	18	2	0	0
2	B	1	20	18	2	0	0
2	C	1	20	18	2	0	0

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$) (labeled as "Ligand of Interest" by depositor).



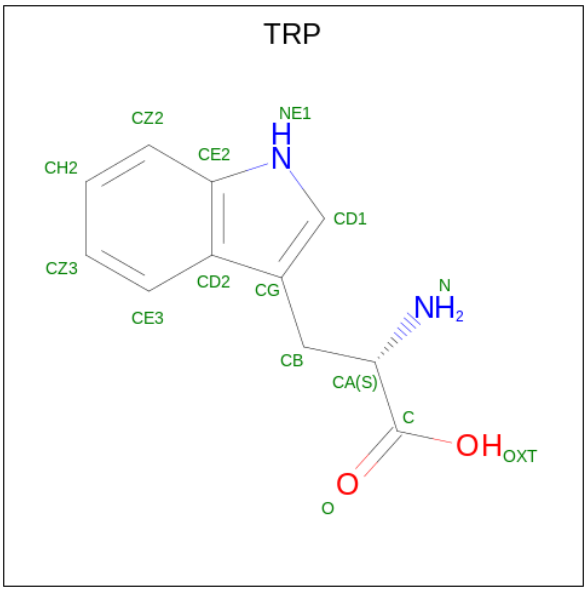
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	10	8	2		0	0
			Total	C	O			
3	A	1	10	8	2		0	0
			Total	C	O			
3	B	1	10	8	2		0	0
			Total	C	O			
3	C	1	10	8	2		0	0
			Total	C	O			
3	C	1	10	8	2		0	0

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



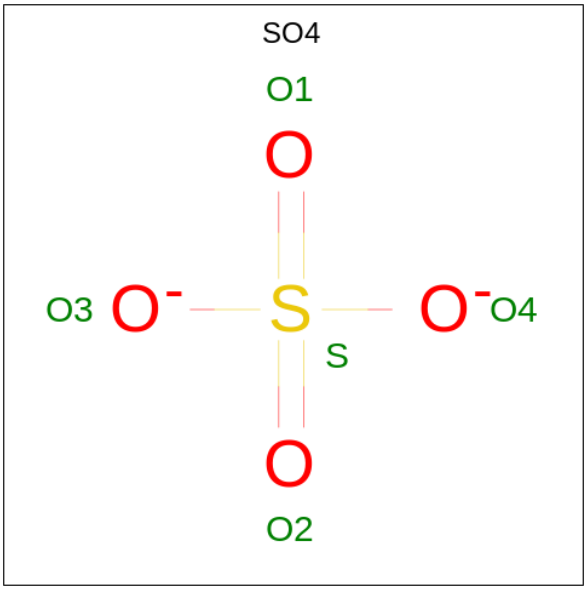
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	18	16	2	0	0
			Total	C	O		
4	B	1	18	16	2	0	0
			Total	C	O		
4	B	1	18	16	2	0	0
			Total	C	O		
4	C	1	18	16	2	0	0

- Molecule 5 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	15	11	2	2	0	0
			Total	C	N	O		
5	B	1	15	11	2	2	0	0
			Total	C	N	O		
5	C	1	15	11	2	2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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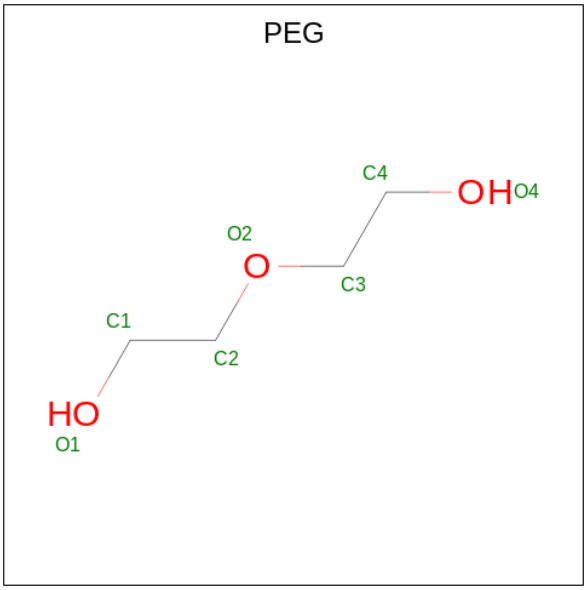
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	B	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O	S		
6	C	1	5	4	1	0	0
			Total	O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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	7	4	3	0	0

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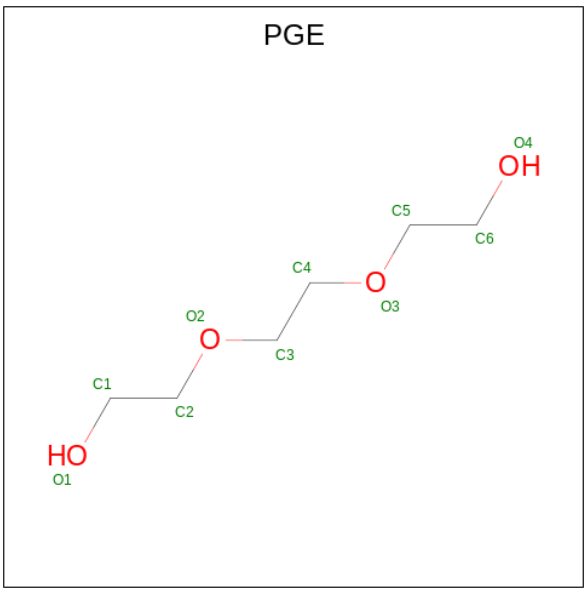
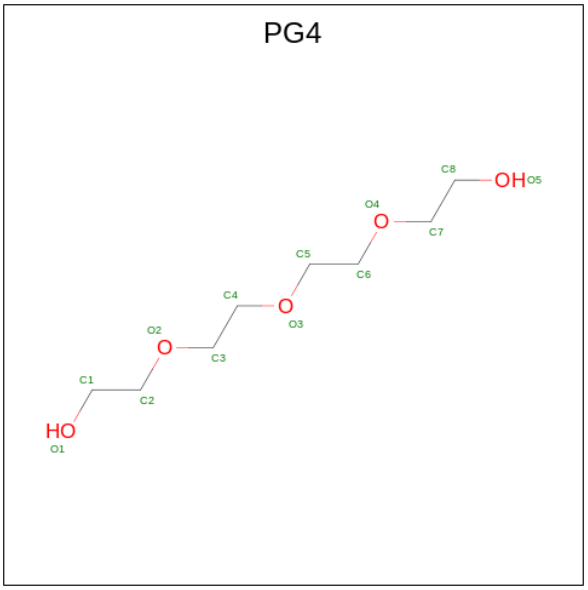
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	A	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	B	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0
			Total	C	O			
7	C	1	7	4	3		0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



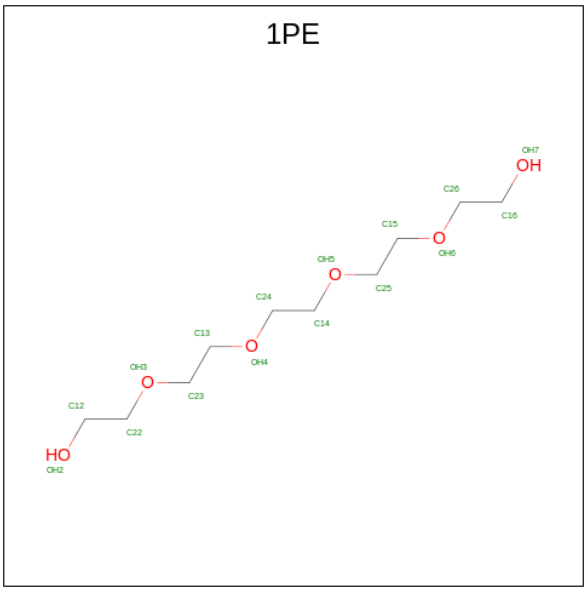
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	10	6	4	0	0
8	B	1	10	6	4	0	0
8	B	1	10	6	4	0	0
8	C	1	10	6	4	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	13	8	5	0	0
9	A	1	13	8	5	0	0
9	B	1	13	8	5	0	0
9	C	1	13	8	5	0	0
9	C	1	13	8	5	0	0

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



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

- Molecule 11 is water.

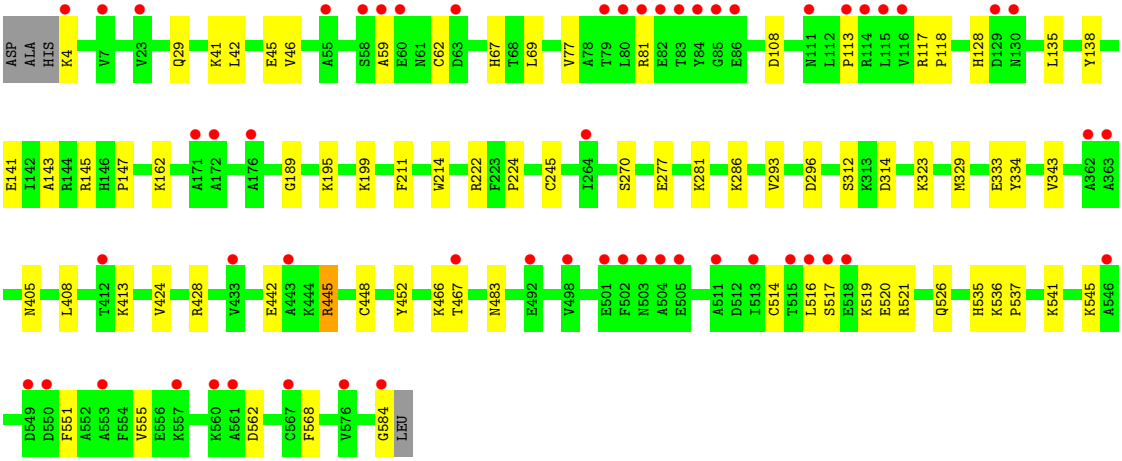
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	143	143	143	0	0
			Total	O		
11	B	176	176	176	0	0
			Total	O		
11	C	142	142	142	0	0

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.

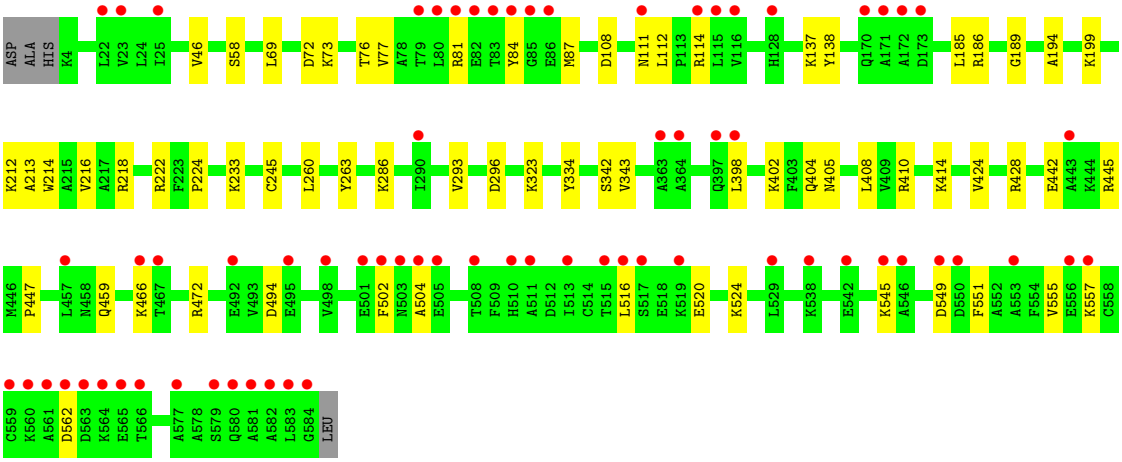
• Molecule 1: Serum albumin

Chain A:



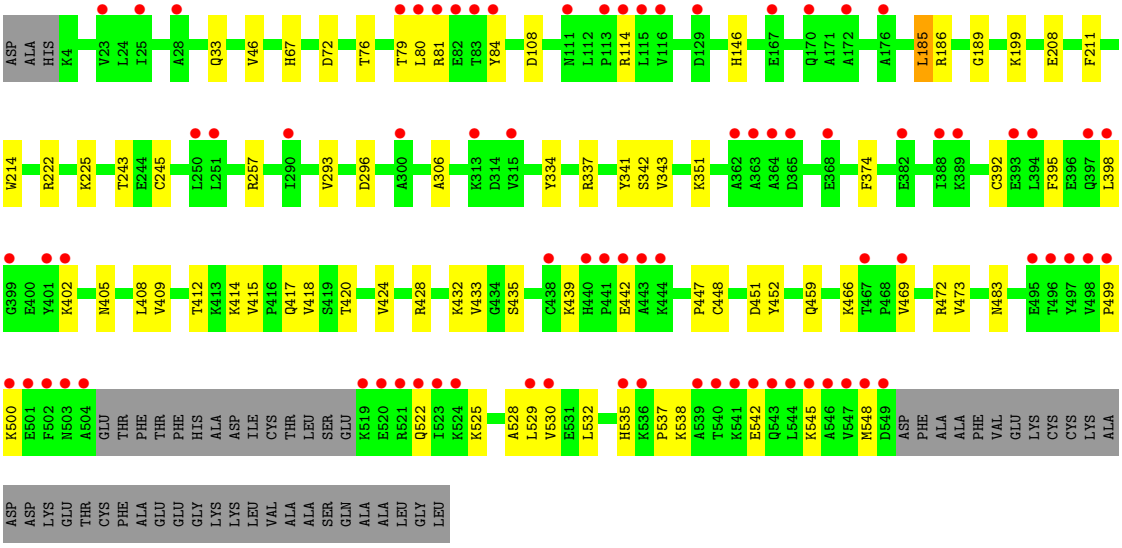
• Molecule 1: Serum albumin

Chain B:



• Molecule 1: Serum albumin

Chain C:


ASP ALA HIS K4 V23 L24 I25 A28 Q33 V46 H67 D72 T76 T79 L80 R81 E82 T83 Y84 D108 N111 L112 P113 R114 L115 V116 D129 H146 E167 Q170 A171 A172 A176 L185 R186 G189 K199 E208 F211
W214 R222 K225 T243 E244 C245 L250 L251 R257 I290 V293 D296 A300 A306 K313 D314 V315 Y334 R337 Y341 S342 V343 K351 A362 A363 A364 D365 E368 F374 E382 I388 K389 C392 E393 L394 F395 E396 Q397 L398
G399 E400 Y401 K402 N405 L408 V409 T412 K413 K414 V415 P416 Q417 V418 S419 T420 V424 R428 K432 V433 G434 S435 C438 K439 H440 P441 E442 A443 K444 P447 C448 D451 Y452 Q459 K466 T467 P468 V469 R472 V473 N483 E496 T496 Y497 V498 P499
K500 E501 F502 N503 A504 GLU THR PHE THR PHE HIS ALA ASP ILE CYS THR LEU SER GLU K519 E520 R521 Q522 I523 K524 K525 A528 L529 V530 E531 L532 H535 K536 P537 K538 A539 T540 K541 E542 Q543 L544 K545 A546 V547 M548 D549 ASP PHE ALA ALA PHE VAL GLU LYS CYS CYS LYS ALA
ASP ASP LYS GLU THR CYS PHE ALA GLU GLU GLY LYS LYS LEU VAL ALA ALA SER GLN ALA ALA LEU GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	203.58Å 113.47Å 86.81Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	19.78 – 2.17 19.78 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.78-2.17) 96.2 (19.78-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.17Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.183 , 0.232 0.183 , 0.232	Depositor DCC
R_{free} test set	4822 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14517	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OCA, PGE, 1PE, CSO, PLM, EIC, SO4, PG4, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/4702	0.50	0/6339
1	B	0.40	0/4713	0.52	0/6353
1	C	0.39	0/4349	0.51	0/5861
All	All	0.39	0/13764	0.51	0/18553

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4621	0	4545	53	0
1	B	4629	0	4558	50	0
1	C	4272	0	4225	65	0
2	A	20	0	31	5	0
2	B	20	0	31	3	0
2	C	20	0	31	7	0
3	A	20	0	30	2	0
3	B	10	0	15	3	0
3	C	20	0	30	2	0
4	A	18	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	36	0	62	15	0
4	C	18	0	31	6	0
5	A	15	0	9	1	0
5	B	15	0	9	1	0
5	C	15	0	9	0	0
6	A	40	0	0	0	0
6	B	35	0	0	0	0
6	C	20	0	0	3	0
7	A	21	0	30	2	0
7	B	49	0	70	3	0
7	C	21	0	30	3	0
8	A	10	0	14	1	0
8	B	20	0	28	4	0
8	C	10	0	14	1	0
9	A	26	0	36	2	0
9	B	13	0	18	0	0
9	C	26	0	36	1	0
10	B	16	0	22	2	0
11	A	143	0	0	2	0
11	B	176	0	0	6	1
11	C	142	0	0	4	0
All	All	14517	0	13945	177	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASN:HA	1:B:408:LEU:HD12	1.70	0.74
1:C:189:GLY:HA3	4:C:603:PLM:H72	1.69	0.73
1:B:69:LEU:HB3	3:B:602:OCA:H72	1.71	0.70
1:B:77:VAL:HG13	1:B:81:ARG:HD2	1.74	0.70
1:A:77:VAL:HG13	1:A:81:ARG:HD2	1.73	0.68
1:B:138:TYR:HE1	4:B:603:PLM:HA2	1.59	0.68
1:A:128:HIS:CD2	1:C:439:LYS:HD2	2.29	0.67
1:C:208:GLU:OE2	11:C:1057:HOH:O	2.12	0.67
1:A:483:ASN:HD21	7:A:617:PEG:H11	1.59	0.67
1:B:185:LEU:HD23	4:B:603:PLM:HA1	1.78	0.66
1:C:337[B]:ARG:NH1	6:C:609:SO4:O1	2.28	0.65
1:C:415:VAL:HG11	1:C:473:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:HE1	4:A:603:PLM:HA2	1.60	0.65
1:A:516:LEU:HB3	1:A:520:GLU:HB2	1.76	0.65
1:B:73:LYS:HD3	3:B:602:OCA:H82	1.80	0.64
1:C:528:ALA:O	1:C:532:LEU:N	2.30	0.64
1:B:516:LEU:HB3	1:B:520:GLU:HB2	1.80	0.64
1:B:323:LYS:HE3	10:B:622:1PE:H241	1.79	0.63
1:B:213:ALA:HB2	4:B:604:PLM:H52	1.81	0.63
1:A:408:LEU:HD11	1:A:526:GLN:HG2	1.80	0.63
1:B:414:LYS:O	1:B:472:ARG:NH2	2.31	0.63
1:B:424:VAL:O	1:B:428:ARG:HG3	1.99	0.62
1:C:114:ARG:HH21	1:C:186:ARG:HH21	1.47	0.62
1:B:216:VAL:HG21	4:B:604:PLM:HA2	1.81	0.62
1:C:414:LYS:O	1:C:472:ARG:NH2	2.30	0.62
1:C:337[A]:ARG:NH1	6:C:609:SO4:O1	2.33	0.61
1:A:199:LYS:NZ	2:A:601:EIC:H31	2.16	0.61
1:B:410:ARG:NH1	5:B:605:TRP:O	2.33	0.61
1:B:73:LYS:NZ	11:B:1154:HOH:O	2.31	0.61
1:C:214:TRP:CD1	1:C:343:VAL:HG11	2.36	0.60
1:C:76:THR:O	1:C:80:LEU:HG	2.02	0.60
1:A:46:VAL:HG22	3:A:602:OCA:H83	1.84	0.59
1:A:189:GLY:HA3	4:A:603:PLM:H72	1.85	0.59
1:C:408:LEU:HD23	1:C:529:LEU:HD23	1.84	0.59
1:C:424:VAL:O	1:C:428:ARG:HG3	2.03	0.58
4:B:604:PLM:CD	11:B:1175:HOH:O	2.50	0.58
1:A:199:LYS:HE2	2:A:601:EIC:H51	1.85	0.58
4:B:604:PLM:HC2	11:B:1175:HOH:O	2.04	0.58
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.39	0.58
1:C:459:GLN:HG2	7:C:615:PEG:H42	1.85	0.57
1:B:442:GLU:HA	1:B:445:ARG:HB2	1.87	0.57
1:C:225:LYS:HB3	8:C:611:PGE:H6	1.85	0.57
1:C:108:ASP:H	1:C:466:LYS:HE2	1.70	0.57
1:C:483:ASN:HD21	7:C:610:PEG:H32	1.69	0.56
1:A:323:LYS:HE2	9:A:618:PG4:H82	1.88	0.55
1:C:114:ARG:NH2	1:C:186:ARG:HH21	2.05	0.55
1:C:420:THR:O	1:C:424:VAL:HG23	2.07	0.55
1:B:46:VAL:HG22	3:B:602:OCA:H83	1.89	0.55
1:B:233:LYS:NZ	8:B:615:PGE:H62	2.22	0.55
1:B:189:GLY:HA3	4:B:603:PLM:H72	1.88	0.54
1:C:499:PRO:HB3	1:C:535:HIS:O	2.08	0.54
1:C:351:LYS:NZ	11:C:1101:HOH:O	2.41	0.54
1:A:541:LYS:HG2	1:A:545:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:604:OCA:O1	11:C:1101:HOH:O	2.17	0.54
1:C:199:LYS:HG2	2:C:601:EIC:H82	1.90	0.53
1:A:108:ASP:H	1:A:466:LYS:NZ	2.07	0.53
1:C:33:GLN:H	1:C:84:TYR:HH	1.56	0.53
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.44	0.52
1:A:555:VAL:HG12	1:A:568:PHE:HE1	1.73	0.52
1:C:398:LEU:HB3	1:C:402:LYS:HB2	1.92	0.52
1:A:281:LYS:O	1:A:286:LYS:NZ	2.40	0.52
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.91	0.52
1:B:138:TYR:CE1	4:B:603:PLM:HA2	2.44	0.52
1:A:162:LYS:NZ	1:C:442:GLU:OE2	2.37	0.52
1:C:214:TRP:CE2	2:C:601:EIC:H111	2.44	0.51
1:B:137:LYS:HD2	7:B:613:PEG:H11	1.93	0.51
1:A:413:LYS:NZ	1:A:537:PRO:O	2.44	0.51
1:B:189:GLY:HA3	4:B:603:PLM:C7	2.41	0.51
1:C:243:THR:HG22	9:C:614:PG4:H32	1.93	0.51
1:C:408:LEU:O	1:C:412:THR:OG1	2.24	0.51
1:B:108:ASP:H	1:B:466:LYS:NZ	2.09	0.50
1:A:535:HIS:O	1:A:536:LYS:HD2	2.11	0.50
1:A:128:HIS:CG	1:C:439:LYS:HD2	2.47	0.50
1:B:404:GLN:HG2	1:B:428:ARG:HA	1.94	0.49
1:B:342:SER:HA	1:B:447:PRO:HA	1.93	0.49
4:B:604:PLM:CC	11:B:1175:HOH:O	2.60	0.49
1:C:342:SER:HA	1:C:447:PRO:HA	1.94	0.49
1:A:189:GLY:HA3	4:A:603:PLM:C7	2.43	0.48
1:B:516:LEU:HD13	1:B:520:GLU:HB3	1.95	0.48
1:B:218[B]:ARG:HH22	2:B:601:EIC:H172	1.78	0.48
4:B:604:PLM:H81	4:B:604:PLM:HB2	1.39	0.48
1:C:451:ASP:HB3	2:C:601:EIC:H171	1.94	0.48
1:A:41:LYS:O	1:A:45:GLU:HG3	2.13	0.48
1:A:69:LEU:HB3	3:A:602:OCA:H72	1.95	0.48
1:C:211:PHE:CE2	2:C:601:EIC:H71	2.48	0.48
1:C:225:LYS:HE2	1:C:296:ASP:OD2	2.14	0.48
1:A:517:SER:O	1:A:521:ARG:HG3	2.14	0.47
1:B:263:TYR:HB2	8:B:615:PGE:H5	1.96	0.47
1:C:522:GLN:HA	1:C:525:LYS:HD3	1.94	0.47
5:A:605:TRP:N	11:A:1100:HOH:O	2.47	0.47
1:B:545:LYS:O	1:B:549:ASP:N	2.47	0.47
1:C:222:ARG:HD3	1:C:293:VAL:HG12	1.96	0.47
1:C:537:PRO:HG2	1:C:538:LYS:HE2	1.96	0.47
1:C:395:PHE:CZ	1:C:435:SER:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ARG:NH2	1:B:494:ASP:HB2	2.31	0.46
1:B:551:PHE:O	1:B:555:VAL:HG23	2.16	0.46
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.97	0.46
1:C:185:LEU:HD12	1:C:185:LEU:HA	1.75	0.46
10:B:622:1PE:H232	10:B:622:1PE:H121	1.61	0.46
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.97	0.46
1:A:270:SER:HA	7:A:619:PEG:H32	1.98	0.45
1:C:146:HIS:HE2	4:C:603:PLM:H41	1.81	0.45
7:B:620:PEG:H12	11:B:1056:HOH:O	2.16	0.45
1:A:211:PHE:CE2	2:A:601:EIC:H71	2.51	0.45
1:A:405:ASN:HA	1:A:408:LEU:HD12	1.97	0.45
1:B:138:TYR:OH	4:B:603:PLM:H81	2.17	0.45
1:C:199:LYS:HE2	2:C:601:EIC:H51	1.98	0.45
1:C:448:CYS:O	1:C:452:TYR:HB2	2.16	0.45
1:C:542:GLU:HA	1:C:545:LYS:HE2	1.98	0.45
1:A:108:ASP:H	1:A:466:LYS:HZ1	1.62	0.45
1:A:517:SER:OG	1:A:519:LYS:HE3	2.16	0.45
1:B:114:ARG:HH22	1:B:186:ARG:HH21	1.64	0.45
1:B:218[B]:ARG:NH2	2:B:601:EIC:H172	2.31	0.45
1:B:260:LEU:HA	8:B:615:PGE:H4	1.98	0.45
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.57	0.45
1:A:424:VAL:O	1:A:428:ARG:HG3	2.16	0.45
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.32	0.45
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.97	0.45
1:A:42:LEU:HD23	1:A:42:LEU:O	2.17	0.45
1:C:189:GLY:CA	4:C:603:PLM:H72	2.42	0.45
1:C:257:ARG:HD3	11:C:1061:HOH:O	2.16	0.45
1:B:194:ALA:HB2	1:B:459:GLN:HE21	1.82	0.45
4:C:603:PLM:HD2	4:C:603:PLM:HG2	1.68	0.44
1:C:341:TYR:O	1:C:447:PRO:HG3	2.18	0.44
1:A:195:LYS:HD3	2:A:601:EIC:H152	1.99	0.44
1:C:500:LYS:HA	1:C:500:LYS:HD2	1.83	0.44
1:A:467:THR:O	1:A:467:THR:OG1	2.33	0.44
1:A:162:LYS:HZ1	1:C:442:GLU:CD	2.20	0.44
1:C:72:ASP:O	1:C:76:THR:HG23	2.17	0.44
1:A:117:ARG:HG2	1:A:118:PRO:O	2.18	0.44
1:B:72:ASP:O	1:B:76:THR:HG23	2.18	0.44
4:B:604:PLM:HD2	11:B:1175:HOH:O	2.13	0.44
1:B:502:PHE:HE1	1:B:504:ALA:HA	1.84	0.43
1:B:557:LYS:HD2	1:B:557:LYS:HA	1.83	0.43
1:A:448:CYS:O	1:A:452:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:604:PLM:HG2	4:B:604:PLM:HD1	1.73	0.43
1:C:392:CYS:HA	1:C:395:PHE:HB3	2.01	0.43
1:A:551:PHE:O	1:A:555:VAL:HG22	2.18	0.43
1:C:199:LYS:NZ	2:C:601:EIC:H31	2.34	0.43
1:B:286:LYS:HB2	1:B:286:LYS:HE3	1.86	0.43
1:C:433:VAL:HG22	1:C:452:TYR:HB3	2.00	0.43
1:A:281:LYS:HG2	8:A:615:PGE:H5	2.01	0.43
1:A:4:LYS:HE3	11:A:1039:HOH:O	2.18	0.42
1:A:442:GLU:HA	1:A:445:ARG:HB2	2.01	0.42
1:A:323:LYS:CE	9:A:618:PG4:H82	2.48	0.42
1:C:79:THR:HG22	1:C:80:LEU:HD23	1.99	0.42
1:B:199:LYS:HE2	2:B:601:EIC:H51	2.01	0.42
1:C:81:ARG:HA	1:C:81:ARG:HD2	1.90	0.42
1:A:312:SER:OG	1:A:314:ASP:OD1	2.38	0.42
1:A:329:MET:O	1:A:333:GLU:HG2	2.20	0.42
1:A:536:LYS:NZ	1:A:584:GLY:HA2	2.35	0.42
1:C:211:PHE:CZ	2:C:601:EIC:H71	2.53	0.42
4:C:603:PLM:HD1	4:C:603:PLM:HA1	1.60	0.41
1:A:277:GLU:H	1:A:277:GLU:CD	2.22	0.41
1:B:111:ASN:O	1:B:112:LEU:HD23	2.20	0.41
1:A:135:LEU:HD11	1:A:162:LYS:HD2	2.02	0.41
1:A:222:ARG:HD3	1:A:293:VAL:HG12	2.02	0.41
1:B:233:LYS:HZ2	8:B:615:PGE:H62	1.85	0.41
1:C:418:VAL:HA	1:C:469:VAL:HG21	2.03	0.41
2:A:601:EIC:H82	2:A:601:EIC:H112	1.87	0.41
1:B:58:SER:HA	7:B:617:PEG:H41	2.01	0.41
1:A:29:GLN:HG3	1:A:143:ALA:HB1	2.03	0.41
1:B:212:LYS:HB3	4:B:604:PLM:H91	2.03	0.41
1:B:524:LYS:HA	1:B:524:LYS:HD3	1.66	0.41
1:C:46:VAL:HG22	3:C:602:OCA:H83	2.02	0.41
1:C:189:GLY:HA3	4:C:603:PLM:C7	2.45	0.41
1:C:417:GLN:HG3	6:C:608:SO4:O1	2.21	0.41
1:C:483:ASN:ND2	7:C:610:PEG:H32	2.34	0.41
1:C:222:ARG:NH1	1:C:293:VAL:O	2.53	0.41
1:C:405:ASN:O	1:C:409:VAL:HG23	2.21	0.41
1:B:84:TYR:HB3	1:B:87:MET:HB3	2.03	0.40
1:B:222:ARG:HD3	1:B:293:VAL:HG12	2.04	0.40
1:C:420:THR:HG23	1:C:530:VAL:HG11	2.03	0.40
1:A:113:PRO:O	1:A:145:ARG:NH2	2.52	0.40
1:C:428:ARG:O	1:C:432:LYS:HG3	2.22	0.40
1:C:529:LEU:HB2	1:C:548:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ALA:HB2	1:C:374:PHE:HE2	1.87	0.40

All (1) 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)
11:B:1052:HOH:O	11:B:1126:HOH:O[4_545]	2.17	0.03

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	578/585 (99%)	565 (98%)	13 (2%)	0	100	100
1	B	579/585 (99%)	569 (98%)	10 (2%)	0	100	100
1	C	529/585 (90%)	515 (97%)	14 (3%)	0	100	100
All	All	1686/1755 (96%)	1649 (98%)	37 (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	507/510 (99%)	501 (99%)	6 (1%)	71	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	508/510 (100%)	505 (99%)	3 (1%)	86 92
1	C	471/510 (92%)	467 (99%)	4 (1%)	81 89
All	All	1486/1530 (97%)	1473 (99%)	13 (1%)	78 87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	245	CYS
1	A	334	TYR
1	A	445	ARG
1	A	514	CYS
1	A	562	ASP
1	B	245	CYS
1	B	334	TYR
1	B	562	ASP
1	C	67	HIS
1	C	185	LEU
1	C	245	CYS
1	C	334	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	67	HIS
1	C	440	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	B	34	1	3,6,7	0.89	0	0,6,8	-	-
1	CSO	C	34	1	3,6,7	0.89	0	0,6,8	-	-
1	CSO	A	34	1	3,6,7	0.89	0	0,6,8	-	-

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
1	CSO	B	34	1	-	0/1/5/7	-
1	CSO	C	34	1	-	0/1/5/7	-
1	CSO	A	34	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

57 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	OCA	C	604	-	9,9,9	1.09	1 (11%)	9,9,9	1.04	2 (22%)
5	TRP	A	605	-	14,16,16	0.75	0	16,22,22	0.82	0
7	PEG	B	620	-	6,6,6	0.49	0	5,5,5	0.20	0
7	PEG	C	615	-	6,6,6	0.50	0	5,5,5	0.33	0
2	EIC	C	601	-	19,19,19	0.71	1 (5%)	19,19,19	0.59	0
8	PGE	B	623	-	9,9,9	0.52	0	8,8,8	0.50	0
9	PG4	A	616	-	12,12,12	0.50	0	11,11,11	0.28	0
3	OCA	A	602	-	9,9,9	0.72	0	9,9,9	0.67	0
6	SO4	A	612	-	4,4,4	0.13	0	6,6,6	0.12	0
2	EIC	A	601	-	19,19,19	0.75	1 (5%)	19,19,19	0.71	0
6	SO4	B	609	-	4,4,4	0.14	0	6,6,6	0.15	0
9	PG4	A	618	-	12,12,12	0.55	0	11,11,11	0.40	0
6	SO4	B	610	-	4,4,4	0.14	0	6,6,6	0.12	0
7	PEG	A	617	-	6,6,6	0.43	0	5,5,5	0.37	0
7	PEG	B	614	-	6,6,6	0.54	0	5,5,5	0.33	0
4	PLM	B	603	-	17,17,17	0.53	0	17,17,17	1.37	2 (11%)
4	PLM	B	604	-	17,17,17	0.88	1 (5%)	17,17,17	0.52	0
5	TRP	C	605	-	14,16,16	0.83	0	16,22,22	1.18	2 (12%)
6	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.19	0
3	OCA	B	602	-	9,9,9	0.56	0	9,9,9	1.32	2 (22%)
6	SO4	C	609	-	4,4,4	0.19	0	6,6,6	0.21	0
7	PEG	B	621	-	6,6,6	0.50	0	5,5,5	0.39	0
8	PGE	A	615	-	9,9,9	0.50	0	8,8,8	0.23	0
4	PLM	C	603	-	17,17,17	0.57	0	17,17,17	1.24	1 (5%)
8	PGE	C	611	-	9,9,9	0.50	0	8,8,8	0.31	0
6	SO4	B	612	-	4,4,4	0.39	0	6,6,6	0.05	0
9	PG4	B	618	-	12,12,12	0.51	0	11,11,11	0.28	0
2	EIC	B	601	-	19,19,19	0.80	1 (5%)	19,19,19	0.62	0
7	PEG	C	610	-	6,6,6	0.45	0	5,5,5	0.33	0
6	SO4	A	607	-	4,4,4	0.15	0	6,6,6	0.17	0
6	SO4	A	608	-	4,4,4	0.15	0	6,6,6	0.19	0
7	PEG	A	614	-	6,6,6	0.50	0	5,5,5	0.29	0
4	PLM	A	603	-	17,17,17	0.52	0	17,17,17	0.49	0
7	PEG	B	617	-	6,6,6	0.43	0	5,5,5	0.33	0
9	PG4	C	614	-	12,12,12	0.49	0	11,11,11	0.47	0
6	SO4	C	606	-	4,4,4	0.19	0	6,6,6	0.34	0
6	SO4	B	606	-	4,4,4	0.10	0	6,6,6	0.16	0
8	PGE	B	615	-	9,9,9	0.49	0	8,8,8	0.29	0
7	PEG	A	619	-	6,6,6	0.46	0	5,5,5	0.46	0
7	PEG	C	613	-	6,6,6	0.47	0	5,5,5	0.48	0
7	PEG	B	613	-	6,6,6	0.53	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	PG4	C	612	-	12,12,12	0.51	0	11,11,11	0.31	0
6	SO4	B	611	-	4,4,4	0.20	0	6,6,6	0.20	0
3	OCA	C	602	-	9,9,9	0.61	0	9,9,9	1.31	2 (22%)
6	SO4	B	608	-	4,4,4	0.14	0	6,6,6	0.14	0
6	SO4	A	611	-	4,4,4	1.45	0	6,6,6	0.42	0
6	SO4	A	610	-	4,4,4	0.16	0	6,6,6	0.09	0
6	SO4	C	607	-	4,4,4	0.13	0	6,6,6	0.34	0
7	PEG	B	616	-	6,6,6	0.49	0	5,5,5	0.31	0
10	1PE	B	622	-	15,15,15	0.53	0	14,14,14	0.41	0
6	SO4	B	607	-	4,4,4	0.13	0	6,6,6	0.16	0
6	SO4	C	608	-	4,4,4	0.15	0	6,6,6	0.13	0
7	PEG	B	619	-	6,6,6	0.47	0	5,5,5	0.30	0
6	SO4	A	613	-	4,4,4	0.15	0	6,6,6	0.12	0
3	OCA	A	604	-	9,9,9	0.91	1 (11%)	9,9,9	0.62	0
5	TRP	B	605	-	14,16,16	0.89	1 (7%)	16,22,22	1.05	2 (12%)
6	SO4	A	609	-	4,4,4	0.14	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	C	604	-	-	7/7/7/7	-
5	TRP	A	605	-	-	3/7/8/8	0/2/2/2
7	PEG	B	620	-	-	1/4/4/4	-
7	PEG	C	615	-	-	2/4/4/4	-
2	EIC	C	601	-	-	14/17/17/17	-
8	PGE	B	623	-	-	4/7/7/7	-
9	PG4	A	616	-	-	4/10/10/10	-
3	OCA	A	602	-	-	5/7/7/7	-
2	EIC	A	601	-	-	11/17/17/17	-
9	PG4	A	618	-	-	6/10/10/10	-
7	PEG	A	617	-	-	3/4/4/4	-
7	PEG	B	614	-	-	3/4/4/4	-
4	PLM	B	603	-	-	7/15/15/15	-
4	PLM	B	604	-	-	15/15/15/15	-
5	TRP	C	605	-	-	5/7/8/8	0/2/2/2
7	PEG	B	621	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	B	602	-	-	4/7/7/7	-
8	PGE	A	615	-	-	3/7/7/7	-
4	PLM	C	603	-	-	8/15/15/15	-
8	PGE	C	611	-	-	2/7/7/7	-
9	PG4	B	618	-	-	0/10/10/10	-
2	EIC	B	601	-	-	11/17/17/17	-
7	PEG	C	610	-	-	2/4/4/4	-
7	PEG	A	614	-	-	4/4/4/4	-
4	PLM	A	603	-	-	10/15/15/15	-
7	PEG	B	617	-	-	2/4/4/4	-
9	PG4	C	614	-	-	5/10/10/10	-
8	PGE	B	615	-	-	5/7/7/7	-
7	PEG	A	619	-	-	3/4/4/4	-
7	PEG	C	613	-	-	1/4/4/4	-
7	PEG	B	613	-	-	2/4/4/4	-
9	PG4	C	612	-	-	6/10/10/10	-
3	OCA	C	602	-	-	3/7/7/7	-
7	PEG	B	616	-	-	2/4/4/4	-
7	PEG	B	619	-	-	4/4/4/4	-
3	OCA	A	604	-	-	6/7/7/7	-
5	TRP	B	605	-	-	5/7/8/8	0/2/2/2
10	1PE	B	622	-	-	5/13/13/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	604	OCA	O2-C1	-3.23	1.19	1.30
4	B	604	PLM	O1-C1	-2.77	1.21	1.30
2	B	601	EIC	O2-C1	-2.45	1.22	1.30
3	A	604	OCA	O2-C1	-2.36	1.22	1.30
5	B	605	TRP	OXT-C	-2.28	1.23	1.30
2	A	601	EIC	O2-C1	-2.05	1.23	1.30
2	C	601	EIC	O2-C1	-2.01	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	PLM	C3-C2-C1	-2.90	107.17	114.47
4	C	603	PLM	C3-C2-C1	-2.86	107.26	114.47
3	B	602	OCA	C3-C2-C1	-2.61	107.89	114.47
5	C	605	TRP	OXT-C-O	-2.57	118.25	124.09
5	C	605	TRP	OXT-C-CA	2.45	121.73	113.38
3	C	602	OCA	C3-C2-C1	-2.39	108.44	114.47
3	C	604	OCA	O2-C1-O1	-2.21	117.78	123.30
5	B	605	TRP	OXT-C-O	-2.20	119.09	124.09
3	B	602	OCA	O1-C1-C2	-2.20	116.01	123.08
5	B	605	TRP	OXT-C-CA	2.19	120.86	113.38
4	B	603	PLM	O1-C1-C2	2.19	121.07	114.03
3	C	604	OCA	C3-C2-C1	-2.03	109.37	114.47
3	C	602	OCA	O2-C1-C2	2.00	120.46	114.03

There are no chirality outliers.

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EIC	C10-C11-C12-C13
5	A	605	TRP	CA-CB-CG-CD1
5	C	605	TRP	CA-CB-CG-CD1
10	B	622	1PE	C12-C22-OH3-C23
7	B	620	PEG	O1-C1-C2-O2
7	B	614	PEG	C4-C3-O2-C2
4	B	604	PLM	C8-C9-CA-CB
9	C	614	PG4	O2-C3-C4-O3
4	B	604	PLM	CB-CC-CD-CE
9	A	616	PG4	O2-C3-C4-O3
9	C	614	PG4	O3-C5-C6-O4
7	C	615	PEG	O1-C1-C2-O2
2	A	601	EIC	C1-C2-C3-C4
4	C	603	PLM	C1-C2-C3-C4
4	B	604	PLM	C1-C2-C3-C4
3	A	604	OCA	C1-C2-C3-C4
4	C	603	PLM	CA-CB-CC-CD
3	C	604	OCA	C1-C2-C3-C4
7	B	616	PEG	O2-C3-C4-O4
7	C	610	PEG	O1-C1-C2-O2
7	C	610	PEG	O2-C3-C4-O4
8	C	611	PGE	O3-C5-C6-O4
9	C	612	PG4	O4-C7-C8-O5
10	B	622	1PE	OH2-C12-C22-OH3
10	B	622	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
9	C	612	PG4	O3-C5-C6-O4
7	A	614	PEG	O2-C3-C4-O4
7	B	613	PEG	O2-C3-C4-O4
7	B	619	PEG	O1-C1-C2-O2
8	B	615	PGE	O1-C1-C2-O2
3	A	604	OCA	C2-C3-C4-C5
4	A	603	PLM	CA-CB-CC-CD
4	A	603	PLM	CC-CD-CE-CF
4	C	603	PLM	C3-C4-C5-C6
4	B	603	PLM	C9-CA-CB-CC
3	A	602	OCA	C1-C2-C3-C4
2	B	601	EIC	C11-C10-C9-C8
4	C	603	PLM	C5-C6-C7-C8
4	C	603	PLM	CB-CC-CD-CE
2	C	601	EIC	C1-C2-C3-C4
4	B	603	PLM	C2-C3-C4-C5
4	B	604	PLM	C6-C7-C8-C9
4	B	604	PLM	CC-CD-CE-CF
4	A	603	PLM	C5-C6-C7-C8
4	B	603	PLM	C5-C6-C7-C8
7	C	615	PEG	O2-C3-C4-O4
2	A	601	EIC	C14-C15-C16-C17
2	A	601	EIC	C4-C5-C6-C7
4	A	603	PLM	C8-C9-CA-CB
2	B	601	EIC	C1-C2-C3-C4
2	B	601	EIC	C6-C7-C8-C9
2	C	601	EIC	C13-C14-C15-C16
4	A	603	PLM	C2-C3-C4-C5
2	C	601	EIC	C14-C15-C16-C17
7	A	619	PEG	O2-C3-C4-O4
9	C	612	PG4	O1-C1-C2-O2
8	B	615	PGE	C1-C2-O2-C3
2	B	601	EIC	C13-C14-C15-C16
3	C	604	OCA	C3-C4-C5-C6
3	C	604	OCA	C4-C5-C6-C7
4	B	604	PLM	C3-C4-C5-C6
2	C	601	EIC	C11-C10-C9-C8
4	B	603	PLM	C8-C9-CA-CB
4	B	604	PLM	C9-CA-CB-CC
9	C	612	PG4	O2-C3-C4-O3
3	C	602	OCA	C1-C2-C3-C4
4	B	604	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
9	A	616	PG4	O3-C5-C6-O4
7	A	614	PEG	O1-C1-C2-O2
7	A	617	PEG	O1-C1-C2-O2
7	A	617	PEG	O2-C3-C4-O4
9	A	616	PG4	O1-C1-C2-O2
9	A	618	PG4	O4-C7-C8-O5
9	C	614	PG4	O4-C7-C8-O5
2	B	601	EIC	C2-C3-C4-C5
2	A	601	EIC	C15-C16-C17-C18
4	A	603	PLM	CD-CE-CF-CG
2	A	601	EIC	C13-C14-C15-C16
3	C	604	OCA	C2-C3-C4-C5
2	C	601	EIC	C2-C3-C4-C5
4	B	603	PLM	CA-CB-CC-CD
9	C	614	PG4	C5-C6-O4-C7
8	A	615	PGE	O1-C1-C2-O2
8	B	623	PGE	O1-C1-C2-O2
4	C	603	PLM	C6-C7-C8-C9
3	C	604	OCA	C5-C6-C7-C8
4	A	603	PLM	C9-CA-CB-CC
3	A	604	OCA	C4-C5-C6-C7
3	A	602	OCA	C4-C5-C6-C7
2	C	601	EIC	C4-C5-C6-C7
3	A	604	OCA	C5-C6-C7-C8
2	B	601	EIC	C14-C15-C16-C17
5	B	605	TRP	OXT-C-CA-N
2	A	601	EIC	C2-C3-C4-C5
2	C	601	EIC	C15-C16-C17-C18
2	B	601	EIC	C10-C11-C12-C13
4	A	603	PLM	C6-C7-C8-C9
5	A	605	TRP	O-C-CA-N
5	B	605	TRP	O-C-CA-N
5	C	605	TRP	O-C-CA-N
4	C	603	PLM	CC-CD-CE-CF
5	B	605	TRP	CA-CB-CG-CD1
10	B	622	1PE	OH6-C15-C25-OH5
7	B	619	PEG	O2-C3-C4-O4
8	A	615	PGE	C3-C4-O3-C5
9	A	618	PG4	C6-C5-O3-C4
4	B	603	PLM	C6-C7-C8-C9
9	A	616	PG4	C1-C2-O2-C3
7	B	619	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	B	604	PLM	CD-CE-CF-CG
7	A	614	PEG	C1-C2-O2-C3
7	A	617	PEG	C1-C2-O2-C3
7	A	614	PEG	C4-C3-O2-C2
8	B	615	PGE	C3-C4-O3-C5
8	A	615	PGE	C1-C2-O2-C3
4	A	603	PLM	C7-C8-C9-CA
2	C	601	EIC	C6-C7-C8-C9
8	B	623	PGE	C6-C5-O3-C4
7	B	613	PEG	O1-C1-C2-O2
7	B	617	PEG	O2-C3-C4-O4
9	C	612	PG4	C1-C2-O2-C3
7	B	621	PEG	O1-C1-C2-O2
3	A	602	OCA	C2-C3-C4-C5
5	B	605	TRP	N-CA-CB-CG
7	B	616	PEG	O1-C1-C2-O2
10	B	622	1PE	C24-C14-OH5-C25
7	A	619	PEG	C4-C3-O2-C2
4	B	604	PLM	C4-C5-C6-C7
7	C	613	PEG	C1-C2-O2-C3
7	B	614	PEG	O1-C1-C2-O2
4	B	604	PLM	C7-C8-C9-CA
9	A	618	PG4	O2-C3-C4-O3
2	C	601	EIC	C11-C12-C13-C14
7	B	621	PEG	O2-C3-C4-O4
7	B	617	PEG	C4-C3-O2-C2
8	C	611	PGE	C3-C4-O3-C5
4	B	604	PLM	CA-CB-CC-CD
7	B	619	PEG	C4-C3-O2-C2
2	C	601	EIC	O1-C1-C2-C3
3	A	604	OCA	O2-C1-C2-C3
8	B	623	PGE	C4-C3-O2-C2
9	A	618	PG4	C3-C4-O3-C5
2	C	601	EIC	O2-C1-C2-C3
3	A	604	OCA	O1-C1-C2-C3
3	C	604	OCA	O1-C1-C2-C3
2	B	601	EIC	C9-C10-C11-C12
2	C	601	EIC	C10-C11-C12-C13
3	B	602	OCA	C3-C4-C5-C6
2	B	601	EIC	C3-C4-C5-C6
2	A	601	EIC	C11-C12-C13-C14
9	A	618	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
2	C	601	EIC	C12-C13-C14-C15
3	C	602	OCA	O2-C1-C2-C3
2	A	601	EIC	O1-C1-C2-C3
2	A	601	EIC	O2-C1-C2-C3
8	B	615	PGE	O2-C3-C4-O3
5	C	605	TRP	O-C-CA-CB
3	B	602	OCA	O2-C1-C2-C3
7	A	619	PEG	C1-C2-O2-C3
9	C	612	PG4	C5-C6-O4-C7
4	B	604	PLM	C2-C3-C4-C5
3	C	602	OCA	O1-C1-C2-C3
2	C	601	EIC	C7-C8-C9-C10
4	B	603	PLM	CB-CC-CD-CE
5	C	605	TRP	OXT-C-CA-N
3	B	602	OCA	O1-C1-C2-C3
2	B	601	EIC	C5-C6-C7-C8
9	C	614	PG4	C6-C5-O3-C4
5	B	605	TRP	C-CA-CB-CG
9	A	618	PG4	C5-C6-O4-C7
4	B	604	PLM	O2-C1-C2-C3
2	A	601	EIC	C12-C13-C14-C15
5	C	605	TRP	OXT-C-CA-CB
5	A	605	TRP	OXT-C-CA-N
3	A	602	OCA	O2-C1-C2-C3
3	C	604	OCA	O2-C1-C2-C3
3	A	602	OCA	O1-C1-C2-C3
4	B	604	PLM	O1-C1-C2-C3
4	C	603	PLM	CD-CE-CF-CG
8	B	615	PGE	C4-C3-O2-C2
7	B	614	PEG	C1-C2-O2-C3
3	B	602	OCA	C1-C2-C3-C4
8	B	623	PGE	O2-C3-C4-O3
4	A	603	PLM	C4-C5-C6-C7
2	B	601	EIC	C7-C8-C9-C10

There are no ring outliers.

28 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	604	OCA	1	0
5	A	605	TRP	1	0
7	B	620	PEG	1	0

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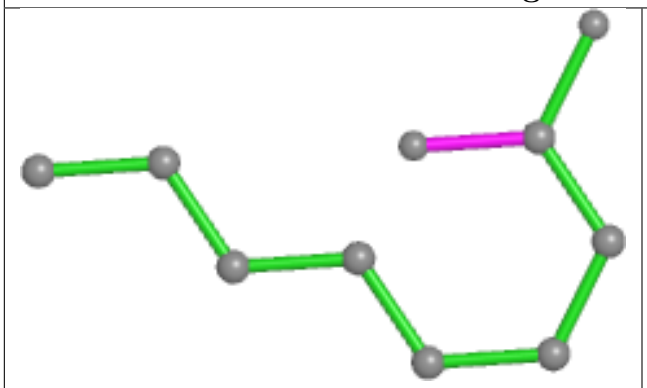
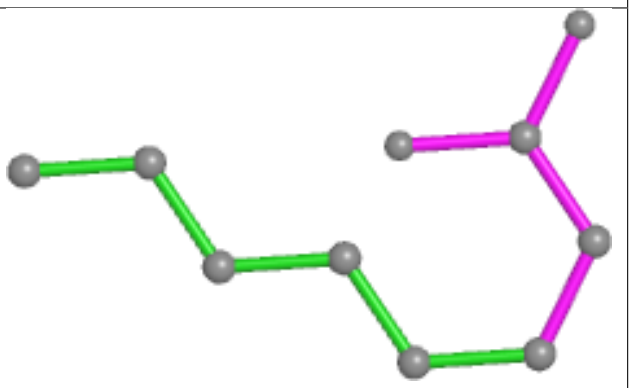
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	615	PEG	1	0
2	C	601	EIC	7	0
3	A	602	OCA	2	0
2	A	601	EIC	5	0
9	A	618	PG4	2	0
7	A	617	PEG	1	0
4	B	603	PLM	6	0
4	B	604	PLM	9	0
3	B	602	OCA	3	0
6	C	609	SO4	2	0
8	A	615	PGE	1	0
4	C	603	PLM	6	0
8	C	611	PGE	1	0
2	B	601	EIC	3	0
7	C	610	PEG	2	0
4	A	603	PLM	3	0
7	B	617	PEG	1	0
9	C	614	PG4	1	0
8	B	615	PGE	4	0
7	A	619	PEG	1	0
7	B	613	PEG	1	0
3	C	602	OCA	1	0
10	B	622	1PE	2	0
6	C	608	SO4	1	0
5	B	605	TRP	1	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.

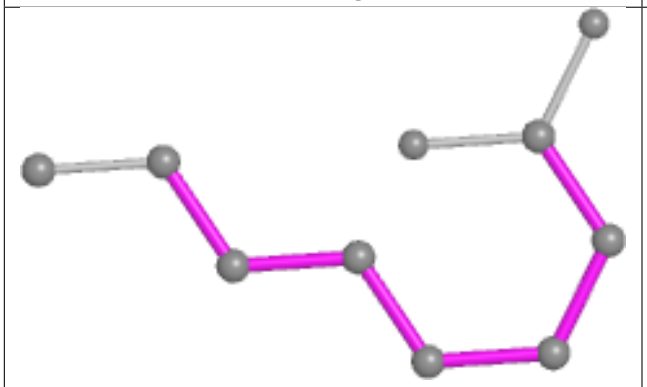
Ligand OCA C 604



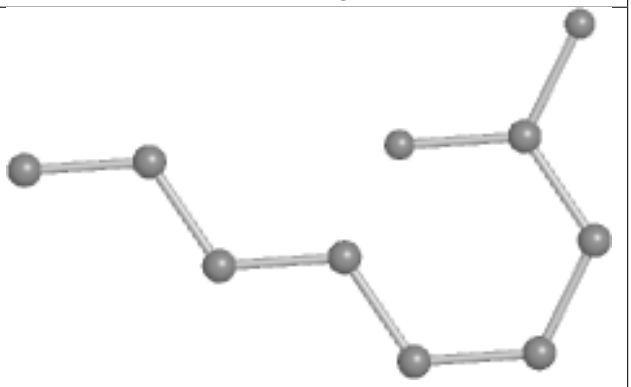
Bond lengths



Bond angles

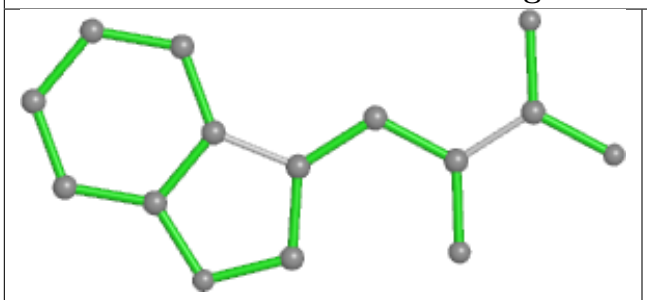


Torsions

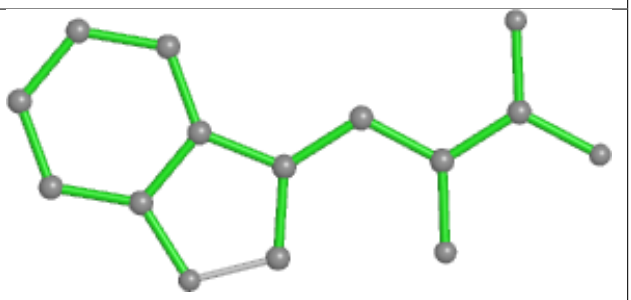


Rings

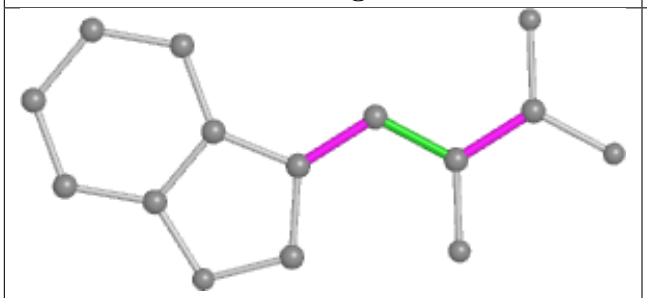
Ligand TRP A 605



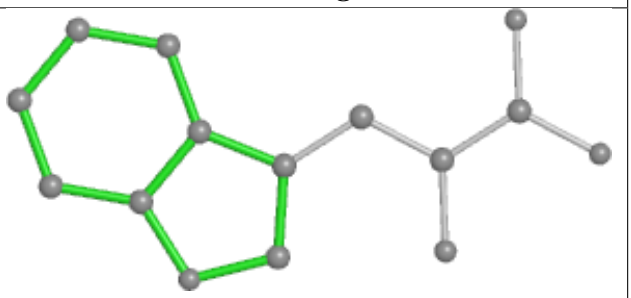
Bond lengths



Bond angles

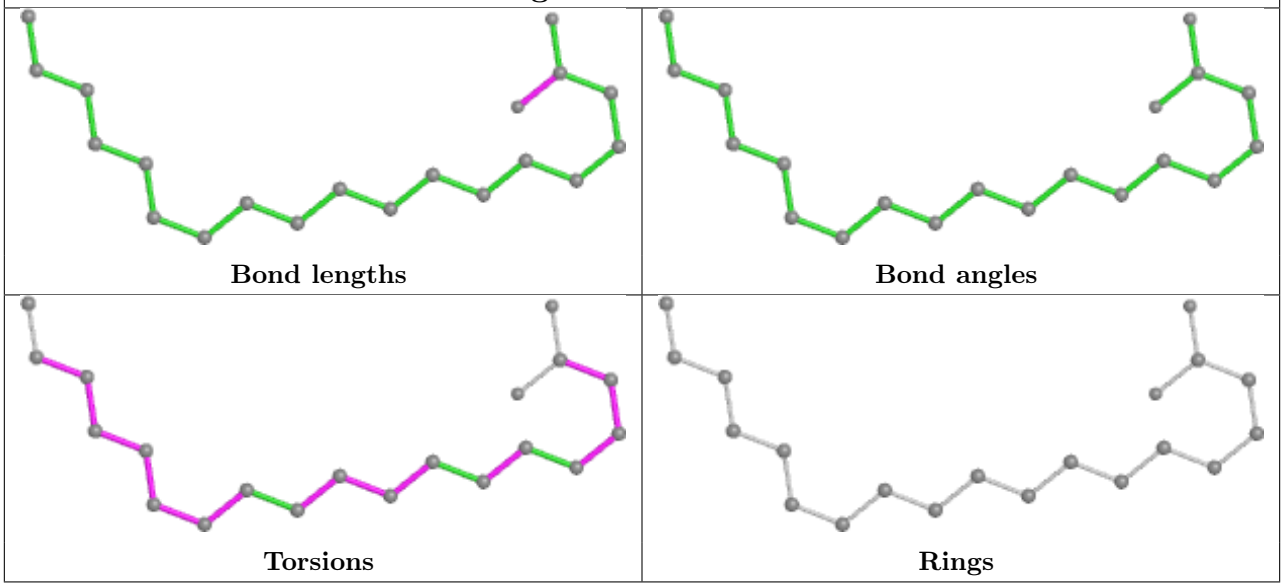


Torsions

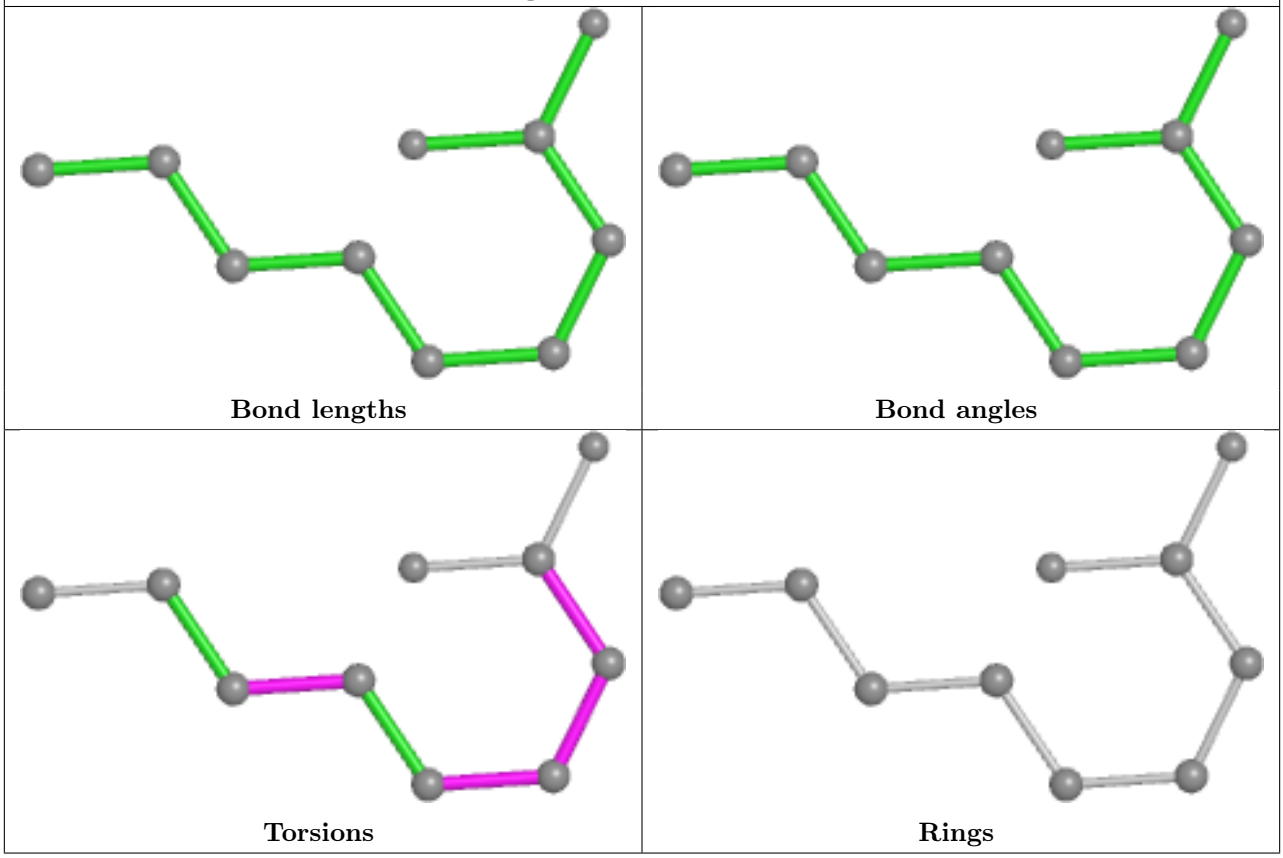


Rings

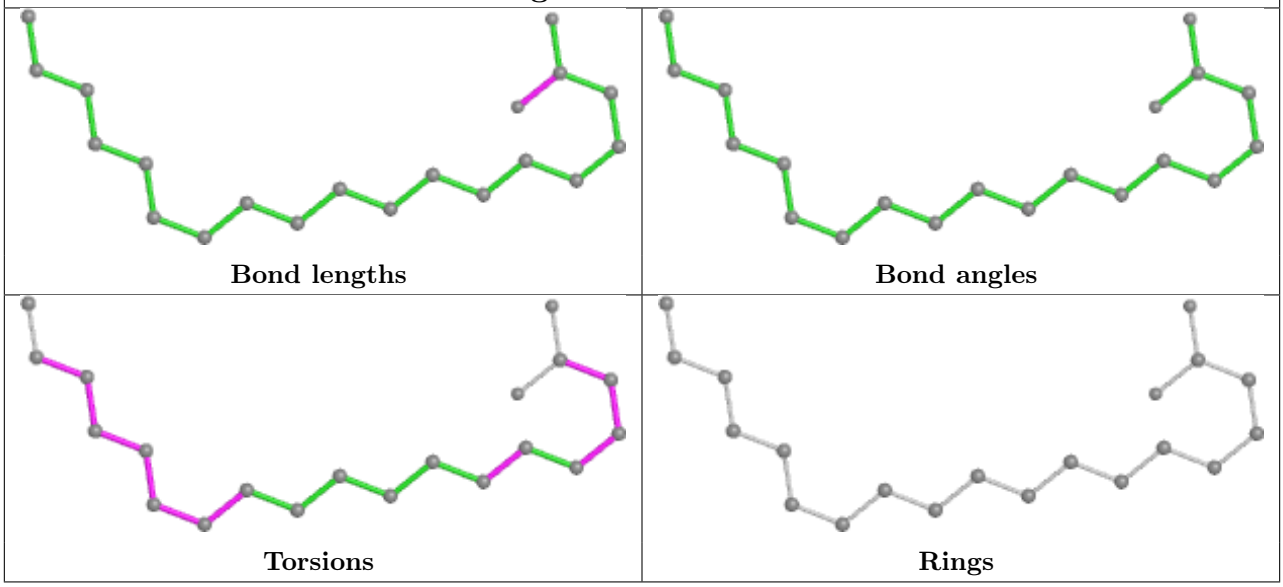
Ligand EIC C 601



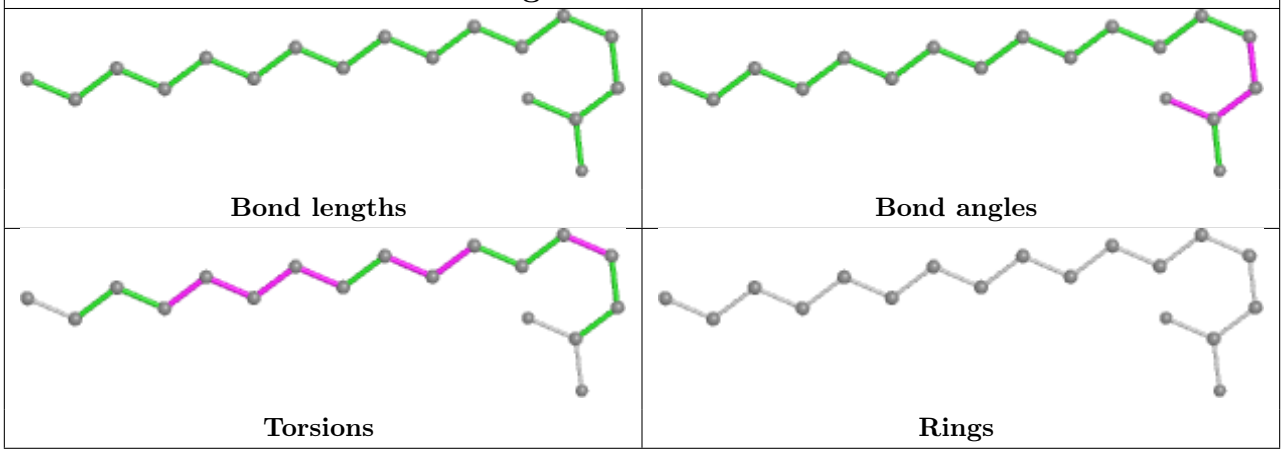
Ligand OCA A 602



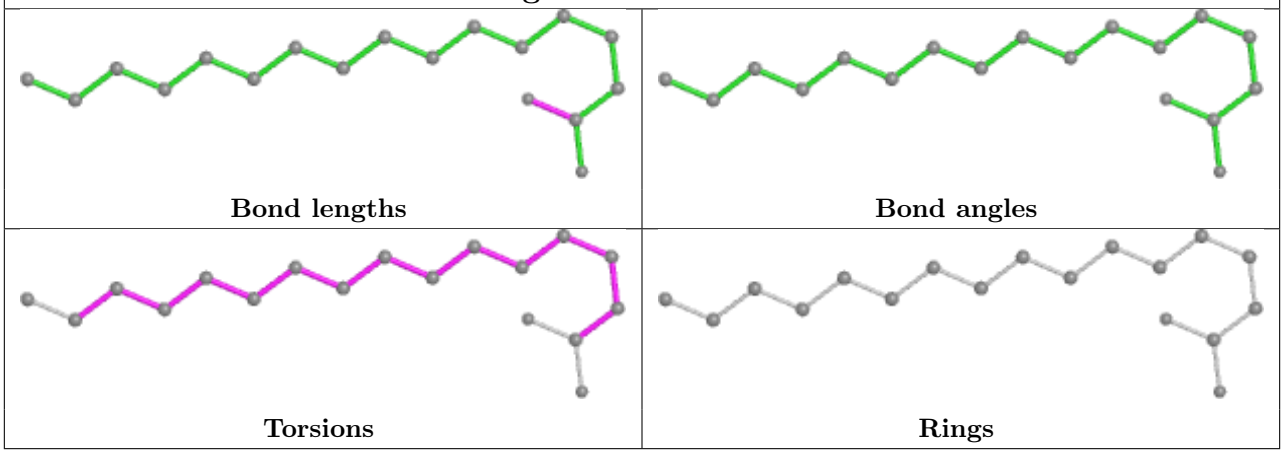
Ligand EIC A 601



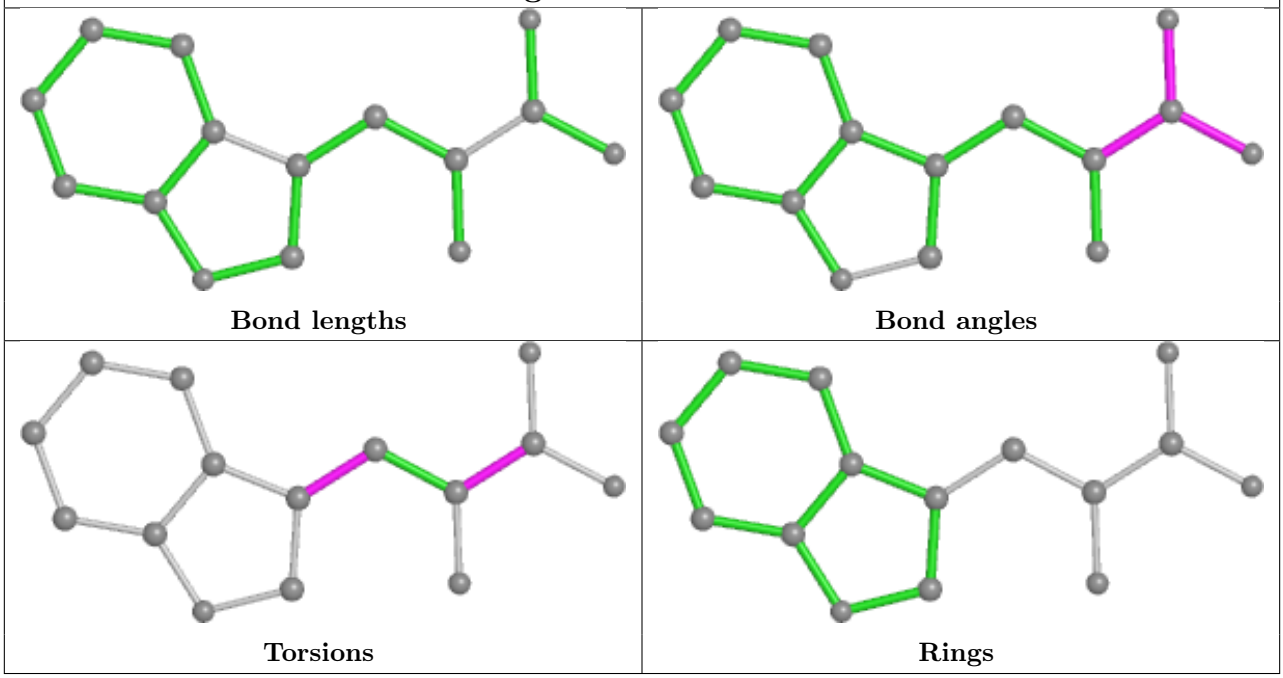
Ligand PLM B 603



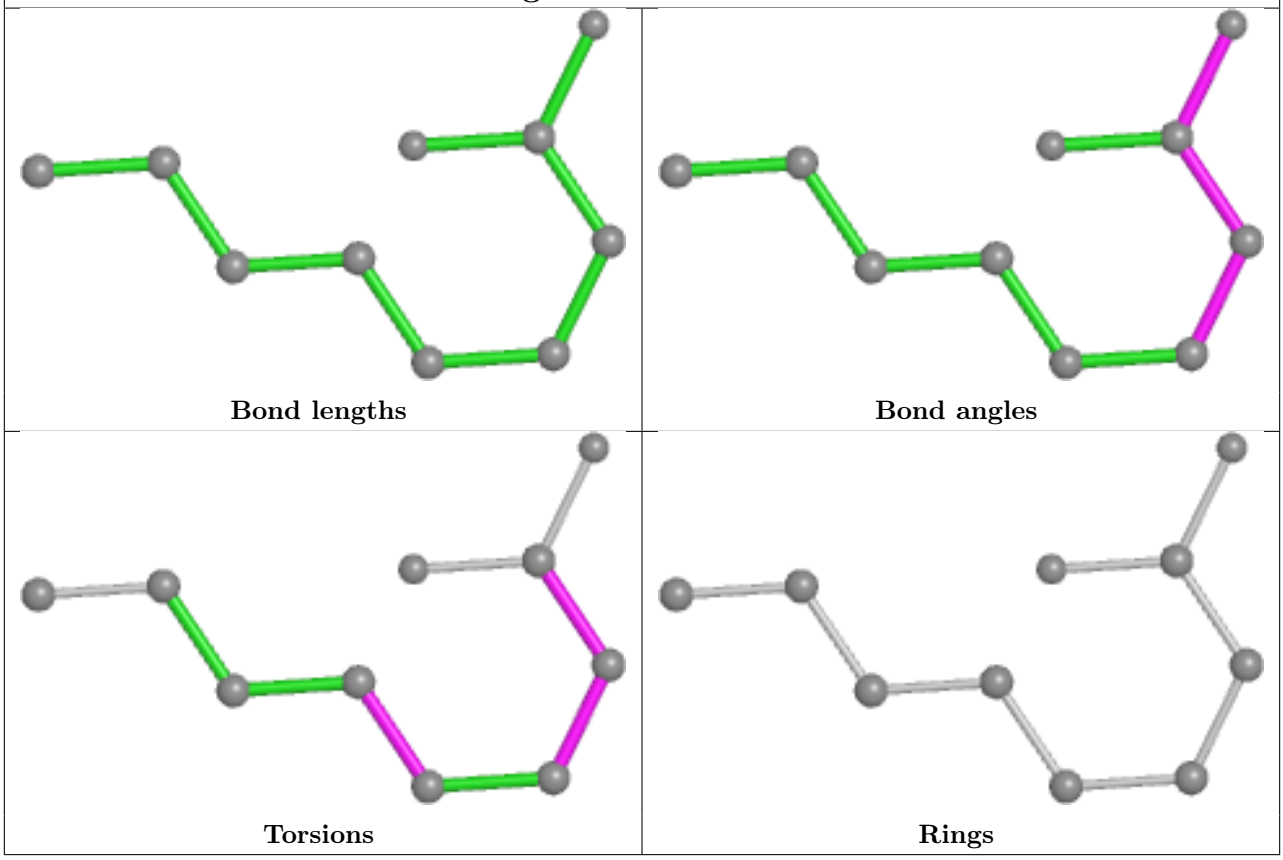
Ligand PLM B 604



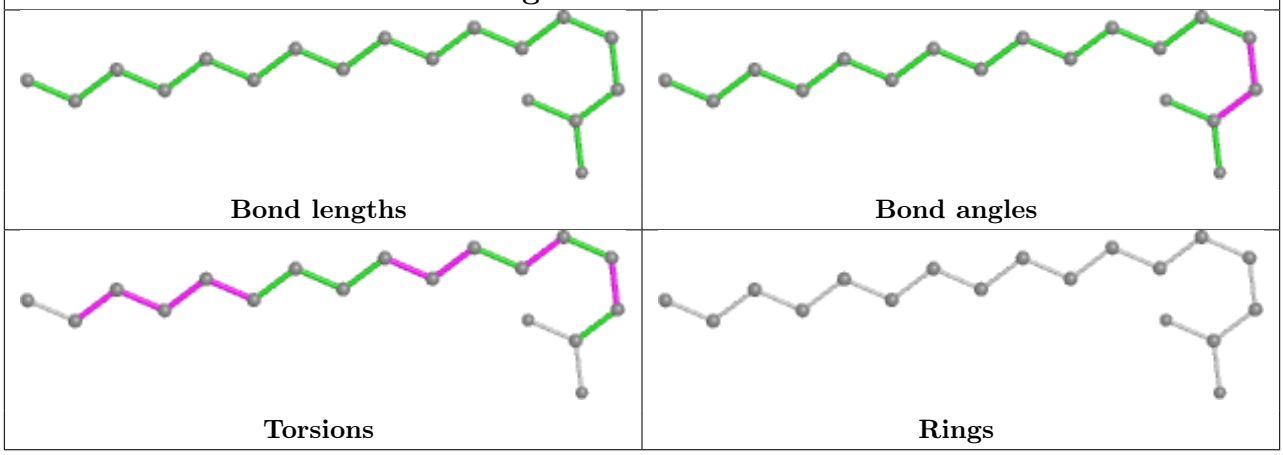
Ligand TRP C 605



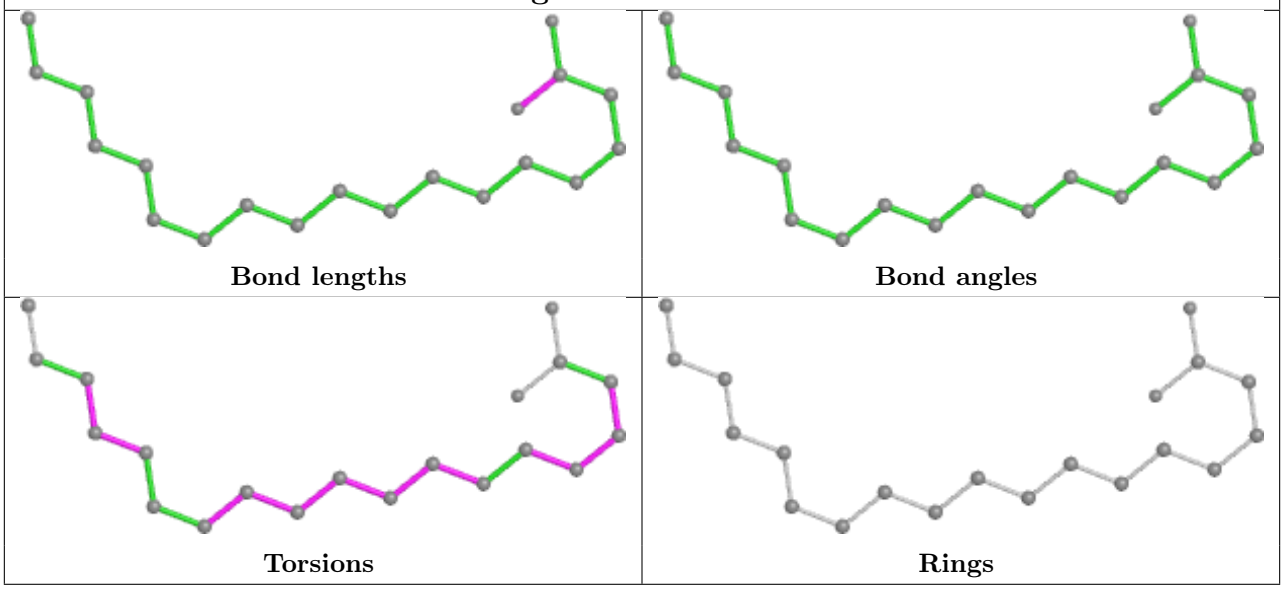
Ligand OCA B 602



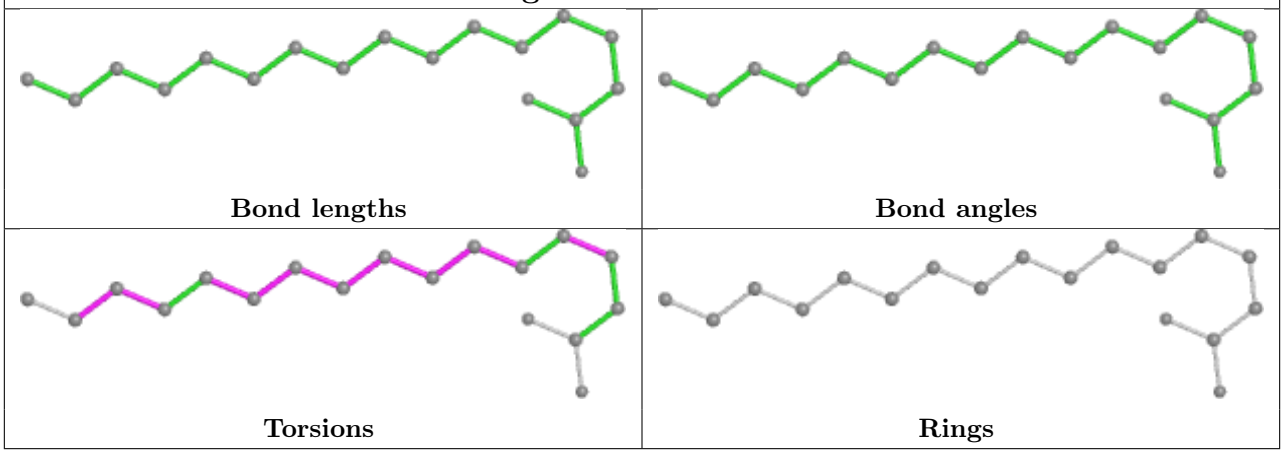
Ligand PLM C 603



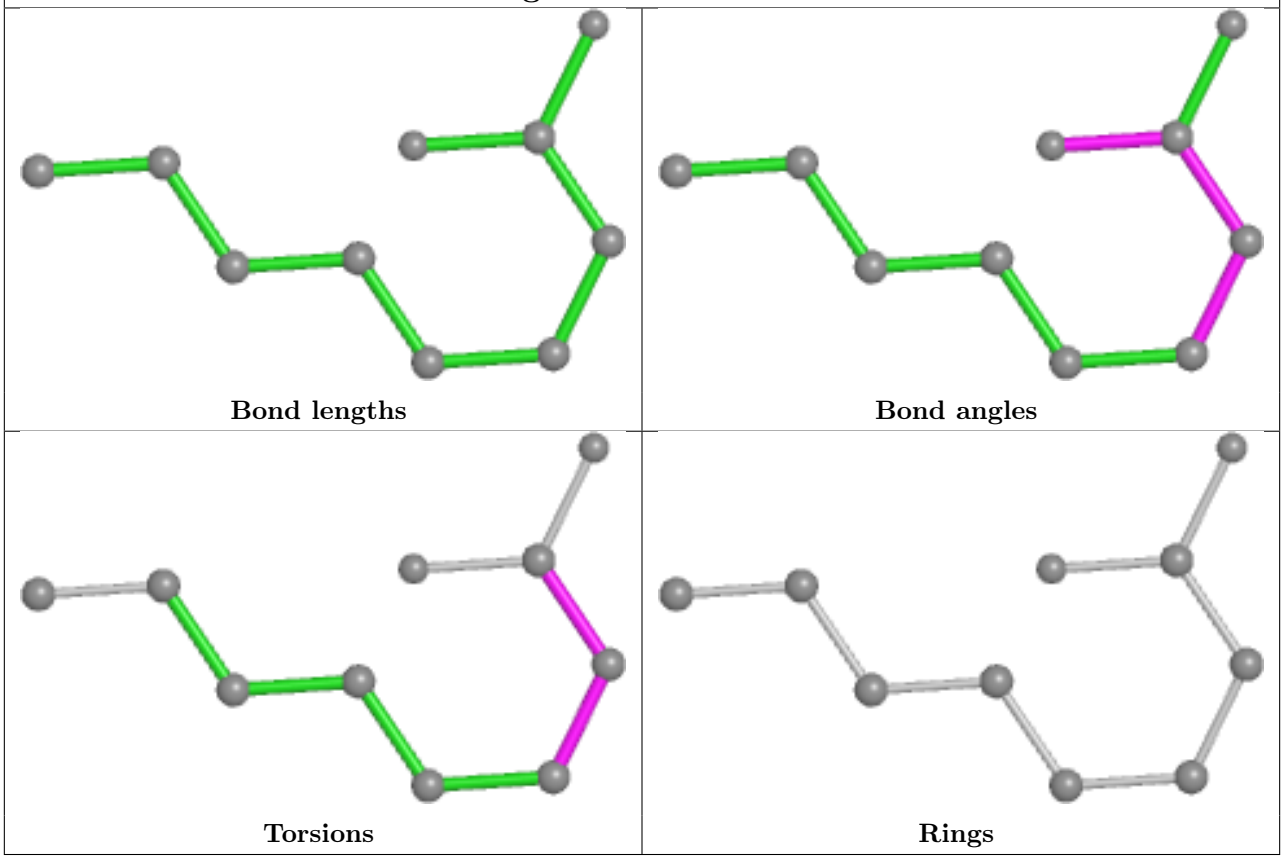
Ligand EIC B 601



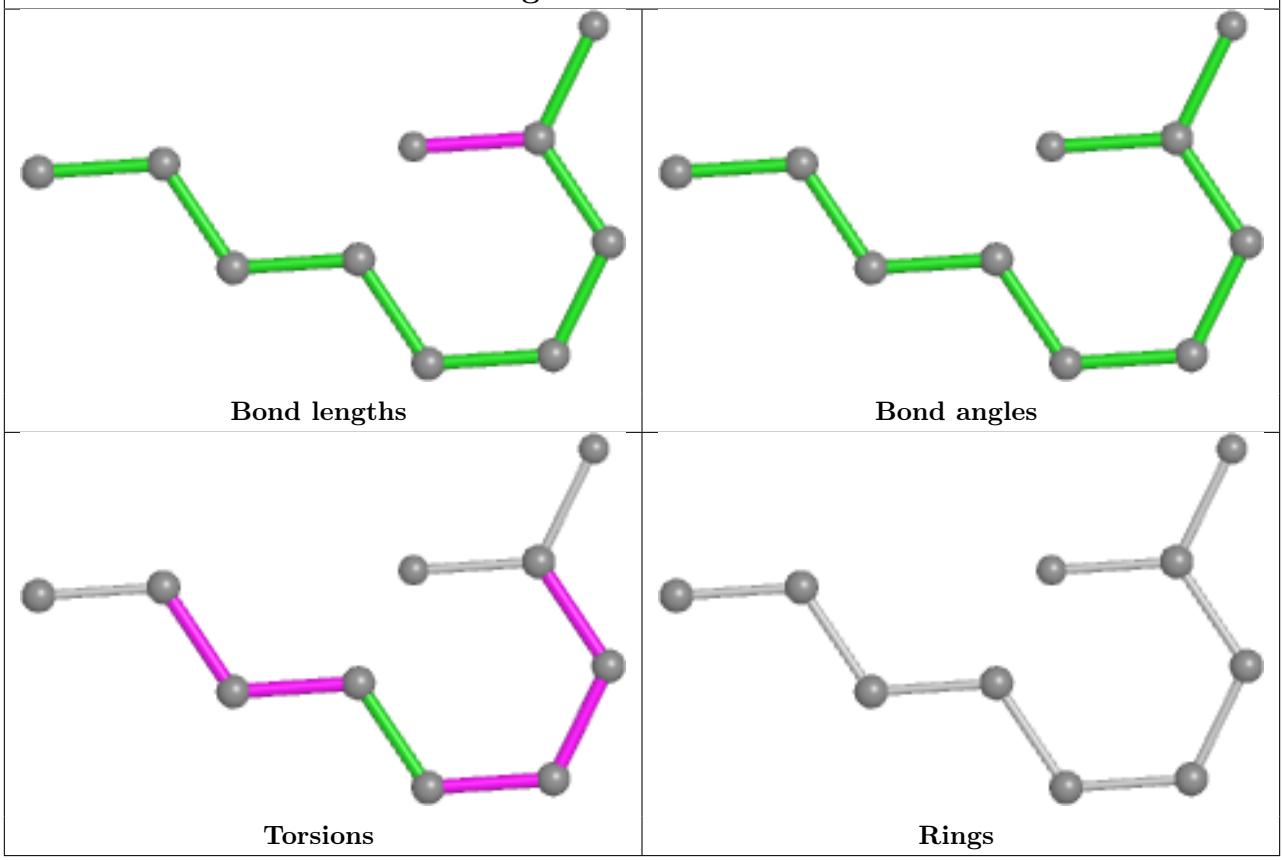
Ligand PLM A 603



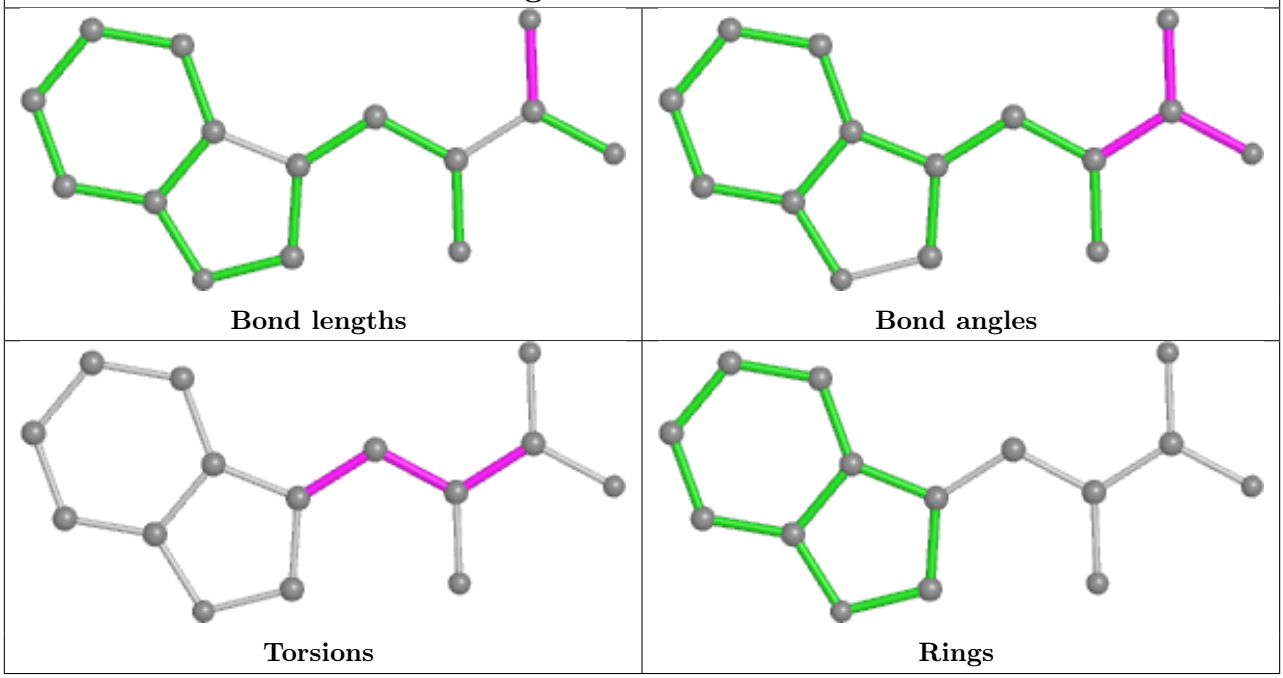
Ligand OCA C 602



Ligand OCA A 604



Ligand TRP B 605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	580/585 (99%)	0.52	56 (9%) 7 8	27, 43, 78, 100	0
1	B	580/585 (99%)	0.54	70 (12%) 4 4	26, 40, 89, 102	0
1	C	531/585 (90%)	0.77	79 (14%) 2 2	28, 43, 89, 122	0
All	All	1691/1755 (96%)	0.60	205 (12%) 4 4	26, 42, 85, 122	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	547	VAL	10.1
1	C	502	PHE	9.7
1	C	497	TYR	8.0
1	C	504	ALA	7.7
1	A	515	THR	7.4
1	A	561	ALA	7.0
1	B	504	ALA	6.9
1	C	521	ARG	6.6
1	B	557	LYS	6.3
1	C	546	ALA	6.2
1	B	82	GLU	6.2
1	A	115	LEU	6.1
1	C	496	THR	5.9
1	C	541	LYS	5.9
1	C	364	ALA	5.8
1	A	83	THR	5.8
1	A	82	GLU	5.7
1	A	172	ALA	5.6
1	C	81	ARG	5.4
1	A	501	GLU	5.3
1	B	116	VAL	5.3
1	C	498	VAL	5.3
1	C	500	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	80	LEU	5.1
1	A	116	VAL	5.1
1	C	522	GLN	5.1
1	C	444	LYS	5.0
1	B	501	GLU	4.9
1	B	553	ALA	4.9
1	C	116	VAL	4.9
1	B	584	GLY	4.8
1	A	504	ALA	4.7
1	C	441	PRO	4.7
1	B	85	GLY	4.7
1	A	58	SER	4.6
1	B	172	ALA	4.6
1	A	516	LEU	4.6
1	C	543	GLN	4.6
1	B	86	GLU	4.5
1	A	81	ARG	4.4
1	C	545	LYS	4.3
1	C	442	GLU	4.2
1	A	80	LEU	4.2
1	A	505	GLU	4.2
1	C	365	ASP	4.2
1	C	398	LEU	4.2
1	C	440	HIS	4.2
1	C	82	GLU	4.1
1	B	519	LYS	4.0
1	C	503	ASN	4.0
1	C	535	HIS	4.0
1	B	515	THR	4.0
1	B	170	GLN	4.0
1	C	363	ALA	4.0
1	B	559	CYS	3.9
1	A	560	LYS	3.9
1	C	397	GLN	3.8
1	A	113	PRO	3.8
1	C	520	GLU	3.7
1	A	549	ASP	3.7
1	C	469	VAL	3.7
1	A	129	ASP	3.7
1	B	516	LEU	3.6
1	C	443	ALA	3.6
1	A	517	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	508	THR	3.6
1	A	59	ALA	3.5
1	A	502	PHE	3.5
1	B	443	ALA	3.5
1	B	550	ASP	3.5
1	C	536	LYS	3.5
1	B	546	ALA	3.5
1	B	83	THR	3.5
1	A	23	VAL	3.5
1	C	172	ALA	3.4
1	B	560	LYS	3.4
1	A	584	GLY	3.4
1	B	128	HIS	3.4
1	C	399	GLY	3.4
1	C	113	PRO	3.4
1	B	510	HIS	3.3
1	C	290	ILE	3.3
1	C	84	TYR	3.3
1	A	114	ARG	3.3
1	B	549	ASP	3.3
1	C	499	PRO	3.3
1	C	114	ARG	3.3
1	C	501	GLU	3.3
1	C	362	ALA	3.3
1	A	79	THR	3.2
1	C	544	LEU	3.2
1	C	524	LYS	3.2
1	C	23	VAL	3.2
1	B	538	LYS	3.2
1	B	545	LYS	3.2
1	C	548	MET	3.2
1	A	63	ASP	3.2
1	C	549	ASP	3.2
1	A	503	ASN	3.1
1	B	565	GLU	3.1
1	C	79	THR	3.1
1	C	519	LYS	3.1
1	B	505	GLU	3.1
1	B	398	LEU	3.1
1	A	86	GLU	3.1
1	C	539	ALA	3.1
1	A	4	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	563	ASP	3.1
1	C	83	THR	3.1
1	B	290	ILE	3.1
1	C	80	LEU	3.0
1	A	557	LYS	3.0
1	B	502	PHE	3.0
1	B	564	LYS	3.0
1	B	556	GLU	3.0
1	A	362	ALA	3.0
1	B	561	ALA	3.0
1	A	85	GLY	3.0
1	C	542	GLU	2.9
1	C	111	ASN	2.9
1	B	562	ASP	2.9
1	C	401	TYR	2.9
1	A	363	ALA	2.9
1	C	393	GLU	2.9
1	B	81	ARG	2.9
1	A	7	VAL	2.8
1	C	438	CYS	2.8
1	C	467	THR	2.8
1	C	251	LEU	2.8
1	B	79	THR	2.7
1	B	397	GLN	2.7
1	B	583	LEU	2.7
1	B	498	VAL	2.7
1	C	382	GLU	2.7
1	A	550	ASP	2.7
1	C	495	GLU	2.7
1	C	388	ILE	2.7
1	B	467	THR	2.7
1	A	84	TYR	2.7
1	C	529	LEU	2.7
1	C	313	LYS	2.6
1	B	503	ASN	2.6
1	C	176	ALA	2.6
1	B	579	SER	2.6
1	C	129	ASP	2.6
1	C	523	ILE	2.6
1	C	540	THR	2.6
1	A	553	ALA	2.5
1	B	111	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	2.5
1	A	546	ALA	2.5
1	B	466	LYS	2.5
1	A	467	THR	2.5
1	B	84	TYR	2.4
1	A	518	GLU	2.4
1	A	171	ALA	2.4
1	B	581	ALA	2.4
1	B	577	ALA	2.4
1	B	22	LEU	2.4
1	B	492	GLU	2.4
1	B	495	GLU	2.4
1	B	566	THR	2.3
1	B	114	ARG	2.3
1	C	115	LEU	2.3
1	A	492	GLU	2.3
1	A	576	VAL	2.3
1	B	582	ALA	2.3
1	C	170	GLN	2.3
1	B	173	ASP	2.3
1	B	513	ILE	2.3
1	B	23	VAL	2.3
1	B	511	ALA	2.2
1	C	389	LYS	2.2
1	C	530	VAL	2.2
1	B	171	ALA	2.2
1	B	364	ALA	2.2
1	B	457	LEU	2.2
1	B	517	SER	2.2
1	A	176	ALA	2.2
1	B	363	ALA	2.2
1	B	542	GLU	2.2
1	A	264	ILE	2.2
1	A	55	ALA	2.2
1	B	115	LEU	2.1
1	A	130	ASN	2.1
1	A	443	ALA	2.1
1	B	529	LEU	2.1
1	B	580	GLN	2.1
1	A	513	ILE	2.1
1	B	25	ILE	2.1
1	C	300	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	60	GLU	2.1
1	A	498	VAL	2.1
1	C	315	VAL	2.1
1	A	412	THR	2.1
1	C	28	ALA	2.1
1	A	567	CYS	2.1
1	C	25	ILE	2.0
1	C	394	LEU	2.0
1	C	167	GLU	2.0
1	C	250	LEU	2.0
1	A	433	VAL	2.0
1	C	368	GLU	2.0
1	A	111	ASN	2.0
1	C	402	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	A	34	7/8	0.84	0.15	38,40,47,48	0
1	CSO	B	34	7/8	0.91	0.12	34,38,45,59	0
1	CSO	C	34	7/8	0.91	0.13	32,34,41,48	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PGE	C	611	10/10	0.70	0.18	43,57,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PLM	A	603	18/18	0.76	0.27	41,54,74,77	0
7	PEG	B	620	7/7	0.77	0.18	63,65,72,74	0
4	PLM	C	603	18/18	0.79	0.24	38,54,76,81	0
3	OCA	C	604	10/10	0.81	0.19	30,38,60,63	0
7	PEG	B	613	7/7	0.81	0.17	48,53,55,60	0
4	PLM	B	603	18/18	0.82	0.24	40,48,76,76	0
3	OCA	A	602	10/10	0.83	0.35	36,46,59,60	0
9	PG4	A	616	13/13	0.83	0.17	42,49,54,55	0
6	SO4	B	609	5/5	0.84	0.41	61,70,78,84	0
7	PEG	C	613	7/7	0.85	0.13	50,53,58,62	0
2	EIC	C	601	20/20	0.85	0.21	28,45,86,87	0
7	PEG	A	614	7/7	0.85	0.18	40,52,60,60	0
7	PEG	B	617	7/7	0.86	0.21	45,54,60,63	0
8	PGE	B	623	10/10	0.86	0.14	39,46,53,57	0
2	EIC	A	601	20/20	0.87	0.19	28,38,71,71	0
4	PLM	B	604	18/18	0.87	0.18	26,45,58,63	0
9	PG4	C	614	13/13	0.87	0.13	37,46,54,54	0
7	PEG	B	614	7/7	0.88	0.15	45,56,65,65	0
3	OCA	B	602	10/10	0.88	0.34	32,38,45,59	0
3	OCA	A	604	10/10	0.89	0.22	29,35,46,53	0
2	EIC	B	601	20/20	0.89	0.17	26,37,56,62	0
7	PEG	B	621	7/7	0.90	0.16	51,55,58,61	0
7	PEG	C	615	7/7	0.90	0.12	51,53,57,58	0
8	PGE	B	615	10/10	0.91	0.25	30,43,46,46	0
7	PEG	C	610	7/7	0.91	0.17	40,48,56,59	0
6	SO4	C	608	5/5	0.91	0.15	67,71,72,86	0
7	PEG	B	619	7/7	0.91	0.19	47,53,59,62	0
8	PGE	A	615	10/10	0.91	0.21	43,50,60,62	0
6	SO4	B	610	5/5	0.92	0.16	72,72,76,81	0
6	SO4	A	613	5/5	0.92	0.24	79,82,92,94	0
6	SO4	A	609	5/5	0.92	0.21	67,70,72,72	0
10	1PE	B	622	16/16	0.92	0.14	28,40,54,60	0
3	OCA	C	602	10/10	0.93	0.31	29,34,49,53	0
6	SO4	B	608	5/5	0.93	0.19	78,79,80,82	0
6	SO4	A	610	5/5	0.93	0.43	63,67,75,79	0
7	PEG	A	619	7/7	0.93	0.12	39,48,54,60	0
5	TRP	C	605	15/15	0.94	0.13	59,63,70,72	0
7	PEG	B	616	7/7	0.94	0.12	36,43,58,64	0
9	PG4	A	618	13/13	0.94	0.11	34,41,52,53	0
9	PG4	B	618	13/13	0.94	0.15	28,43,69,70	0
6	SO4	B	607	5/5	0.94	0.14	54,66,68,72	0
6	SO4	A	612	5/5	0.94	0.39	70,73,75,85	0

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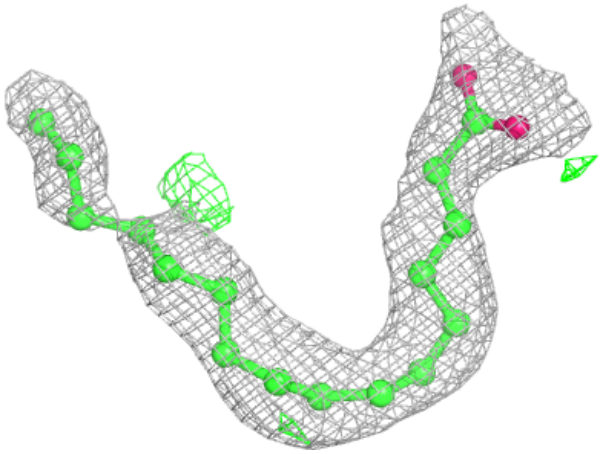
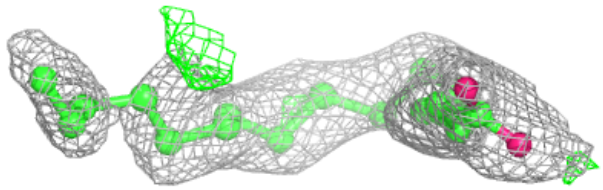
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	611	5/5	0.95	0.14	31,36,44,51	0
6	SO4	A	606	5/5	0.95	0.14	58,65,75,78	0
9	PG4	C	612	13/13	0.95	0.11	37,45,51,54	0
6	SO4	A	607	5/5	0.95	0.11	40,46,56,69	0
7	PEG	A	617	7/7	0.95	0.12	42,43,51,56	0
5	TRP	A	605	15/15	0.96	0.12	29,33,60,66	0
6	SO4	A	608	5/5	0.97	0.11	51,55,64,69	0
5	TRP	B	605	15/15	0.97	0.16	28,31,60,67	0
6	SO4	B	612	5/5	0.97	0.20	79,80,88,93	0
6	SO4	C	607	5/5	0.97	0.10	36,41,58,69	0
6	SO4	C	609	5/5	0.98	0.20	58,60,66,71	0
6	SO4	B	606	5/5	0.98	0.09	35,36,52,58	0
6	SO4	B	611	5/5	0.99	0.07	28,35,36,39	0
6	SO4	C	606	5/5	0.99	0.08	35,37,41,42	0

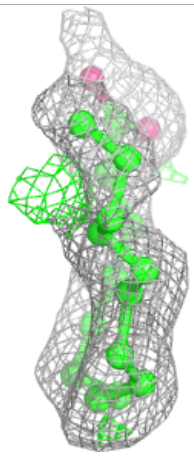
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLM A 603:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

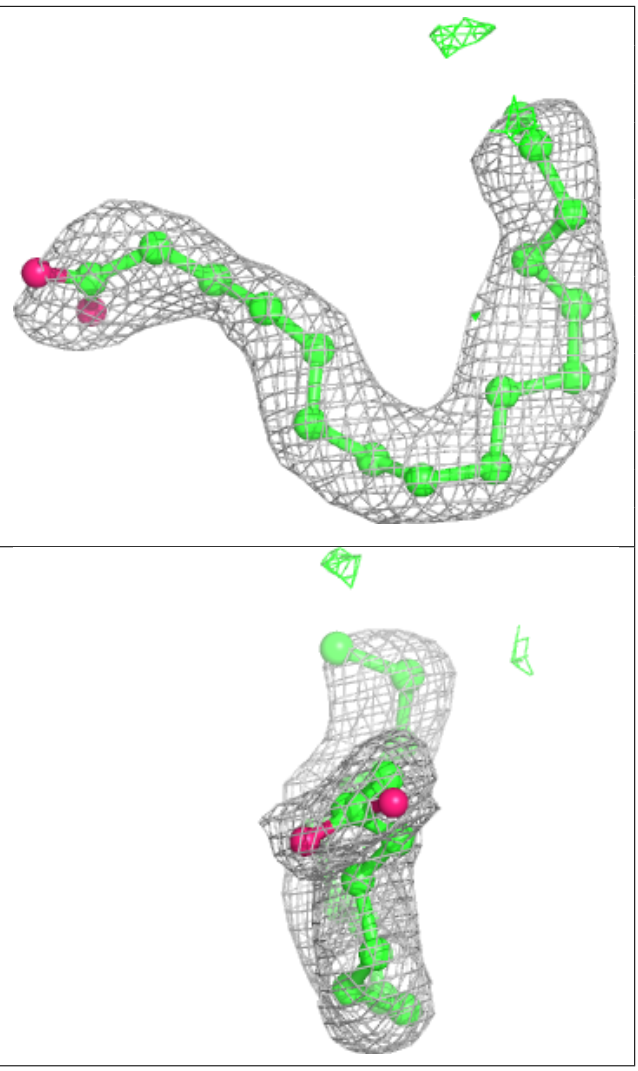






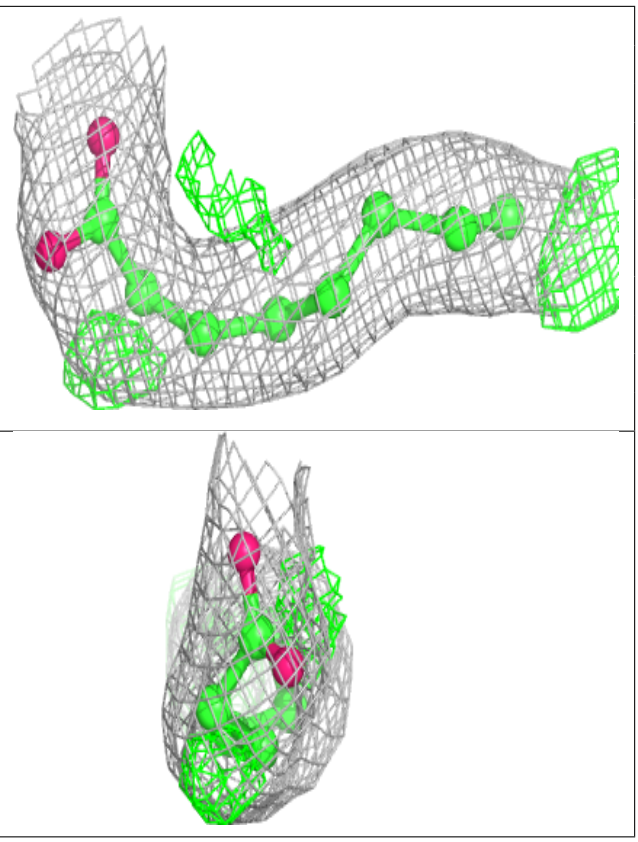
Electron density around PLM C 603:

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



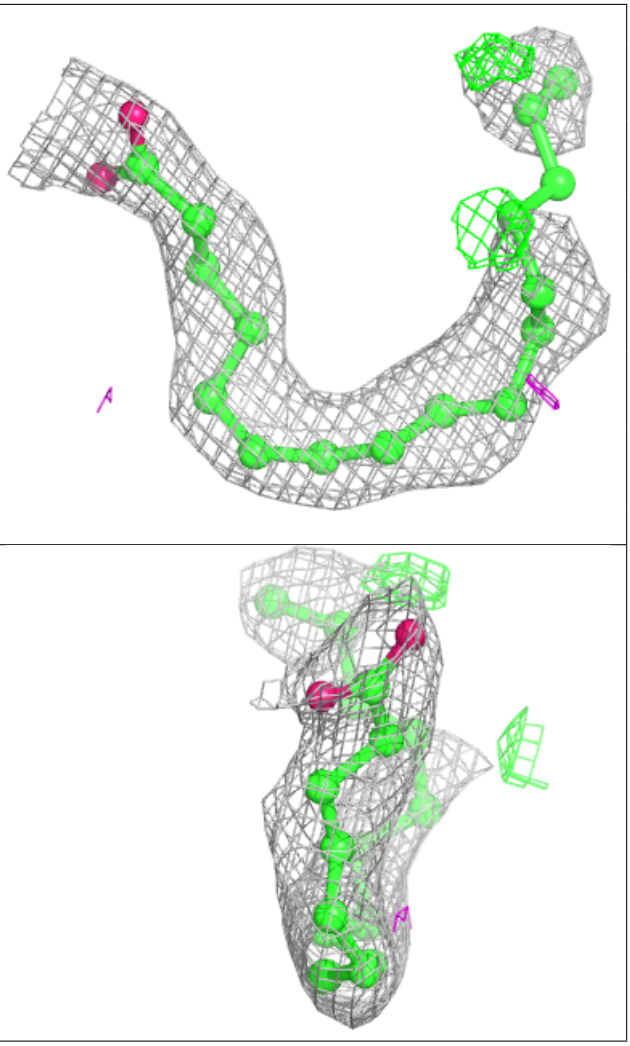
Electron density around OCA C 604:

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



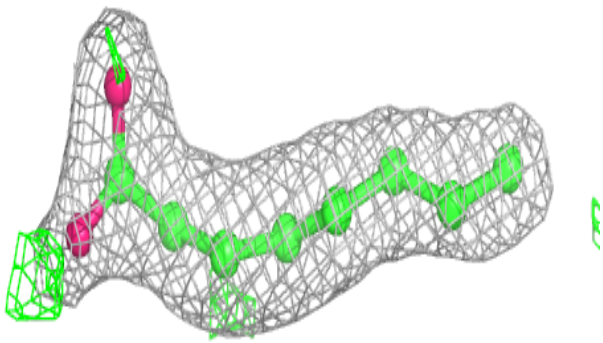
Electron density around PLM B 603:

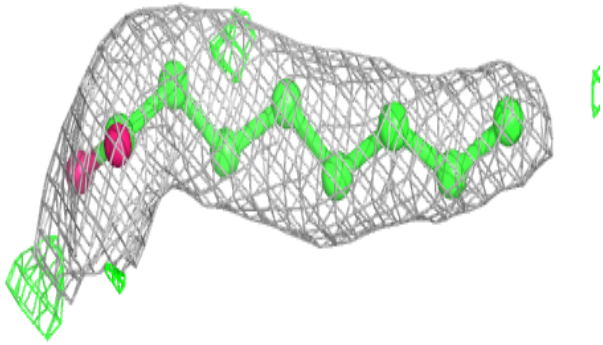
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

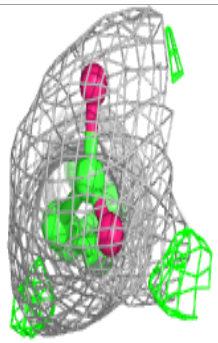


Electron density around OCA A 602:

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

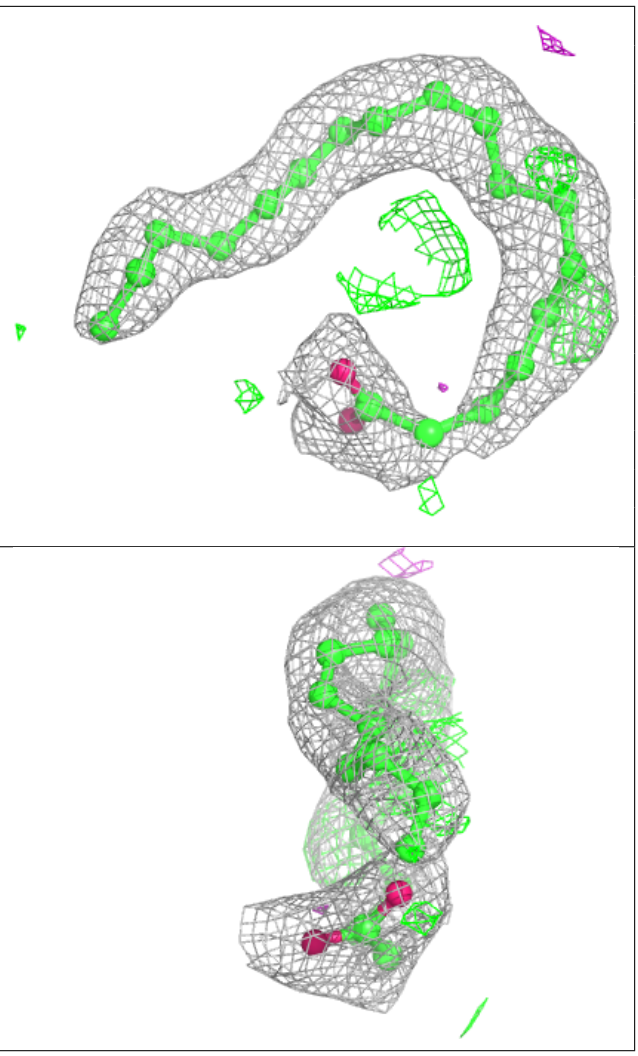






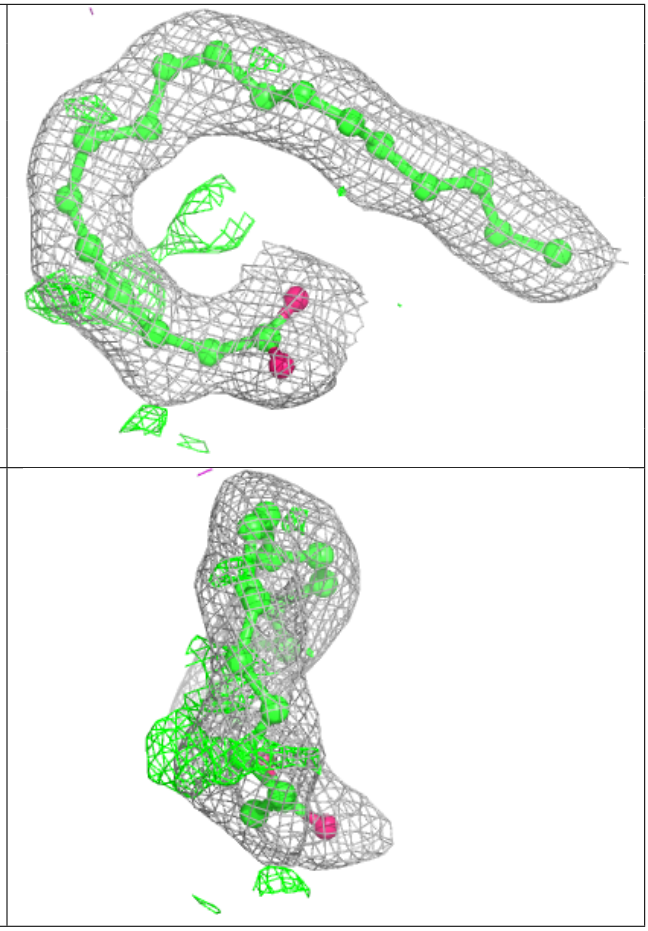
Electron density around EIC C 601:

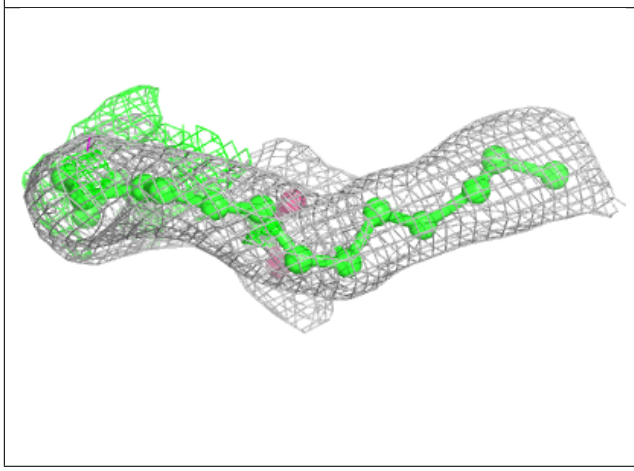
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EIC A 601:

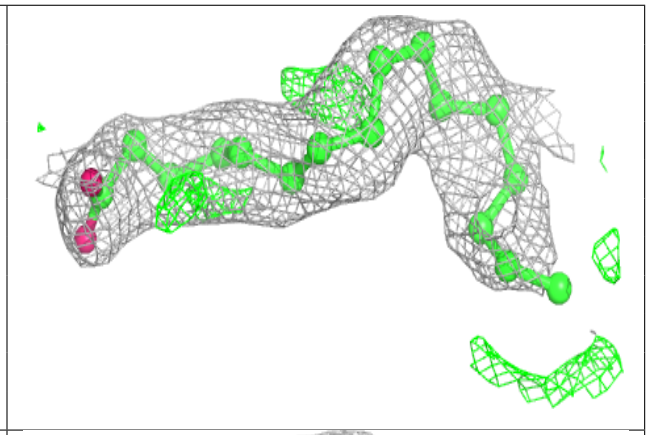
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

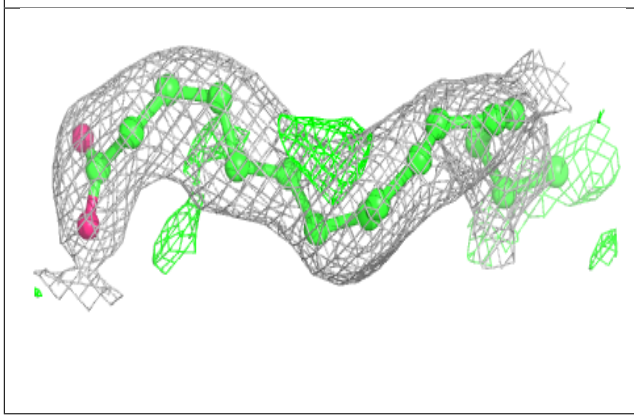




Electron density around PLM B 604:

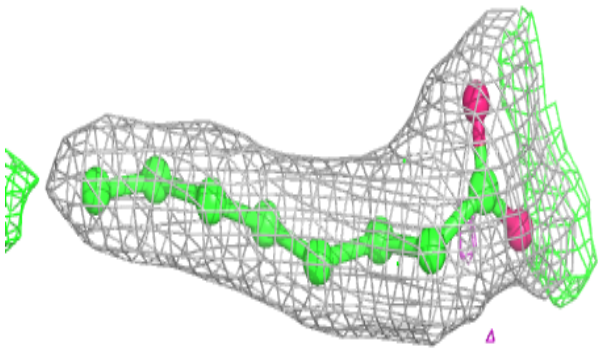
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

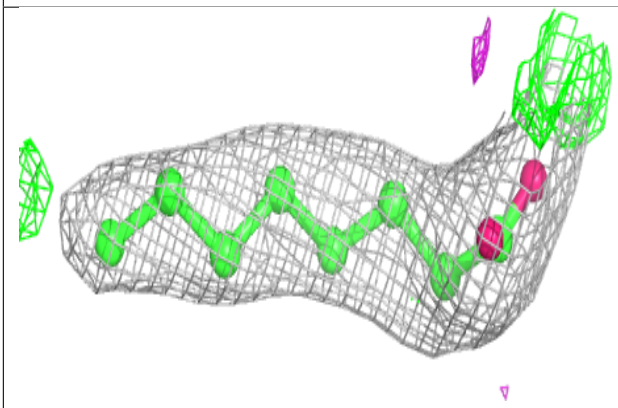


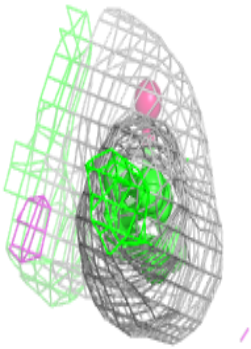


Electron density around OCA B 602:

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

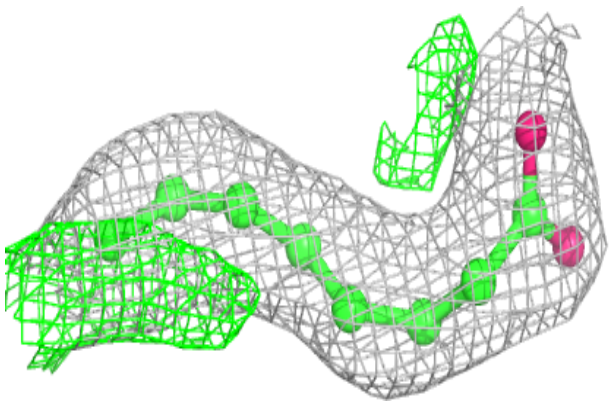


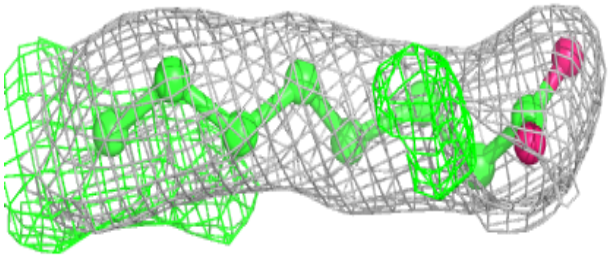


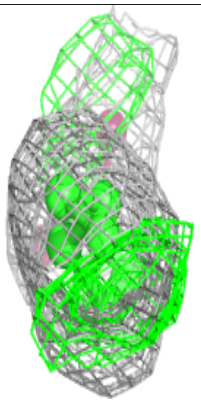


Electron density around OCA A 604:

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

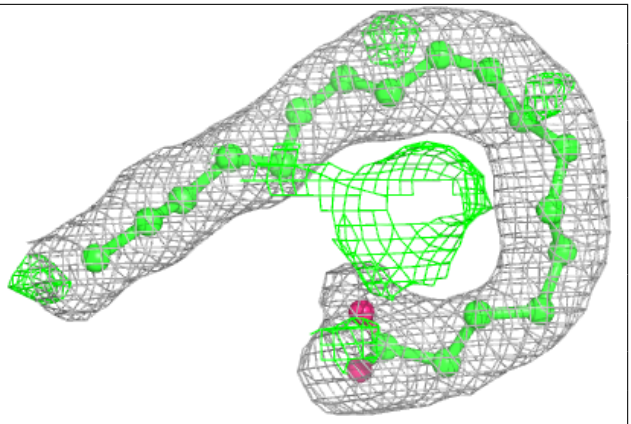


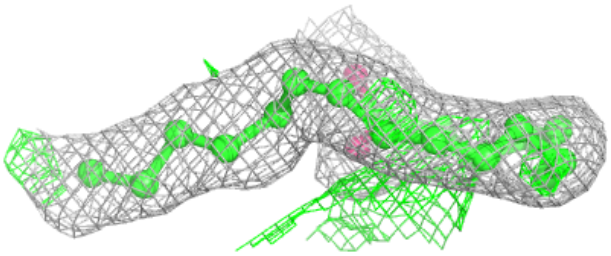


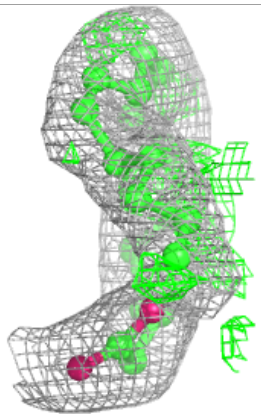


Electron density around EIC B 601:

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

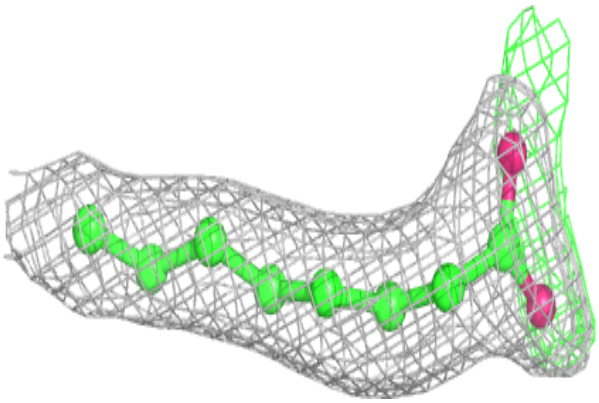


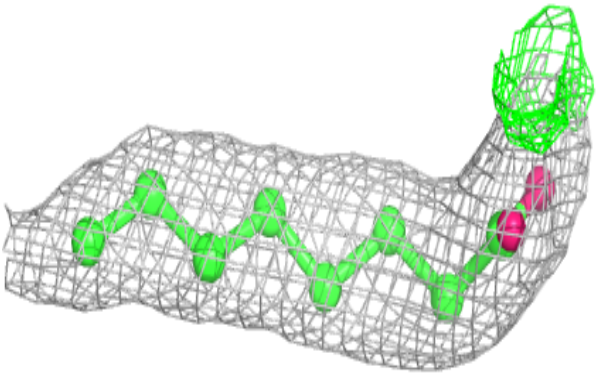


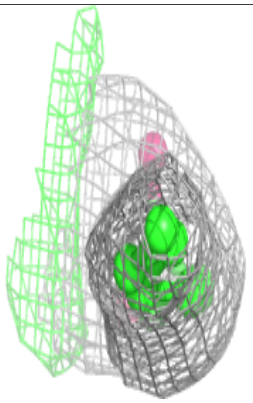


Electron density around OCA C 602:

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

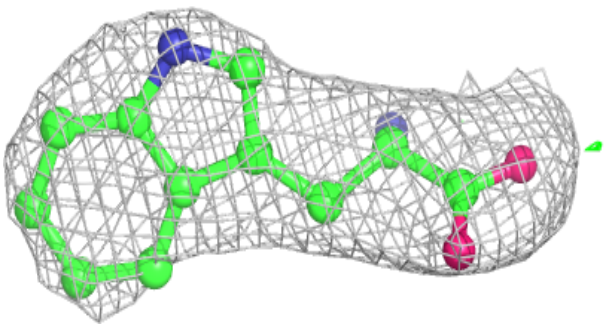


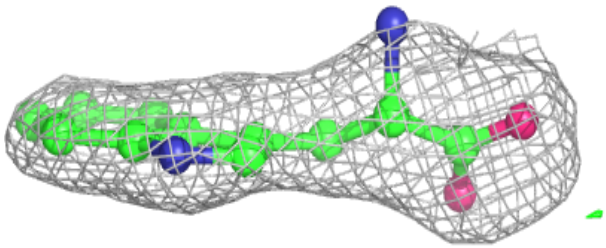


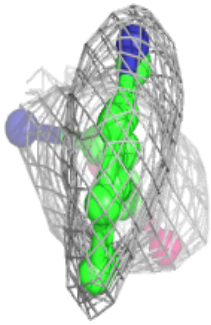


Electron density around TRP C 605:

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

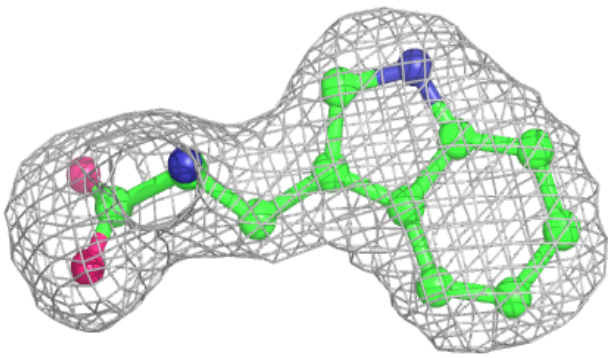


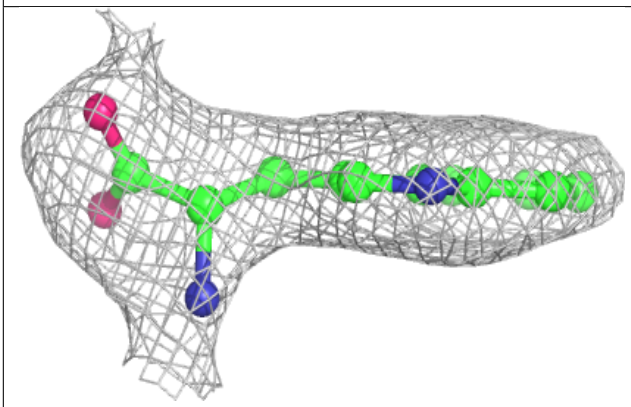


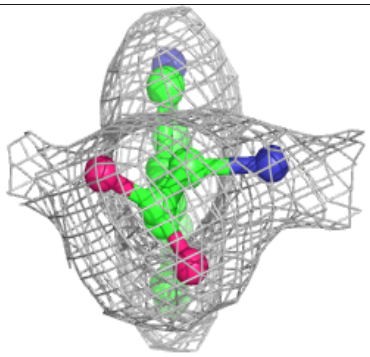


Electron density around TRP A 605:

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

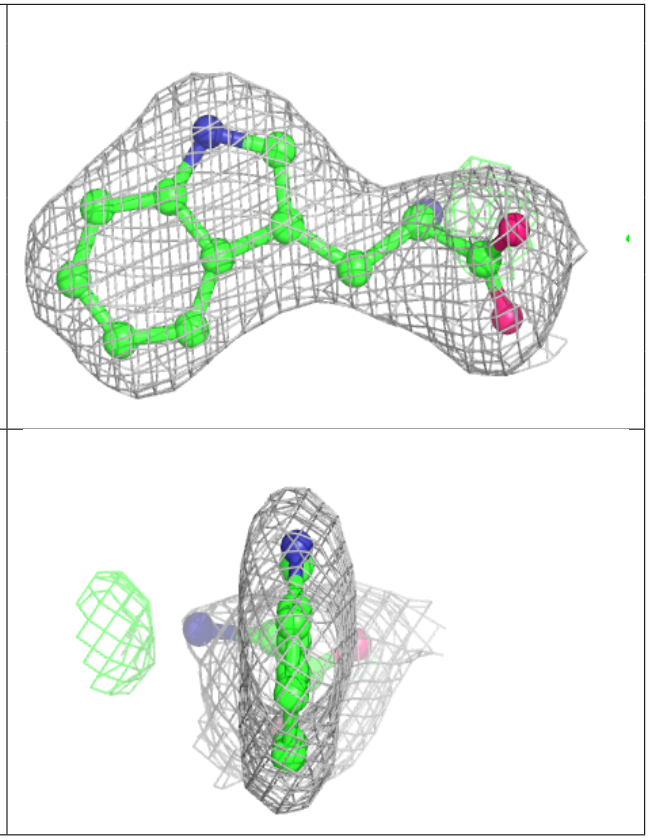






Electron density around TRP B 605:

$2mF_o$-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.