



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:50 PM UTC

PDB ID : 5EGF / pdb_00005egf
Title : The crystal structure of SeMet-CT
Authors : Zhang, J.R.; Tang, Y.; Zhou, J.H.
Deposited on : 2015-10-27
Resolution : 2.29 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

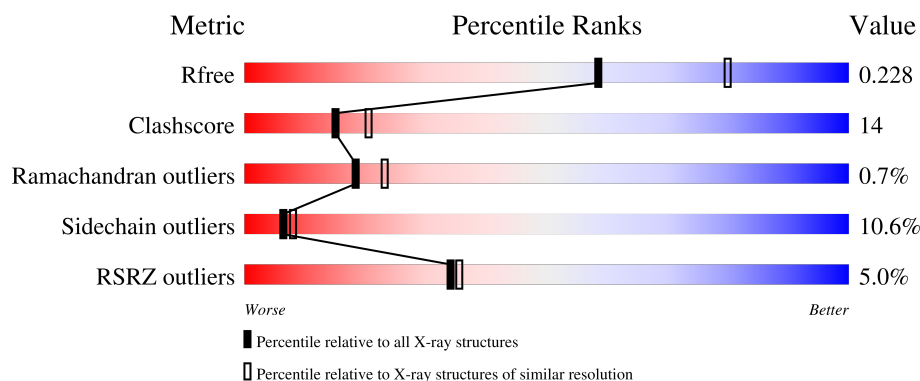
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	486	5% 63% 24% • 9%
1	B	486	3% 66% 22% • 9%
1	C	486	6% 62% 26% • 9%
1	D	486	5% 61% 26% • 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
2	EDO	A	504	-	-	X	-
2	EDO	B	502	-	-	X	-
2	EDO	B	506	-	-	X	-
2	EDO	B	508	-	-	X	-
2	EDO	C	501	-	-	X	-
2	EDO	C	504	-	-	X	-
3	C8E	A	508	-	-	X	-
3	C8E	B	512	-	-	X	-
3	C8E	C	509	-	-	X	-
3	C8E	D	511	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14879 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 TqaA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			
1	B	443	Total	C	N	O	S	Se	0	1	0
			3527	2252	609	653	7	6			
1	C	444	Total	C	N	O	S	Se	0	2	0
			3544	2265	612	654	7	6			
1	D	442	Total	C	N	O	S	Se	0	1	0
			3529	2257	609	650	7	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP F1CWE4
A	3	HIS	-	expression tag	UNP F1CWE4
A	4	HIS	-	expression tag	UNP F1CWE4
A	5	HIS	-	expression tag	UNP F1CWE4
A	6	HIS	-	expression tag	UNP F1CWE4
A	7	HIS	-	expression tag	UNP F1CWE4
A	35	ALA	LYS	engineered mutation	UNP F1CWE4
A	36	ALA	GLU	engineered mutation	UNP F1CWE4
B	2	HIS	-	expression tag	UNP F1CWE4
B	3	HIS	-	expression tag	UNP F1CWE4
B	4	HIS	-	expression tag	UNP F1CWE4
B	5	HIS	-	expression tag	UNP F1CWE4
B	6	HIS	-	expression tag	UNP F1CWE4
B	7	HIS	-	expression tag	UNP F1CWE4
B	35	ALA	LYS	engineered mutation	UNP F1CWE4
B	36	ALA	GLU	engineered mutation	UNP F1CWE4
C	2	HIS	-	expression tag	UNP F1CWE4
C	3	HIS	-	expression tag	UNP F1CWE4
C	4	HIS	-	expression tag	UNP F1CWE4
C	5	HIS	-	expression tag	UNP F1CWE4
C	6	HIS	-	expression tag	UNP F1CWE4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	7	HIS	-	expression tag	UNP F1CWE4
C	35	ALA	LYS	engineered mutation	UNP F1CWE4
C	36	ALA	GLU	engineered mutation	UNP F1CWE4
D	2	HIS	-	expression tag	UNP F1CWE4
D	3	HIS	-	expression tag	UNP F1CWE4
D	4	HIS	-	expression tag	UNP F1CWE4
D	5	HIS	-	expression tag	UNP F1CWE4
D	6	HIS	-	expression tag	UNP F1CWE4
D	7	HIS	-	expression tag	UNP F1CWE4
D	35	ALA	LYS	engineered mutation	UNP F1CWE4
D	36	ALA	GLU	engineered mutation	UNP F1CWE4

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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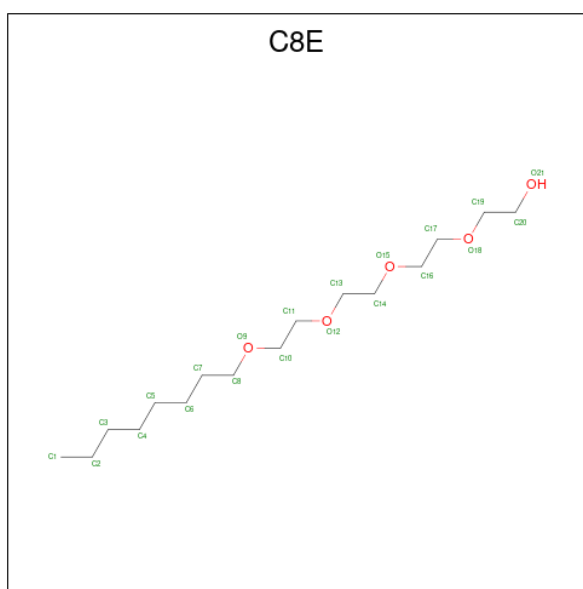
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 16 5	0	0
3	B	1	Total C O 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	179	Total	O	0	0
			179	179		
4	C	134	Total	O	0	0
			134	134		
4	D	98	Total	O	0	0
			98	98		

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.

Chain A:

5% 63% 24% 9%

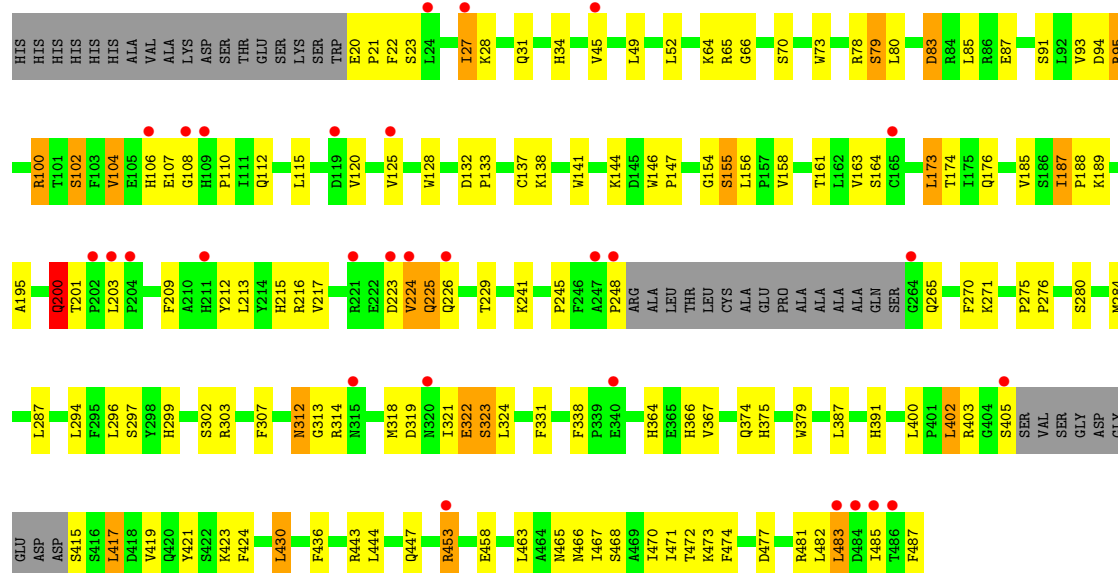
HIS HIS HIS HIS HIS HIS HIS VAL VAL LYS LYS ASP SER THR GLU SER LYS SER W19 E20 S25 P26 I27 K28 H34 I43 P44 V45 T46 S47 L48 L49 L52 L53 H60 R65 W73 S79 M82 R86 R89 T101 S102 F103 E105 P110 P111 Q12 L115 A116 M117 E124 D132 P133 K138 W141 D142 K144 K145 W146 P147 V151 L156 P157 V158 R159 L162 G167 N168 V172 L173 Q176 V185 S186 I187 P188 A189 L190 D193 N199 Q200 T206 S207 D208 Y214 R216 S219 V224 Q225 T229 F230 Q231 F232 W233 R234 A240 V244 A247 P248 ARG A249 LEU THR CYS A251 ALA GLU PRO A253 ALA ALA ALA A255 ALA GLN SER Q264 Q265 G272 G273 V274 P275 P276 T277 L278 P279 T282 T283 K284 K285 T286 L287 V288 K289 H299 S302 R303 H309 H310 V311 N312 G313 R314 M318 D319 N320 I321 W323 E322 S323 L324 L325 R335 F338 P339 E340 D341 S342 T343 D344 M348 T356 T359 R360 A361 L362 S363 H364 E365 D371 I372 F373 Q374 H375 S376 T377 N378 Q390 L396 S399 G404 SER VAL SER GLY ASP GLY L440 A441 D442 R443 L444 Q447 R453 E462 T471 T472 K473 T476 D477 P478 T479 A480 R481 L482 L483 D484 T485 T486 PHE

Chain B:

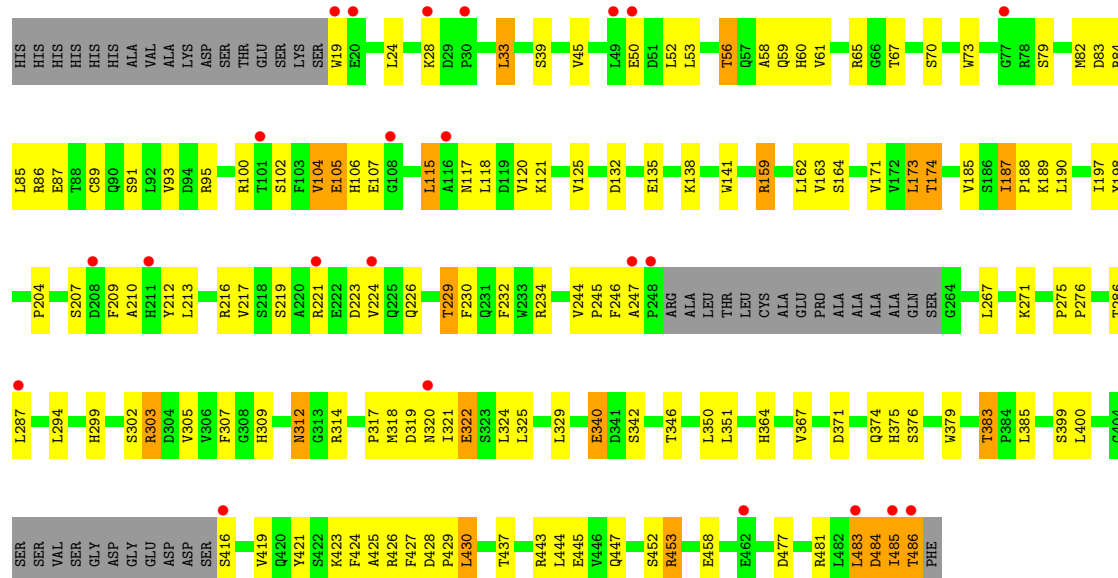
Category	Percentage
Red	3%
Green	66%
Yellow	22%
Grey	9%



• Molecule 1: TqaA



• Molecule 1: TqaA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.60Å 100.28Å 128.23Å 90.00° 100.18° 90.00°	Depositor
Resolution (Å)	29.75 – 2.29 29.75 – 2.29	Depositor EDS
% Data completeness (in resolution range)	85.4 (29.75-2.29) 85.0 (29.75-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.225 , 0.266 0.227 , 0.228	Depositor DCC
R_{free} test set	1880 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14879	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, C8E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/3626	0.90	2/4946 (0.0%)
1	B	0.61	1/3623 (0.0%)	0.94	8/4941 (0.2%)
1	C	0.54	1/3645 (0.0%)	0.89	2/4970 (0.0%)
1	D	0.51	0/3626	0.89	6/4946 (0.1%)
All	All	0.56	2/14520 (0.0%)	0.91	18/19803 (0.1%)

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
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	ILE	CA-CB	5.30	1.57	1.53
1	C	187	ILE	CA-CB	5.13	1.57	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ILE	N-CA-C	9.61	120.08	111.81
1	D	477	ASP	CA-C-N	6.99	126.69	119.56
1	D	477	ASP	C-N-CA	6.99	126.69	119.56
1	B	247	ALA	N-CA-C	6.75	124.74	109.81
1	B	109	HIS	CA-C-N	6.47	126.23	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	484	ASP	Peptide
1	B	247	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3529	0	3454	93	0
1	B	3527	0	3452	80	0
1	C	3544	0	3466	104	0
1	D	3529	0	3454	100	0
2	A	28	0	42	9	0
2	B	40	0	60	20	0
2	C	32	0	48	16	0
2	D	40	0	60	9	0
3	A	21	0	34	9	0
3	B	21	0	34	16	0
3	C	21	0	34	12	0
3	D	21	0	34	9	0
4	A	115	0	0	2	0
4	B	179	0	0	6	0
4	C	134	0	0	9	0
4	D	98	0	0	5	0
All	All	14879	0	14172	392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 392 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)
2:B:502:EDO:H11	3:B:512:C8E:H13	1.34	1.08
2:C:501:EDO:H21	3:C:509:C8E:H81	1.36	1.02
2:B:502:EDO:H22	3:B:512:C8E:H32	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:HH21	1:B:203:LEU:HB3	1.25	0.98
1:D:56:THR:HG22	1:D:59:GLN:H	1.30	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/486 (90%)	410 (94%)	24 (6%)	3 (1%)	18	23
1	B	438/486 (90%)	413 (94%)	21 (5%)	4 (1%)	14	17
1	C	440/486 (90%)	415 (94%)	22 (5%)	3 (1%)	18	23
1	D	437/486 (90%)	412 (94%)	22 (5%)	3 (1%)	18	23
All	All	1752/1944 (90%)	1650 (94%)	89 (5%)	13 (1%)	18	23

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	ASP
1	B	247	ALA
1	B	249	ARG
1	D	247	ALA
1	B	485	ILE

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	397/424 (94%)	353 (89%)	44 (11%)	6	7
1	B	398/424 (94%)	361 (91%)	37 (9%)	8	11
1	C	400/424 (94%)	357 (89%)	43 (11%)	6	7
1	D	397/424 (94%)	353 (89%)	44 (11%)	6	7
All	All	1592/1696 (94%)	1424 (89%)	168 (11%)	6	8

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	430	LEU
1	D	219	SER
1	C	468	SER
1	D	67	THR
1	D	312	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	31	GLN
1	D	109	HIS
1	D	312	ASN
1	B	69	HIS
1	B	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

39 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	B	503	-	3,3,3	0.62	0	2,2,2	0.15	0
2	EDO	B	504	-	3,3,3	0.69	0	2,2,2	0.12	0
2	EDO	B	507	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	A	507	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.37	0
3	C8E	C	509	-	20,20,20	0.40	0	19,19,19	0.76	0
3	C8E	B	512	-	20,20,20	0.34	0	19,19,19	0.63	0
2	EDO	D	502	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	D	508	-	3,3,3	0.49	0	2,2,2	0.37	0
2	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	D	504	-	3,3,3	0.52	0	2,2,2	0.19	0
2	EDO	B	508	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	B	511	-	3,3,3	0.47	0	2,2,2	0.41	0
2	EDO	D	507	-	3,3,3	0.48	0	2,2,2	0.18	0
2	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.28	0
3	C8E	D	511	-	20,20,20	0.46	0	19,19,19	0.40	0
2	EDO	D	503	-	3,3,3	0.53	0	2,2,2	0.19	0
2	EDO	B	502	-	3,3,3	0.38	0	2,2,2	0.39	0
2	EDO	C	506	-	3,3,3	0.43	0	2,2,2	0.31	0
2	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.15	0
2	EDO	D	510	-	3,3,3	0.50	0	2,2,2	0.60	0
2	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	C	504	-	3,3,3	0.59	0	2,2,2	0.21	0
2	EDO	A	502	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	B	509	-	3,3,3	0.50	0	2,2,2	0.30	0
2	EDO	C	501	-	3,3,3	0.44	0	2,2,2	0.30	0
2	EDO	C	507	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.38	0
2	EDO	B	506	-	3,3,3	0.35	0	2,2,2	0.38	0
2	EDO	D	509	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	D	506	-	3,3,3	0.45	0	2,2,2	0.31	0
2	EDO	C	508	-	3,3,3	0.47	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	B	501	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	A	504	-	3,3,3	0.43	0	2,2,2	0.44	0
3	C8E	A	508	-	20,20,20	0.44	0	19,19,19	0.38	0
2	EDO	A	505	-	3,3,3	0.59	0	2,2,2	0.17	0
2	EDO	A	501	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	D	501	-	3,3,3	0.47	0	2,2,2	0.37	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
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	B	504	-	-	0/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
3	C8E	C	509	-	-	12/18/18/18	-
3	C8E	B	512	-	-	10/18/18/18	-
2	EDO	D	502	-	-	1/1/1/1	-
2	EDO	D	508	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	D	504	-	-	1/1/1/1	-
2	EDO	B	508	-	-	1/1/1/1	-
2	EDO	B	511	-	-	1/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	D	505	-	-	1/1/1/1	-
3	C8E	D	511	-	-	13/18/18/18	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	C	506	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	D	510	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	509	-	-	1/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	C	507	-	-	0/1/1/1	-
2	EDO	C	505	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	506	-	-	0/1/1/1	-
2	EDO	D	509	-	-	1/1/1/1	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	C	508	-	-	1/1/1/1	-
2	EDO	C	503	-	-	0/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
3	C8E	A	508	-	-	9/18/18/18	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	509	C8E	O9-C10-C11-O12
3	D	511	C8E	O12-C13-C14-O15
3	A	508	C8E	C6-C7-C8-O9
3	C	509	C8E	O18-C19-C20-O21
3	D	511	C8E	O18-C19-C20-O21

There are no ring outliers.

25 monomers are involved in 75 short contacts:

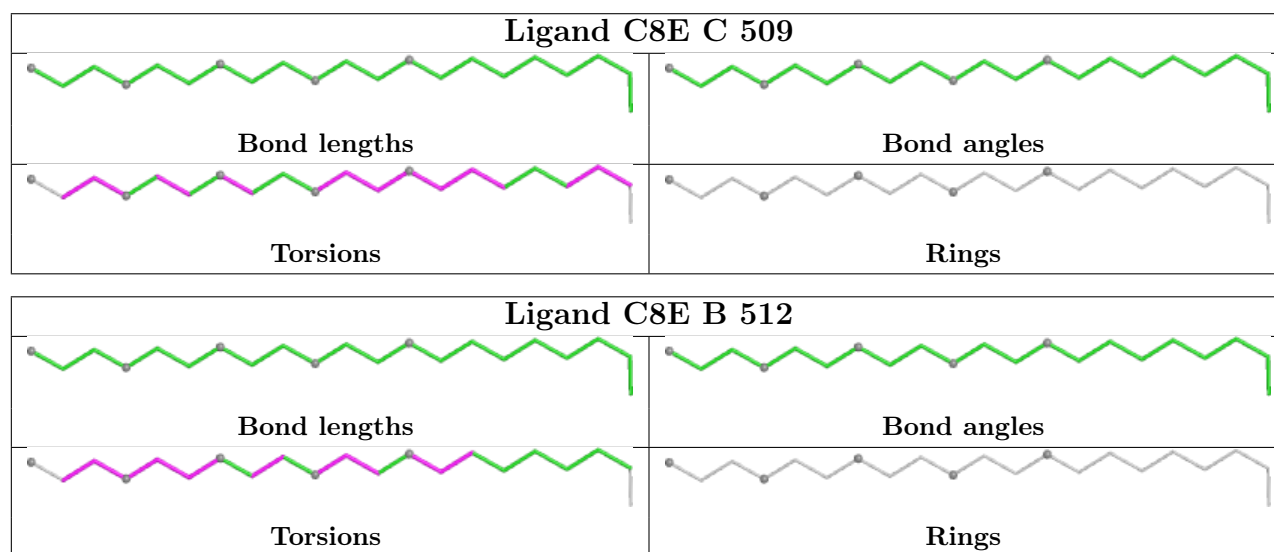
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	EDO	1	0
2	B	505	EDO	3	0
3	C	509	C8E	12	0
3	B	512	C8E	16	0
2	D	502	EDO	1	0
2	D	508	EDO	1	0
2	C	502	EDO	1	0
2	D	504	EDO	1	0
2	B	508	EDO	4	0
2	D	507	EDO	1	0
3	D	511	C8E	9	0
2	D	503	EDO	3	0

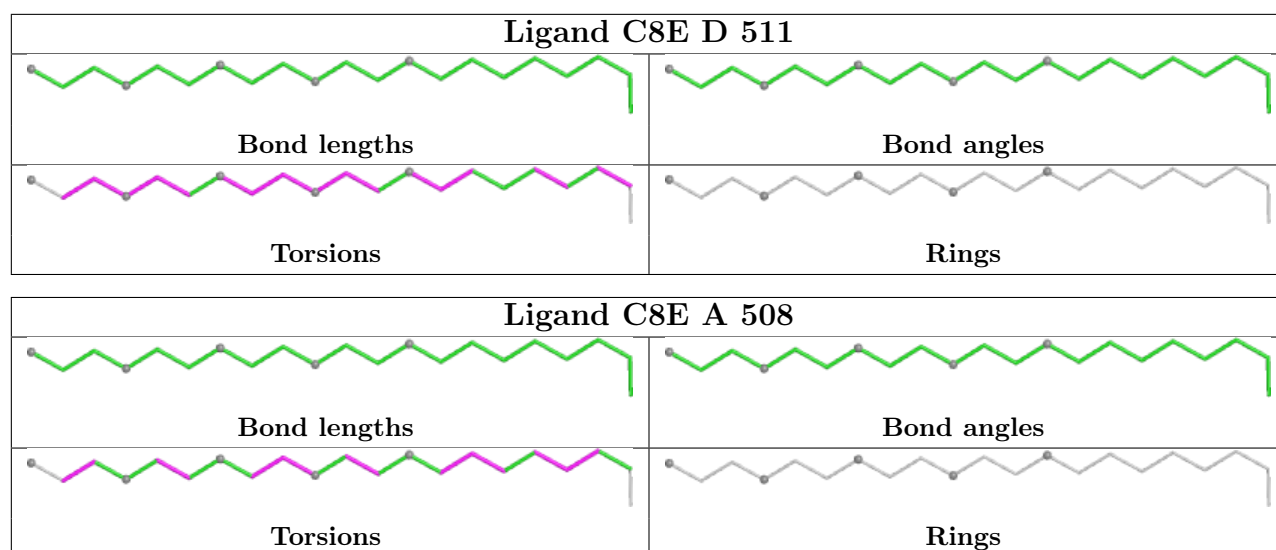
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	EDO	6	0
2	C	506	EDO	1	0
2	A	503	EDO	3	0
2	D	510	EDO	1	0
2	A	506	EDO	1	0
2	C	504	EDO	4	0
2	C	501	EDO	9	0
2	C	505	EDO	1	0
2	B	506	EDO	6	0
2	D	506	EDO	1	0
2	A	504	EDO	4	0
3	A	508	C8E	9	0
2	A	505	EDO	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/486 (89%)	0.49	23 (5%) 32 34	31, 53, 85, 153	1 (0%)
1	B	437/486 (89%)	0.27	13 (2%) 52 54	25, 44, 79, 139	1 (0%)
1	C	438/486 (90%)	0.46	29 (6%) 24 26	27, 50, 92, 144	2 (0%)
1	D	436/486 (89%)	0.62	23 (5%) 32 34	34, 56, 91, 133	1 (0%)
All	All	1747/1944 (89%)	0.46	88 (5%) 34 35	25, 51, 88, 153	5 (0%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	ILE	5.9
1	A	485	ILE	5.4
1	D	19	TRP	4.9
1	B	485	ILE	4.9
1	B	250	ALA	4.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

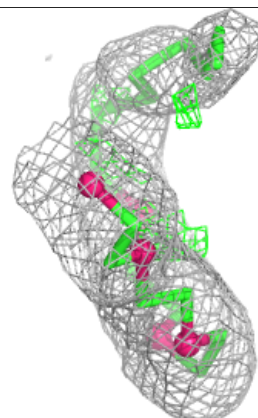
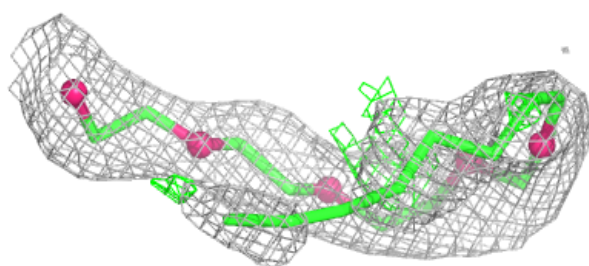
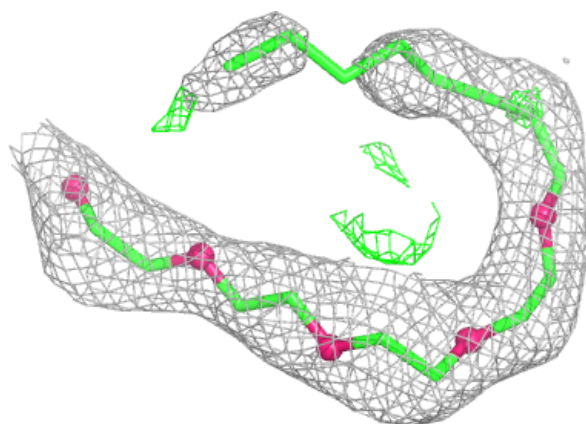
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	D	509	4/4	0.60	0.17	85,85,85,85	0
2	EDO	D	501	4/4	0.66	0.18	78,78,78,78	0
2	EDO	A	507	4/4	0.69	0.23	84,84,84,84	0
2	EDO	D	506	4/4	0.73	0.16	83,83,83,83	0
2	EDO	C	508	4/4	0.75	0.26	82,82,82,82	0
2	EDO	D	505	4/4	0.76	0.27	91,91,91,91	0
2	EDO	A	503	4/4	0.77	0.18	65,65,65,65	0
2	EDO	A	505	4/4	0.79	0.16	64,64,64,64	0
2	EDO	B	508	4/4	0.80	0.21	58,58,58,58	0
2	EDO	B	509	4/4	0.83	0.17	62,62,62,62	0
2	EDO	C	504	4/4	0.84	0.21	51,51,51,51	0
2	EDO	D	504	4/4	0.85	0.18	68,68,68,68	0
2	EDO	B	503	4/4	0.85	0.16	56,56,56,56	0
2	EDO	A	504	4/4	0.86	0.23	54,54,54,54	0
2	EDO	B	507	4/4	0.87	0.15	67,67,67,67	0
2	EDO	A	506	4/4	0.87	0.11	72,72,72,72	0
2	EDO	D	510	4/4	0.87	0.10	57,57,57,57	0
3	C8E	A	508	21/21	0.88	0.17	66,66,66,66	0
3	C8E	D	511	21/21	0.89	0.14	65,65,65,65	0
2	EDO	B	511	4/4	0.90	0.14	71,71,71,71	0
2	EDO	B	501	4/4	0.90	0.12	62,62,62,62	0
2	EDO	D	502	4/4	0.90	0.13	71,71,71,71	0
2	EDO	D	508	4/4	0.90	0.12	67,67,67,67	0
2	EDO	A	502	4/4	0.91	0.12	74,74,74,74	0
2	EDO	C	501	4/4	0.91	0.23	53,53,53,53	0
2	EDO	A	501	4/4	0.91	0.11	45,45,45,45	0
2	EDO	C	505	4/4	0.91	0.19	60,60,60,60	0
2	EDO	B	504	4/4	0.91	0.12	38,38,38,38	0
2	EDO	B	502	4/4	0.92	0.17	48,48,48,48	0
2	EDO	D	503	4/4	0.93	0.08	49,49,49,49	0
2	EDO	C	506	4/4	0.93	0.12	63,63,63,63	0
2	EDO	B	506	4/4	0.93	0.19	42,42,42,42	0
2	EDO	D	507	4/4	0.94	0.09	44,44,44,44	0
2	EDO	C	507	4/4	0.94	0.09	38,38,38,38	0
3	C8E	B	512	21/21	0.94	0.10	42,42,42,42	0
3	C8E	C	509	21/21	0.94	0.09	42,42,42,42	0
2	EDO	B	505	4/4	0.94	0.07	45,45,45,45	0
2	EDO	C	502	4/4	0.95	0.11	59,59,59,59	0
2	EDO	C	503	4/4	0.96	0.18	57,57,57,57	0

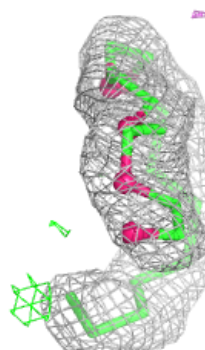
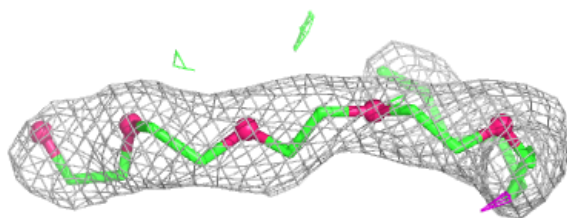
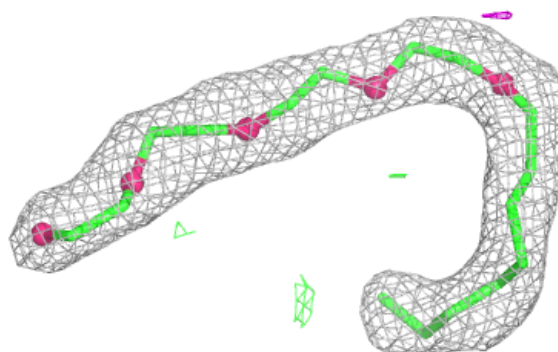
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E A 508:

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

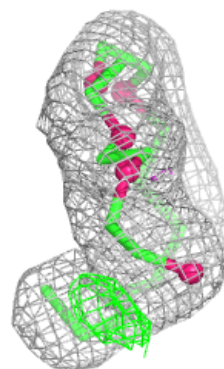
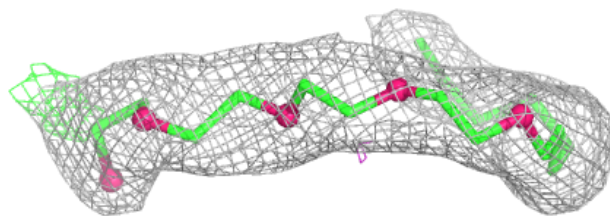
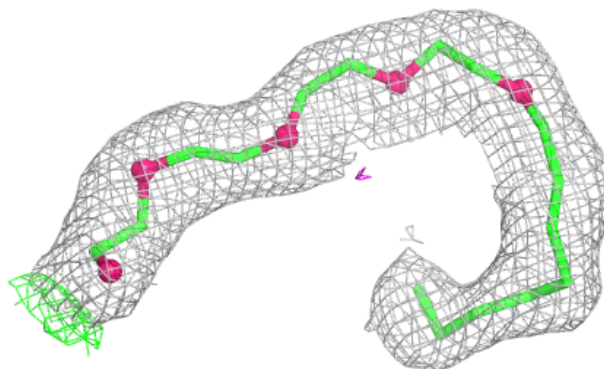
**Electron density around C8E D 511:**

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

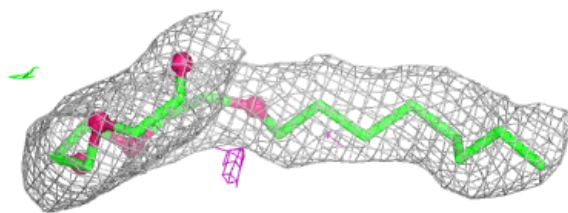
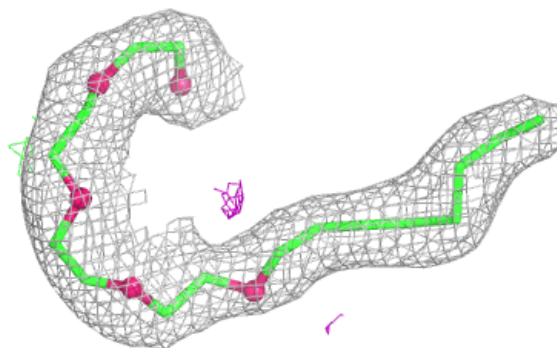


Electron density around C8E B 512:

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

**Electron density around C8E C 509:**

$2mF_o-DF_c$ (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.