



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 PM UTC

PDB ID : 7PYT / pdb_00007pyt
Title : Benzoylsuccinyl-CoA thiolase with coenzyme A
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Deposited on : 2021-10-11
Resolution : 1.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

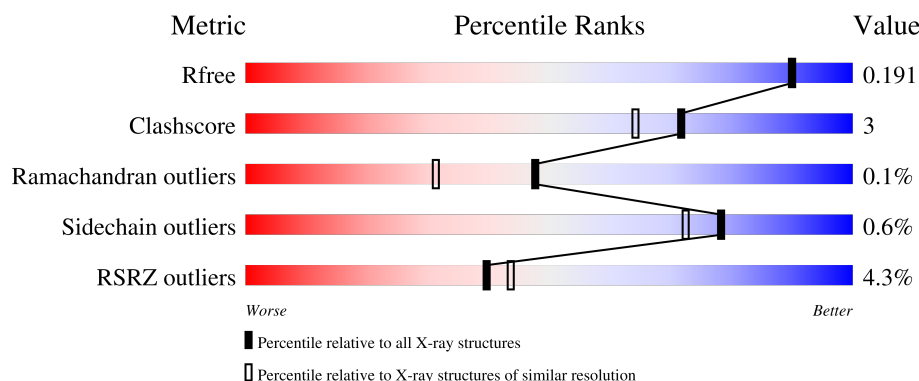
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	146	5% 86% 6% 8%
1	C	146	5% 88% • 9%
2	B	392	5% 94% 6%
2	D	392	3% 93% 6% •

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
4	PE8	A	202	-	-	X	-
7	COA	D	401	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8859 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 Benzoylsuccinyl-CoA thiolase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	1	0
			1099	707	175	209	8			
1	C	133	Total	C	N	O	S	0	2	0
			1102	709	178	206	9			

- Molecule 2 is a protein called Benzoylsuccinyl-CoA thiolase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	392	Total	C	N	O	S	0	12	0
			2960	1839	521	566	34			
2	D	392	Total	C	N	O	S	0	3	0
			2917	1812	516	557	32			

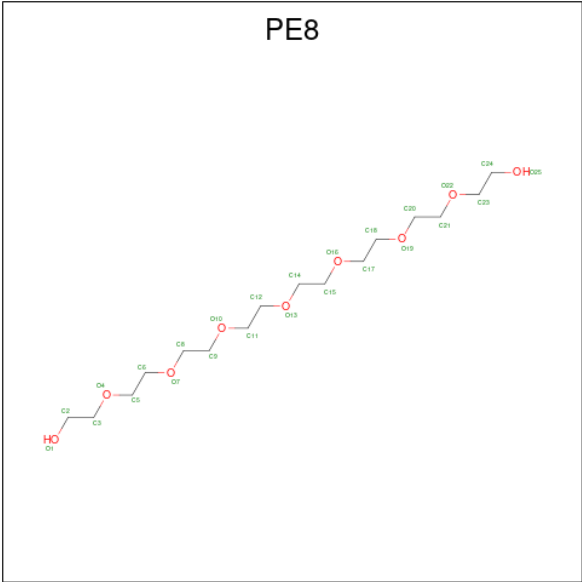
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	391	GLY	-	expression tag	UNP Q39VG1
B	392	SER	-	expression tag	UNP Q39VG1
D	391	GLY	-	expression tag	UNP Q39VG1
D	392	SER	-	expression tag	UNP Q39VG1

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

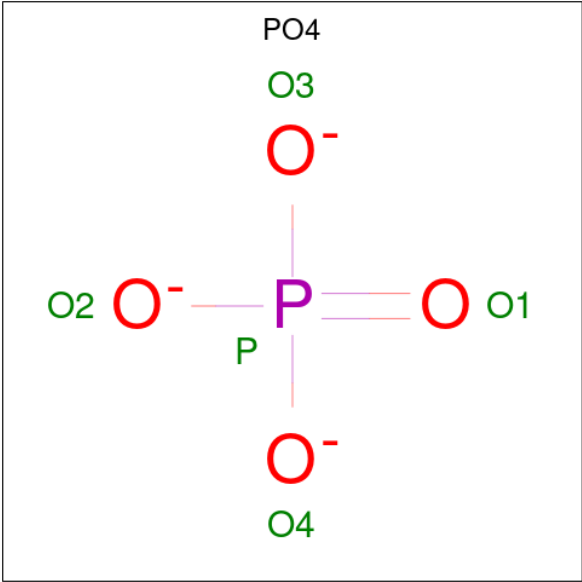
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	14	8		
4	B	1	Total	C	O	0	1
			22	14	8		
4	C	1	Total	C	O	0	0
			25	16	9		
4	D	1	Total	C	O	0	0
			22	14	8		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

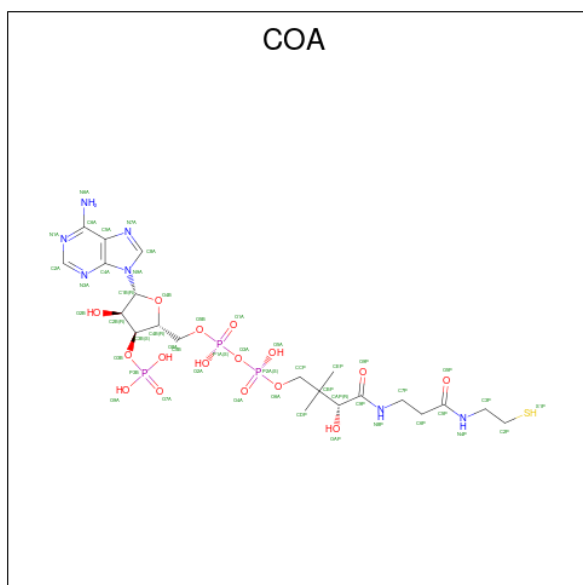


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).

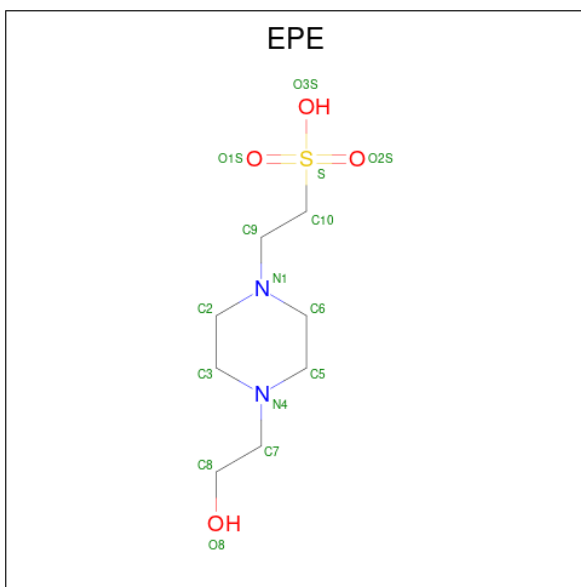


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

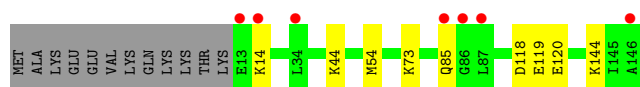
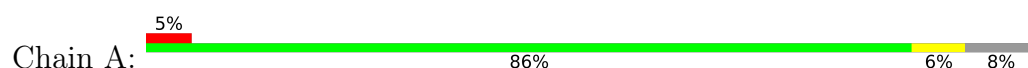
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	79	Total	O	0	0
			79	79		
10	B	226	Total	O	0	0
			226	226		
10	C	88	Total	O	0	1
			89	89		
10	D	217	Total	O	0	2
			219	219		

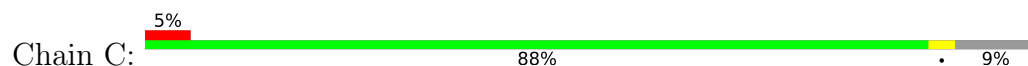
3 Residue-property plots [i](#)

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.

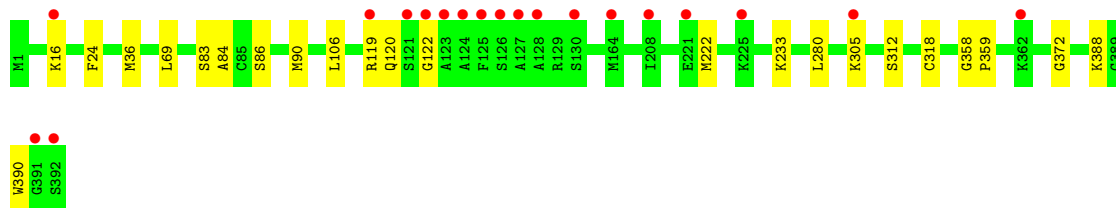
- Molecule 1: Benzoylsuccinyl-CoA thiolase subunit



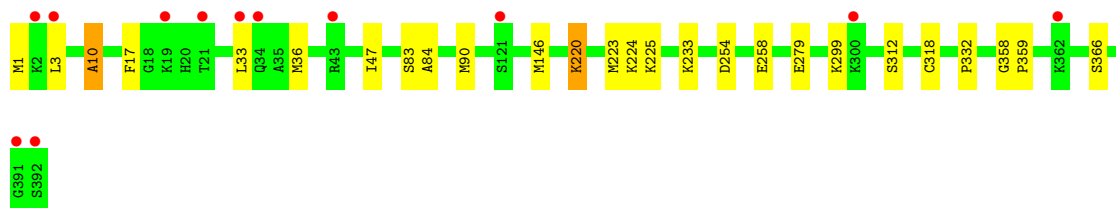
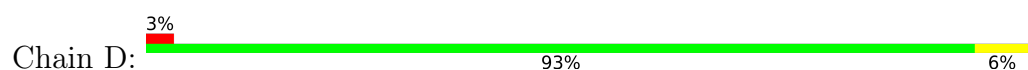
- Molecule 1: Benzoylsuccinyl-CoA thiolase subunit



- Molecule 2: Benzoylsuccinyl-CoA thiolase subunit



- Molecule 2: Benzoylsuccinyl-CoA thiolase subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.34Å 117.34Å 228.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 1.70 47.67 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.67-1.70) 99.9 (47.67-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.158 , 0.181 0.173 , 0.191	Depositor DCC
R_{free} test set	8656 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8859	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: CL, COA, PO4, MG, EPE, PE8, ZN

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	0.51	0/1126	0.70	0/1521
1	C	0.55	0/1129	0.74	0/1523
2	B	0.66	0/3013	0.82	4/4062 (0.1%)
2	D	0.66	1/2970 (0.0%)	0.82	4/4006 (0.1%)
All	All	0.62	1/8238 (0.0%)	0.80	8/11112 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	146	MET	C-O	-5.22	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	GLN	CB-CA-C	7.05	121.76	110.19
2	B	122	GLY	N-CA-C	-5.98	107.19	113.58
2	D	10	ALA	CA-C-N	5.80	126.46	120.60
2	D	10	ALA	C-N-CA	5.80	126.46	120.60
2	D	84	ALA	CB-CA-C	5.53	121.42	110.42
2	B	16	LYS	O-C-N	-5.49	116.38	122.86
2	D	10	ALA	CB-CA-C	5.23	120.84	110.42
2	B	84	ALA	CB-CA-C	5.14	120.66	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1099	0	1069	15	0
1	C	1102	0	1077	4	0
2	B	2960	0	2938	10	0
2	D	2917	0	2893	17	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	22	0	29	15	0
4	B	22	0	29	1	0
4	C	25	0	34	3	0
4	D	22	0	29	5	0
5	B	10	0	0	0	0
6	B	1	0	0	0	0
7	D	48	0	32	0	0
8	D	1	0	0	0	0
9	D	15	0	17	1	0
10	A	79	0	0	1	0
10	B	226	0	0	2	0
10	C	89	0	0	1	0
10	D	219	0	0	3	0
All	All	8859	0	8147	54	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 3.

All (54) 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:D:220:LYS:HE3	2:D:224:LYS:HE2	1.68	0.73
1:A:73:LYS:NZ	4:A:202:PE8:H141	2.05	0.72
4:A:202:PE8:H212	4:A:202:PE8:H22	1.73	0.70
1:A:120:GLU:CD	4:A:202:PE8:H171	2.22	0.65
4:C:202:PE8:H202	10:C:377:HOH:O	1.97	0.64
4:B:404[A]:PE8:H51	10:B:666:HOH:O	1.96	0.64
1:A:73:LYS:HZ3	4:A:202:PE8:H141	1.62	0.63
4:A:202:PE8:H62	4:A:202:PE8:H211	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:202:PE8:H22	4:A:202:PE8:C21	2.32	0.59
2:D:233:LYS:HZ3	4:D:403:PE8:H181	1.70	0.57
1:C:50:PHE:CD2	4:C:202:PE8:H231	2.40	0.56
2:D:233:LYS:NZ	4:D:403:PE8:H152	2.19	0.56
2:B:119:ARG:HG2	2:B:119:ARG:HH11	1.71	0.55
2:D:233:LYS:HZ1	4:D:403:PE8:H121	1.72	0.54
1:A:73:LYS:HZ3	4:A:202:PE8:H122	1.71	0.54
1:A:85:GLN:HA	1:A:85:GLN:OE1	2.08	0.52
1:A:73:LYS:HD3	4:A:202:PE8:H91	1.90	0.52
2:D:220:LYS:HE3	2:D:224:LYS:CE	2.40	0.51
2:D:233:LYS:HD2	4:D:403:PE8:H212	1.92	0.51
2:D:312:SER:HA	2:D:318:CYS:O	2.11	0.49
2:B:312:SER:HA	2:B:318:CYS:O	2.13	0.48
1:A:54:MET:HE1	2:D:33:LEU:HD21	1.94	0.48
2:B:24:PHE:C	2:B:24:PHE:CD1	2.92	0.48
2:D:254:ASP:O	2:D:258:GLU:HG3	2.14	0.47
1:A:118:ASP:HB3	4:A:202:PE8:H111	1.96	0.47
1:A:119:GLU:OE1	1:A:144:LYS:NZ	2.48	0.47
1:A:120:GLU:OE2	4:A:202:PE8:H171	2.14	0.47
2:B:83:SER:HB2	2:B:90:MET:SD	2.55	0.47
9:D:404:EPE:H32	9:D:404:EPE:H81	1.65	0.45
2:B:36[B]:MET:HE1	2:B:69:LEU:HD13	1.97	0.45
2:D:1:MET:HE3	2:D:3:LEU:HD23	1.98	0.45
2:D:83:SER:HB2	2:D:90:MET:SD	2.57	0.45
2:D:10:ALA:HB2	2:D:223:MET:SD	2.57	0.45
4:A:202:PE8:O22	4:A:202:PE8:H52	2.17	0.45
1:A:73:LYS:HZ3	4:A:202:PE8:C12	2.30	0.44
2:B:358:GLY:HA2	2:B:359:PRO:C	2.42	0.44
2:D:358:GLY:HA2	2:D:359:PRO:C	2.42	0.44
1:A:14:LYS:HD3	1:A:14:LYS:HA	1.85	0.44
2:B:106:LEU:HD13	2:B:222:MET:HG2	1.99	0.44
4:C:202:PE8:H211	10:D:592:HOH:O	2.17	0.44
2:D:233:LYS:HZ3	4:D:403:PE8:H152	1.84	0.43
1:A:44:LYS:NZ	10:A:305:HOH:O	2.51	0.43
1:C:85:GLN:CG	10:D:582:HOH:O	2.65	0.43
1:A:73:LYS:CE	4:A:202:PE8:H141	2.49	0.42
2:B:388:LYS:NZ	2:B:390:TRP:O	2.52	0.42
4:A:202:PE8:H62	4:A:202:PE8:C21	2.49	0.42
1:C:27:GLU:HB2	1:C:38:LYS:HD3	2.02	0.42
1:A:73:LYS:NZ	4:A:202:PE8:H122	2.35	0.42
2:D:279:GLU:O	2:D:366:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:MET:SD	2:D:47:ILE:HD12	2.59	0.41
2:D:17:PHE:CE2	2:D:332:PRO:HG2	2.55	0.41
2:B:233:LYS:NZ	10:B:515:HOH:O	2.54	0.40
1:C:85:GLN:HG2	10:D:582:HOH:O	2.21	0.40
2:B:280:LEU:C	2:B:280:LEU:HD12	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/146 (91%)	132 (99%)	1 (1%)	0	100	100
1	C	133/146 (91%)	128 (96%)	5 (4%)	0	100	100
2	B	398/392 (102%)	388 (98%)	9 (2%)	1 (0%)	36	22
2	D	393/392 (100%)	385 (98%)	8 (2%)	0	100	100
All	All	1057/1076 (98%)	1033 (98%)	23 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	372	GLY

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	122/132 (92%)	122 (100%)	0	100	100
1	C	122/132 (92%)	122 (100%)	0	100	100
2	B	310/302 (103%)	308 (99%)	2 (1%)	78	72
2	D	304/302 (101%)	301 (99%)	3 (1%)	68	58
All	All	858/868 (99%)	853 (99%)	5 (1%)	78	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	SER
2	B	305	LYS
2	D	220	LYS
2	D	225	LYS
2	D	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	GLN
1	C	47	GLN
2	D	120	GLN
2	D	192	ASN
2	D	204	GLN
2	D	281	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PE8	A	202	-	21,21,24	0.56	0	20,20,23	0.41	0
4	PE8	D	403	-	21,21,24	0.55	0	20,20,23	0.31	0
5	PO4	B	401	-	4,4,4	0.79	0	6,6,6	0.84	0
9	EPE	D	404	-	15,15,15	2.26	3 (20%)	19,20,20	2.81	8 (42%)
4	PE8	B	404[A]	-	21,21,24	0.58	0	20,20,23	0.36	0
7	COA	D	401	-	47,50,50	2.96	21 (44%)	69,75,75	1.88	12 (17%)
5	PO4	B	402	-	4,4,4	0.88	0	6,6,6	0.70	0
4	PE8	C	202	-	24,24,24	0.60	0	23,23,23	1.22	2 (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
4	PE8	A	202	-	-	12/19/19/22	-
4	PE8	D	403	-	-	12/19/19/22	-
9	EPE	D	404	-	-	4/9/19/19	0/1/1/1
4	PE8	B	404[A]	-	-	7/19/19/22	-
7	COA	D	401	-	1/1/11/13	2/48/64/64	0/3/3/3
4	PE8	C	202	-	-	14/22/22/22	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	401	COA	C2B-C3B	-11.81	1.27	1.53
9	D	404	EPE	C10-S	-7.26	1.67	1.77
7	D	401	COA	O4B-C1B	-5.68	1.28	1.42
7	D	401	COA	C5A-N7A	-4.67	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	401	COA	C8A-N9A	-4.63	1.29	1.37
7	D	401	COA	O9P-C9P	-4.46	1.14	1.23
7	D	401	COA	O5P-C5P	-4.32	1.14	1.23
7	D	401	COA	C6A-N6A	3.76	1.43	1.34
7	D	401	COA	P2A-O4A	-3.66	1.38	1.50
7	D	401	COA	C5P-N4P	3.46	1.41	1.33
7	D	401	COA	C9P-N8P	3.42	1.41	1.33
9	D	404	EPE	O1S-S	3.39	1.54	1.45
9	D	404	EPE	O2S-S	3.06	1.53	1.45
7	D	401	COA	C2B-C1B	2.99	1.62	1.53
7	D	401	COA	P2A-O5A	-2.82	1.42	1.55
7	D	401	COA	P1A-O2A	-2.75	1.42	1.55
7	D	401	COA	OAP-CAP	-2.65	1.37	1.42
7	D	401	COA	C4A-N9A	-2.53	1.32	1.37
7	D	401	COA	O4B-C4B	2.48	1.50	1.45
7	D	401	COA	O6A-CCP	-2.32	1.36	1.43
7	D	401	COA	C2A-N3A	-2.28	1.29	1.33
7	D	401	COA	C6A-N1A	-2.21	1.29	1.35
7	D	401	COA	P3B-O3B	2.10	1.63	1.59
7	D	401	COA	P1A-O1A	-2.08	1.43	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	404	EPE	O2S-S-C10	7.07	117.42	106.73
7	D	401	COA	C5A-C4A-N3A	-6.02	118.43	126.72
9	D	404	EPE	C7-N4-C5	-5.57	96.40	111.24
7	D	401	COA	C2B-C1B-N9A	5.07	125.89	113.30
9	D	404	EPE	O3S-S-C10	4.76	115.31	106.00
7	D	401	COA	C3B-C2B-C1B	4.38	109.52	99.89
7	D	401	COA	C4A-C5A-N7A	-4.14	105.85	110.58
7	D	401	COA	N3A-C2A-N1A	-4.08	122.41	128.58
7	D	401	COA	N3A-C4A-N9A	4.01	133.98	127.17
4	C	202	PE8	O1-C2-C3	4.00	135.35	111.82
7	D	401	COA	C2A-N3A-C4A	3.80	121.11	111.83
7	D	401	COA	C5A-N7A-C8A	3.79	109.40	103.45
9	D	404	EPE	O3S-S-O1S	-3.46	102.75	111.40
4	C	202	PE8	C5-O4-C3	2.96	126.21	113.26
7	D	401	COA	O2B-C2B-C1B	2.90	120.09	110.10
7	D	401	COA	N9A-C8A-N7A	-2.88	109.85	113.94
7	D	401	COA	C2P-C3P-N4P	-2.64	106.32	112.31
9	D	404	EPE	O3S-S-O2S	-2.56	104.99	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	COA	O3B-C3B-C2B	-2.22	103.71	111.68
9	D	404	EPE	C5-C6-N1	-2.20	106.21	110.65
9	D	404	EPE	C9-N1-C6	2.15	116.97	111.24
9	D	404	EPE	O2S-S-O1S	-2.05	107.17	113.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	401	COA	C2B

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	404	EPE	C10-C9-N1-C6
4	A	202	PE8	C2-C3-O4-C5
9	D	404	EPE	C8-C7-N4-C3
4	B	404[A]	PE8	O13-C14-C15-O16
4	C	202	PE8	O10-C11-C12-O13
4	A	202	PE8	O13-C14-C15-O16
4	C	202	PE8	O13-C14-C15-O16
4	C	202	PE8	O1-C2-C3-O4
4	C	202	PE8	O4-C5-C6-O7
4	B	404[A]	PE8	O10-C11-C12-O13
4	B	404[A]	PE8	O19-C20-C21-O22
4	B	404[A]	PE8	O1-C2-C3-O4
4	A	202	PE8	O16-C17-C18-O19
4	D	403	PE8	O4-C5-C6-O7
4	C	202	PE8	O19-C20-C21-O22
4	D	403	PE8	O7-C8-C9-O10
9	D	404	EPE	S-C10-C9-N1
4	A	202	PE8	O1-C2-C3-O4
4	A	202	PE8	O19-C20-C21-O22
4	D	403	PE8	O19-C20-C21-O22
9	D	404	EPE	C10-C9-N1-C2
4	C	202	PE8	O16-C17-C18-O19
4	A	202	PE8	O4-C5-C6-O7
4	D	403	PE8	C12-C11-O10-C9
4	D	403	PE8	C21-C20-O19-C18
4	B	404[A]	PE8	C5-C6-O7-C8
4	D	403	PE8	C8-C9-O10-C11
4	A	202	PE8	C8-C9-O10-C11
4	B	404[A]	PE8	C11-C12-O13-C14

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Mol	Chain	Res	Type	Atoms
4	C	202	PE8	C17-C18-O19-C20
4	D	403	PE8	O10-C11-C12-O13
4	C	202	PE8	C20-C21-O22-C23
4	C	202	PE8	C2-C3-O4-C5
4	D	403	PE8	O16-C17-C18-O19
4	C	202	PE8	C18-C17-O16-C15
4	A	202	PE8	C9-C8-O7-C6
4	C	202	PE8	C15-C14-O13-C12
4	A	202	PE8	C12-C11-O10-C9
4	C	202	PE8	C14-C15-O16-C17
4	A	202	PE8	C15-C14-O13-C12
4	B	404[A]	PE8	C18-C17-O16-C15
4	D	403	PE8	C2-C3-O4-C5
7	D	401	COA	C3B-O3B-P3B-O7A
4	D	403	PE8	C15-C14-O13-C12
4	D	403	PE8	C6-C5-O4-C3
4	D	403	PE8	O13-C14-C15-O16
4	C	202	PE8	C11-C12-O13-C14
7	D	401	COA	P1A-O3A-P2A-O5A
4	C	202	PE8	C24-C23-O22-C21
4	A	202	PE8	O10-C11-C12-O13
4	A	202	PE8	O7-C8-C9-O10

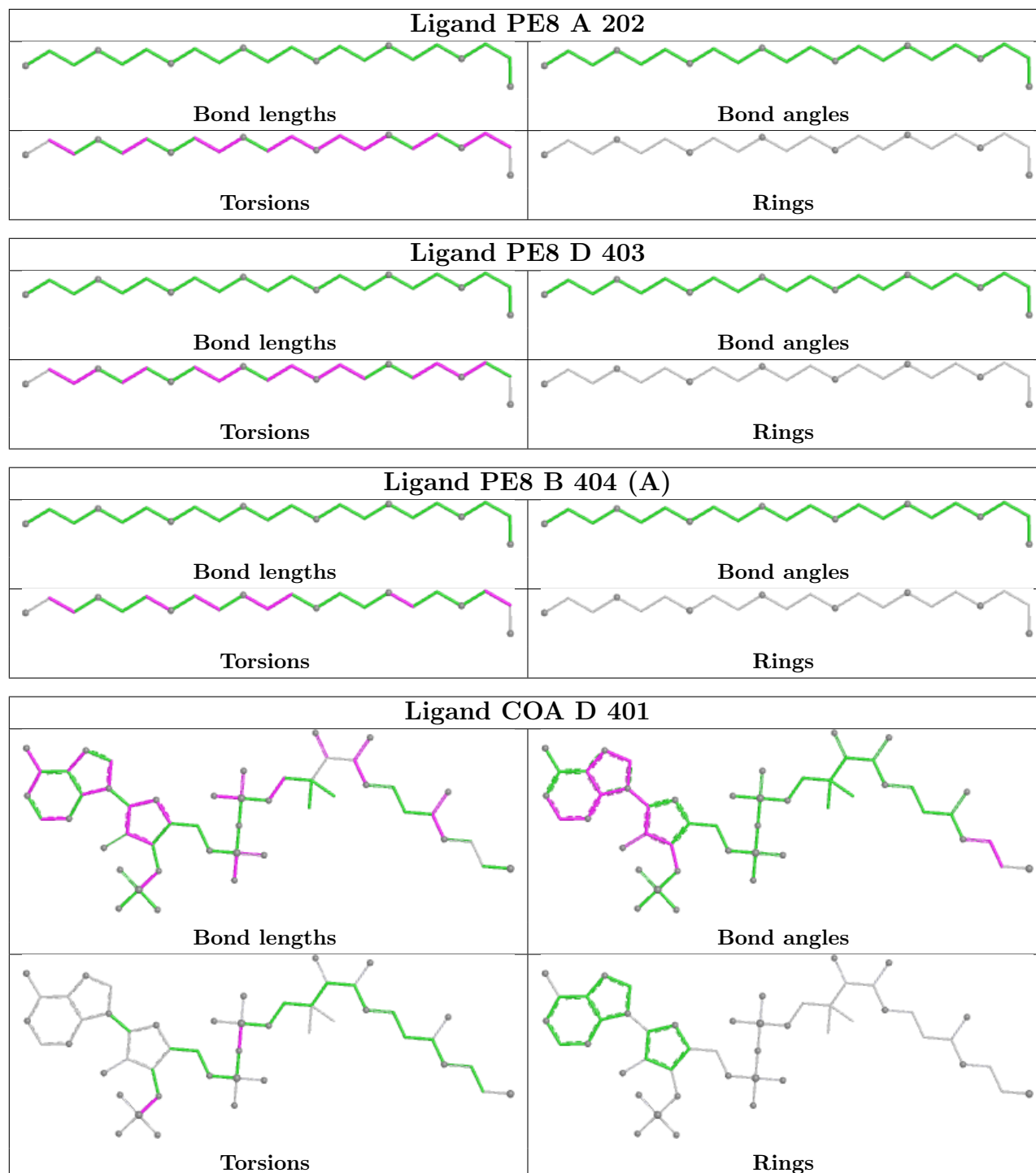
There are no ring outliers.

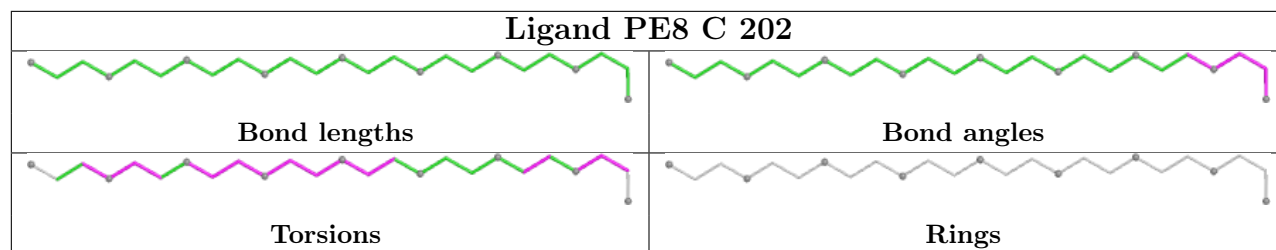
5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	202	PE8	15	0
4	D	403	PE8	5	0
9	D	404	EPE	1	0
4	B	404[A]	PE8	1	0
4	C	202	PE8	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	134/146 (91%)	0.53	7 (5%) 33 36	22, 45, 71, 107	1 (0%)
1	C	133/146 (91%)	0.41	7 (5%) 32 35	18, 41, 82, 115	2 (1%)
2	B	392/392 (100%)	0.02	19 (4%) 35 39	14, 32, 56, 112	8 (2%)
2	D	392/392 (100%)	0.07	12 (3%) 51 55	16, 34, 57, 109	3 (0%)
All	All	1051/1076 (97%)	0.15	45 (4%) 40 44	14, 35, 65, 115	14 (1%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	391	GLY	6.2
1	A	146	ALA	5.9
2	D	392	SER	5.5
2	B	123	ALA	5.2
1	C	146	ALA	5.1
2	B	124	ALA	4.7
2	B	130	SER	4.1
2	B	391	GLY	4.0
2	B	392	SER	4.0
2	B	125	PHE	3.8
2	B	122	GLY	3.7
2	B	127	ALA	3.7
1	C	14	LYS	3.6
2	B	126	SER	3.3
1	A	14	LYS	3.3
2	B	225	LYS	3.1
1	C	31	ASP	3.1
2	B	305	LYS	3.0
2	B	121	SER	2.9
1	A	13	GLU	2.9
2	B	128	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	19	LYS	2.8
2	D	34	GLN	2.7
1	A	87	LEU	2.7
1	C	73	LYS	2.6
2	D	300	LYS	2.6
2	B	362	LYS	2.6
2	D	2	LYS	2.6
2	D	21	THR	2.5
2	D	121	SER	2.4
2	B	16	LYS	2.3
2	D	362	LYS	2.3
2	B	164[A]	MET	2.3
1	C	70[A]	ARG	2.3
1	A	34	LEU	2.3
2	D	3	LEU	2.2
2	B	221	GLU	2.2
1	A	86	GLY	2.2
2	D	43	ARG	2.2
1	A	85	GLN	2.1
2	B	208	ILE	2.1
1	C	34	LEU	2.1
2	D	33	LEU	2.1
1	C	134	ASN	2.0
2	B	119	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

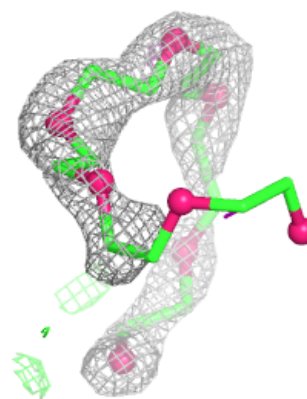
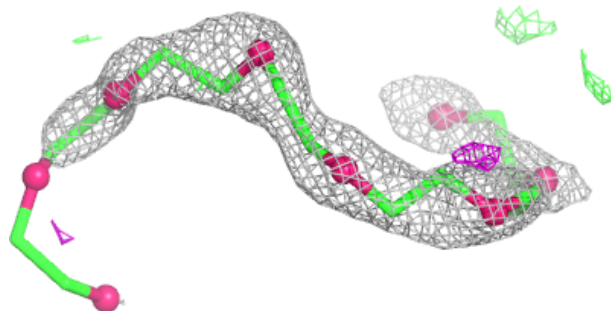
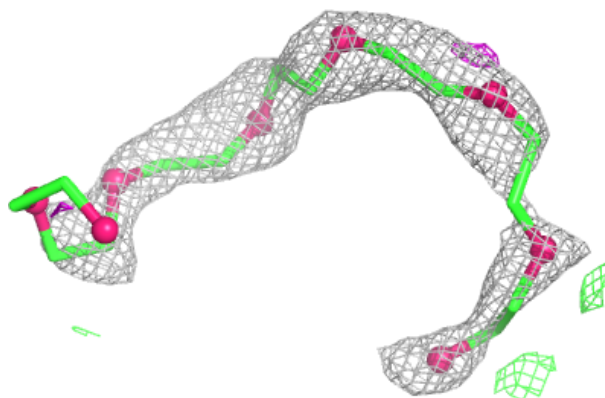
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EPE	D	404	15/15	0.78	0.25	82,103,110,110	0
4	PE8	D	403	22/25	0.79	0.20	74,80,99,111	0
5	PO4	B	402	5/5	0.84	0.11	69,75,87,111	0
4	PE8	C	202	25/25	0.84	0.24	43,64,83,104	0
4	PE8	A	202	22/25	0.87	0.18	62,74,100,114	0
5	PO4	B	401	5/5	0.88	0.13	67,67,82,87	0
4	PE8	B	404[A]	22/25	0.94	0.22	64,67,71,71	22
7	COA	D	401	48/48	0.96	0.09	27,37,89,92	0
8	CL	D	402	1/1	0.97	0.11	53,53,53,53	0
6	MG	B	403	1/1	0.98	0.18	44,44,44,44	0
3	ZN	A	201	1/1	0.99	0.04	36,36,36,36	0
3	ZN	C	201	1/1	0.99	0.03	31,31,31,31	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.

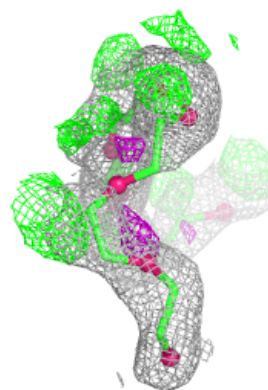
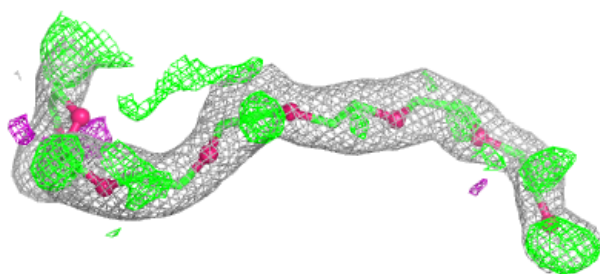
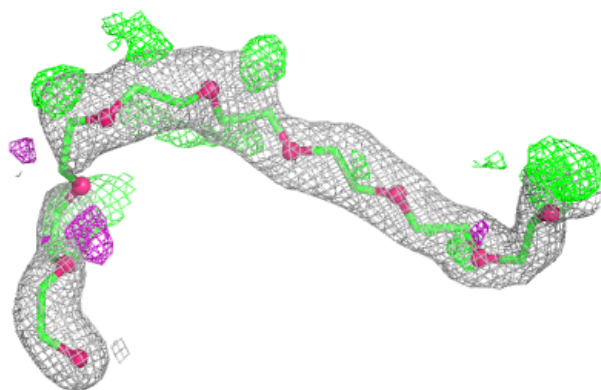
Electron density around PE8 D 403:

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



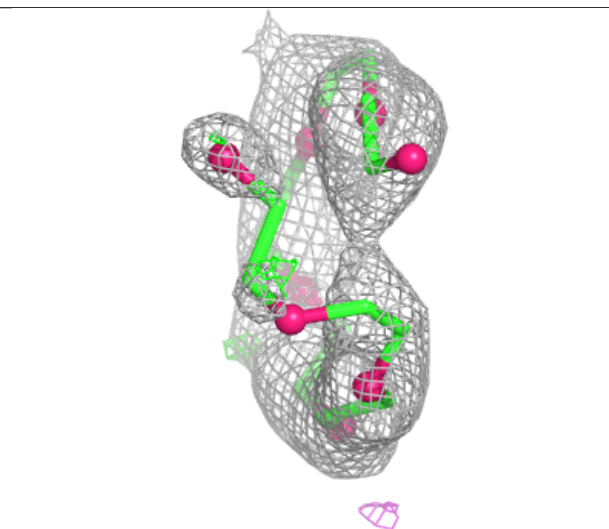
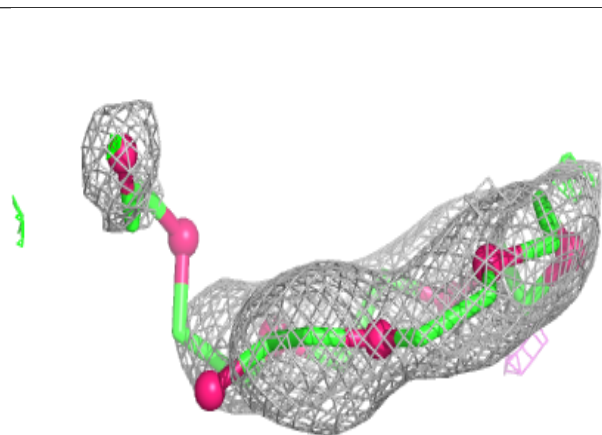
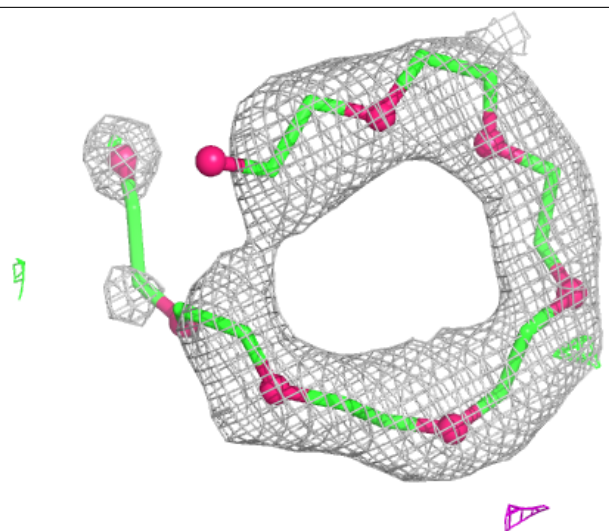
Electron density around PE8 C 202:

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



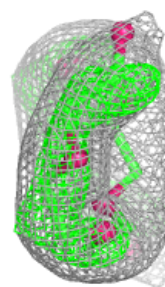
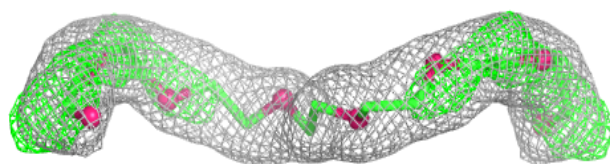
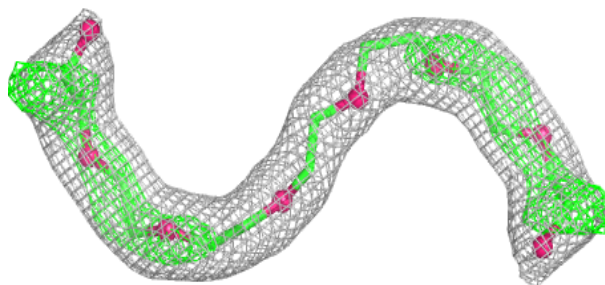
Electron density around PE8 A 202:

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

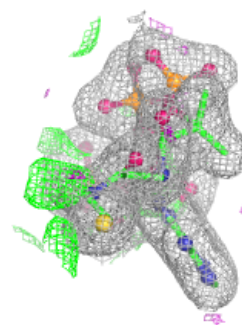
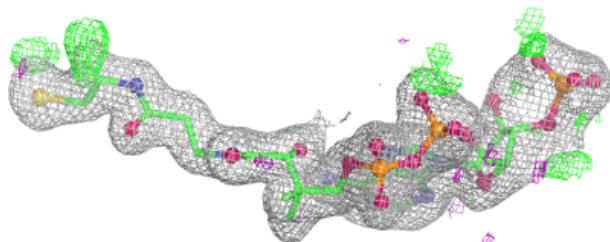
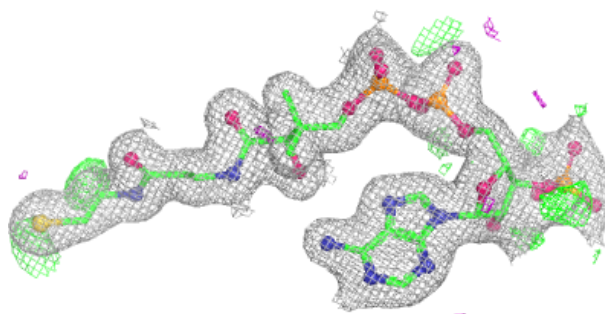


Electron density around PE8 B 404 (A):

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

**Electron density around COA D 401:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.