



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:30 PM UTC

PDB ID : 9FOL / pdb\_00009fol  
Title : Succinyl-CoA:(R)-benzylsuccinate CoA-transferase (BbsEF), D178-CoA adduct + succinate (weakly occupied)  
Authors : Ermler, U.; Heider, J.; Demmer, U.  
Deposited on : 2024-06-12  
Resolution : 1.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

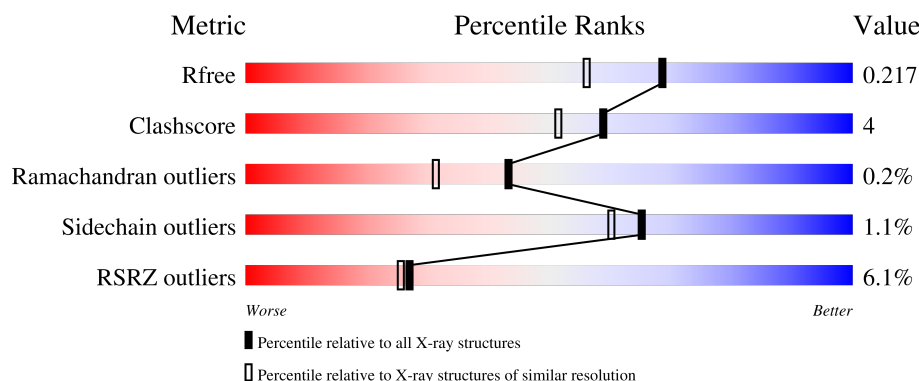
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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  $\geq 3$ , 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	410	<div> <div>2%</div> <div>93%</div> <div>6%</div> </div>
1	C	410	<div> <div>13%</div> <div>89%</div> <div>9%</div> </div>
2	B	409	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
2	D	409	<div> <div>3%</div> <div>92%</div> <div>7%</div> </div>

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	PGE	D	506	-	X	-	-
7	SIN	D	509	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13732 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.

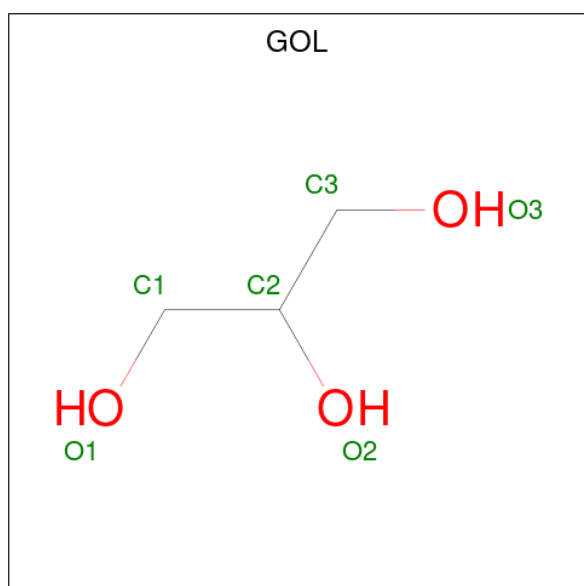
- Molecule 1 is a protein called Subunit of Benzylsuccinate CoA-transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	6	0
			3202	2016	573	598	15			
1	C	408	Total	C	N	O	S	0	5	0
			3220	2026	578	601	15			

- Molecule 2 is a protein called Subunit of Benzylsuccinate CoA-transferase.

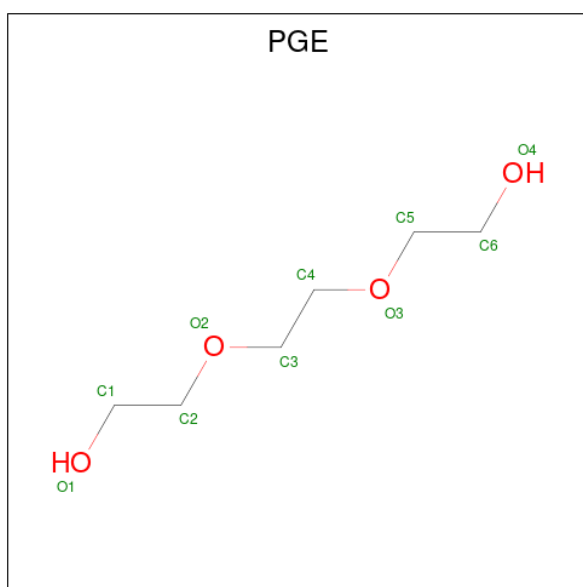
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	4	0
			3147	1976	566	588	17			
2	D	405	Total	C	N	O	S	0	7	0
			3156	1985	565	588	18			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



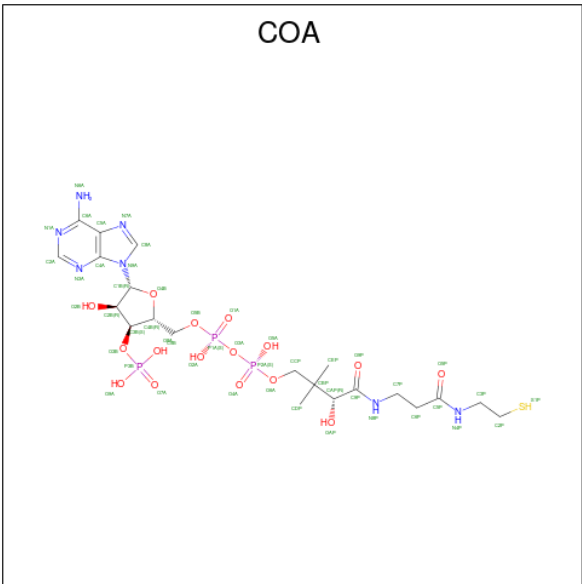
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



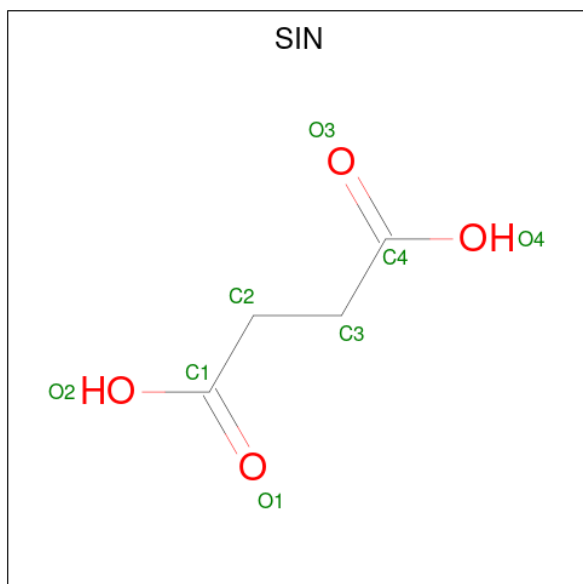
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is SUCCINIC ACID (CCD ID: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 8 is water.

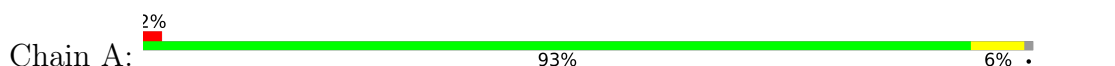
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	180	Total 181	O 181	0	1
8	B	172	Total 172	O 172	0	0
8	C	188	Total 190	O 190	0	2
8	D	218	Total 218	O 218	0	0



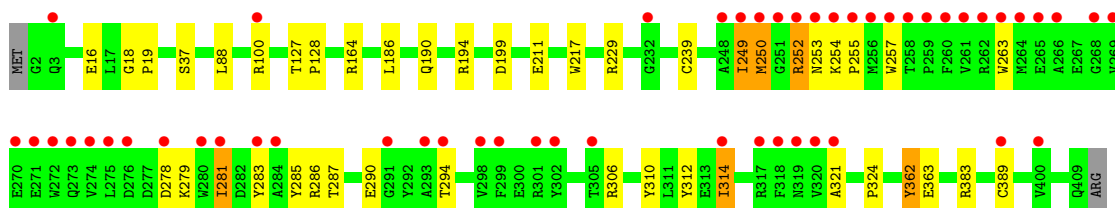
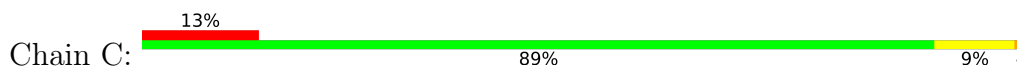
### 3 Residue-property plots [i](#)

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.

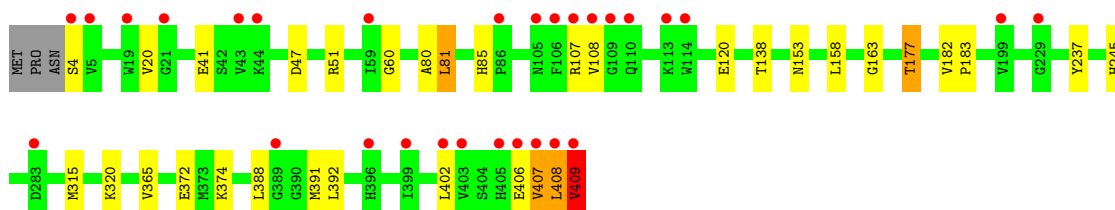
- Molecule 1: Subunit of Benzylsuccinate CoA-transferase



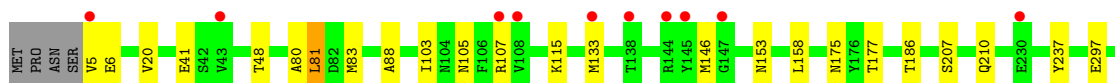
- Molecule 1: Subunit of Benzylsuccinate CoA-transferase



- Molecule 2: Subunit of Benzylsuccinate CoA-transferase



- Molecule 2: Subunit of Benzylsuccinate CoA-transferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.21Å 100.63Å 192.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 1.80 48.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.67-1.80) 94.8 (48.67-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.183 , 0.213 0.189 , 0.217	Depositor DCC
$R_{free}$ test set	7849 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIN, GOL, TRS, COA, PGE

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	0.28	0/3289	0.49	0/4461
1	C	0.46	6/3304 (0.2%)	0.66	7/4481 (0.2%)
2	B	0.37	5/3227 (0.2%)	0.58	5/4379 (0.1%)
2	D	0.29	0/3245	0.50	0/4403
All	All	0.36	11/13065 (0.1%)	0.56	12/17724 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	217	TRP	C-O	-7.82	1.15	1.24
2	B	408	LEU	C-O	-7.40	1.14	1.23
2	B	81	LEU	C-O	-7.32	1.15	1.24
1	C	255	PRO	N-CA	6.04	1.55	1.47
1	C	253	ASN	CA-C	5.87	1.60	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	LYS	O-C-N	-9.65	111.46	120.92
1	C	253	ASN	CA-C-N	8.58	130.26	120.06
1	C	253	ASN	C-N-CA	8.58	130.26	120.06
2	B	408	LEU	CA-C-N	8.01	136.11	121.70
2	B	408	LEU	C-N-CA	8.01	136.11	121.70

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	3202	0	3072	12	0
1	C	3220	0	3090	32	0
2	B	3147	0	3082	36	0
2	D	3156	0	3101	29	0
3	A	12	0	15	0	0
3	B	12	0	16	0	0
3	C	18	0	23	3	0
3	D	24	0	31	2	0
4	A	10	0	14	0	0
4	B	10	0	14	3	0
4	C	20	0	28	9	0
4	D	20	0	25	0	0
5	B	48	0	31	6	0
5	D	48	0	30	5	0
6	B	8	0	11	0	0
6	D	8	0	11	0	0
7	D	8	0	4	1	0
8	A	181	0	0	0	0
8	B	172	0	0	1	0
8	C	190	0	0	2	0
8	D	218	0	0	3	0
All	All	13732	0	12598	113	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 4.

The worst 5 of 113 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:107:ARG:HD3	5:B:502:COA:O1A	1.73	0.88
2:B:409:VAL:CG1	2:B:409:VAL:OXT	2.28	0.81
1:C:37:SER:HB3	4:C:602:PGE:H22	1.62	0.81
2:B:153:ASN:OD1	2:B:177[A]:THR:HG23	1.82	0.80
2:B:107:ARG:CD	5:B:502:COA:O1A	2.32	0.78

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	408/410 (100%)	399 (98%)	8 (2%)	1 (0%)	43	31
1	C	411/410 (100%)	401 (98%)	9 (2%)	1 (0%)	43	31
2	B	408/409 (100%)	401 (98%)	6 (2%)	1 (0%)	43	31
2	D	410/409 (100%)	403 (98%)	6 (2%)	1 (0%)	43	31
All	All	1637/1638 (100%)	1604 (98%)	29 (2%)	4 (0%)	43	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20	VAL
1	A	211	GLU
2	D	20	VAL
1	C	211	GLU

### 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	319/317 (101%)	315 (99%)	4 (1%)	61	54
1	C	320/317 (101%)	313 (98%)	7 (2%)	45	34
2	B	321/320 (100%)	318 (99%)	3 (1%)	70	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	323/320 (101%)	321 (99%)	2 (1%)	78	77
All	All	1283/1274 (101%)	1267 (99%)	16 (1%)	65	57

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	5	VAL
1	C	362[B]	TYR
1	C	249	ILE
1	C	362[A]	TYR
1	C	100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	374	ASN
2	D	235	GLN
2	B	401	ASN
1	C	346	GLN
1	C	354	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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
6	TRS	B	503	-	7,7,7	1.23	0	9,9,9	0.93	1 (11%)
3	GOL	C	604	-	5,5,5	1.16	0	5,5,5	1.88	1 (20%)
3	GOL	C	603	-	5,5,5	1.40	1 (20%)	5,5,5	1.63	1 (20%)
4	PGE	C	601	-	9,9,9	0.64	0	8,8,8	1.34	1 (12%)
4	PGE	A	702	-	9,9,9	0.40	0	8,8,8	0.96	0
5	COA	D	503	2	47,50,50	3.52	16 (34%)	69,75,75	1.85	16 (23%)
3	GOL	A	701	-	5,5,5	0.80	0	5,5,5	1.13	0
4	PGE	D	506	-	9,9,9	1.88	3 (33%)	8,8,8	1.34	2 (25%)
3	GOL	A	703	-	5,5,5	0.82	0	5,5,5	0.62	0
4	PGE	B	505	-	9,9,9	0.47	0	8,8,8	1.34	1 (12%)
4	PGE	C	602	-	9,9,9	0.45	0	8,8,8	1.23	1 (12%)
3	GOL	C	605	-	5,5,5	0.62	0	5,5,5	0.64	0
5	COA	B	502	2	47,50,50	2.46	13 (27%)	69,75,75	2.46	24 (34%)
7	SIN	D	509	-	7,7,7	1.33	1 (14%)	8,8,8	1.95	3 (37%)
3	GOL	D	507	-	5,5,5	0.81	0	5,5,5	0.92	0
3	GOL	B	501	-	5,5,5	0.87	0	5,5,5	1.08	0
3	GOL	B	504	-	5,5,5	0.77	0	5,5,5	1.03	0
3	GOL	D	508	-	5,5,5	0.71	0	5,5,5	1.05	0
6	TRS	D	504	-	7,7,7	1.22	0	9,9,9	0.83	0
4	PGE	D	505	-	9,9,9	1.14	1 (11%)	8,8,8	1.30	0
3	GOL	D	501	-	5,5,5	0.70	0	5,5,5	0.92	0
3	GOL	D	502	-	5,5,5	1.74	2 (40%)	5,5,5	1.65	1 (20%)

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
6	TRS	B	503	-	-	2/9/9/9	-
3	GOL	C	604	-	-	2/4/4/4	-
3	GOL	C	603	-	-	1/4/4/4	-
4	PGE	C	601	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	702	-	-	6/7/7/7	-
5	COA	D	503	2	-	17/48/64/64	0/3/3/3
3	GOL	A	701	-	-	2/4/4/4	-
4	PGE	D	506	-	-	6/7/7/7	-
3	GOL	A	703	-	-	2/4/4/4	-
4	PGE	B	505	-	-	5/7/7/7	-
4	PGE	C	602	-	-	6/7/7/7	-
3	GOL	C	605	-	-	4/4/4/4	-
5	COA	B	502	2	-	14/48/64/64	0/3/3/3
7	SIN	D	509	-	-	5/5/5/5	-
3	GOL	D	507	-	-	2/4/4/4	-
3	GOL	B	501	-	-	0/4/4/4	-
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	D	508	-	-	4/4/4/4	-
6	TRS	D	504	-	-	0/9/9/9	-
4	PGE	D	505	-	-	5/7/7/7	-
3	GOL	D	501	-	-	0/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	COA	C3B-C4B	-9.95	1.27	1.52
5	D	503	COA	C2B-C1B	-9.11	1.24	1.53
5	D	503	COA	O4B-C1B	8.38	1.61	1.42
5	D	503	COA	C2B-C3B	7.46	1.69	1.53
5	B	502	COA	P1A-O3A	7.34	1.67	1.59

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	COA	O5P-C5P-N4P	-7.40	108.52	123.03
5	B	502	COA	C6P-C5P-N4P	6.64	128.45	116.34
5	B	502	COA	C7P-N8P-C9P	5.68	132.74	122.55
5	B	502	COA	C5A-C4A-N3A	-5.66	118.93	126.72
5	D	503	COA	C7P-C6P-C5P	5.02	120.76	112.39

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

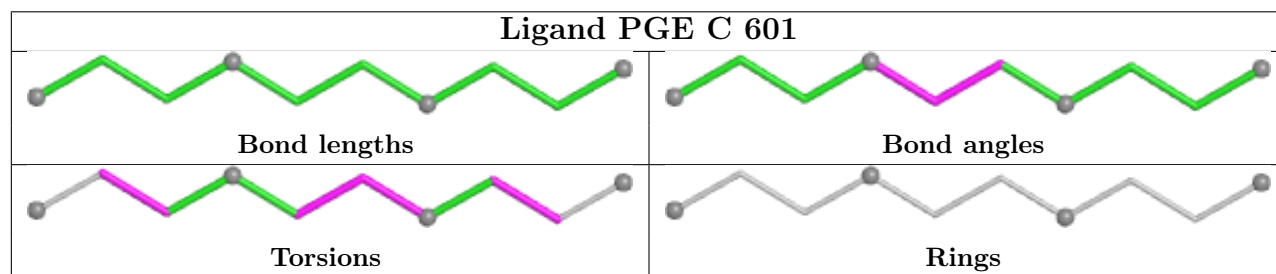
Mol	Chain	Res	Type	Atoms
3	A	703	GOL	O1-C1-C2-C3
3	C	604	GOL	C1-C2-C3-O3
3	C	605	GOL	O1-C1-C2-O2
3	C	605	GOL	O1-C1-C2-C3
3	C	605	GOL	C1-C2-C3-O3

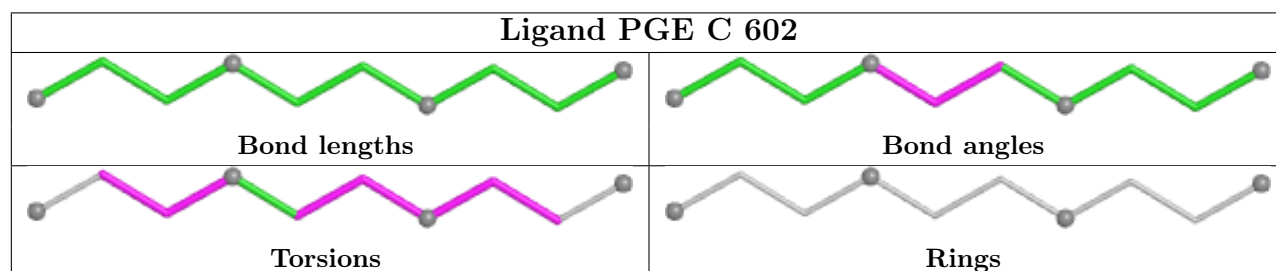
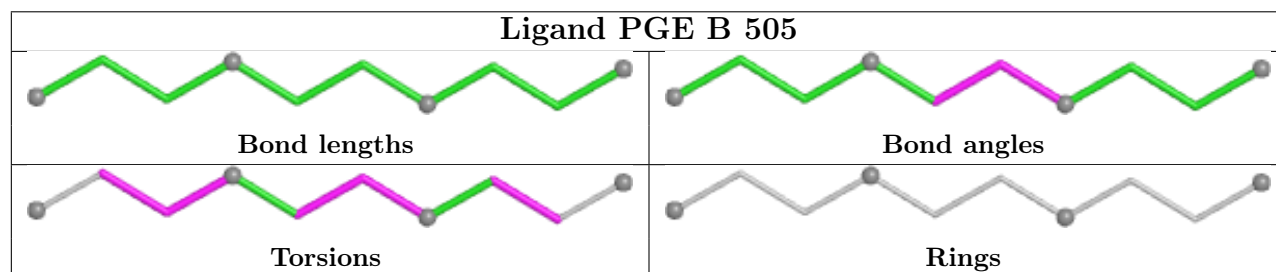
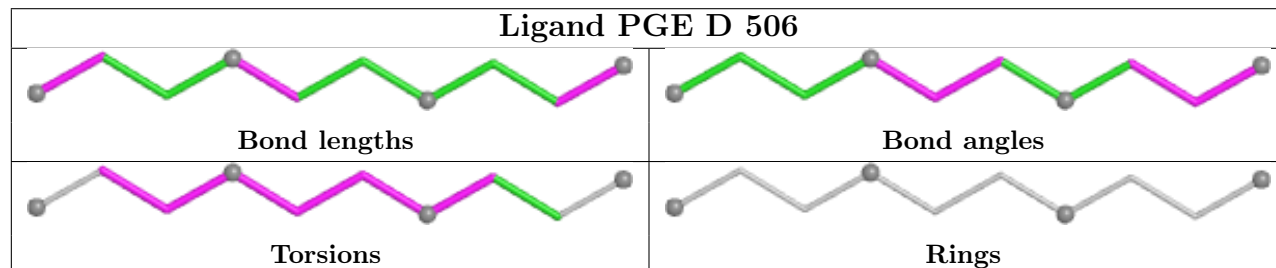
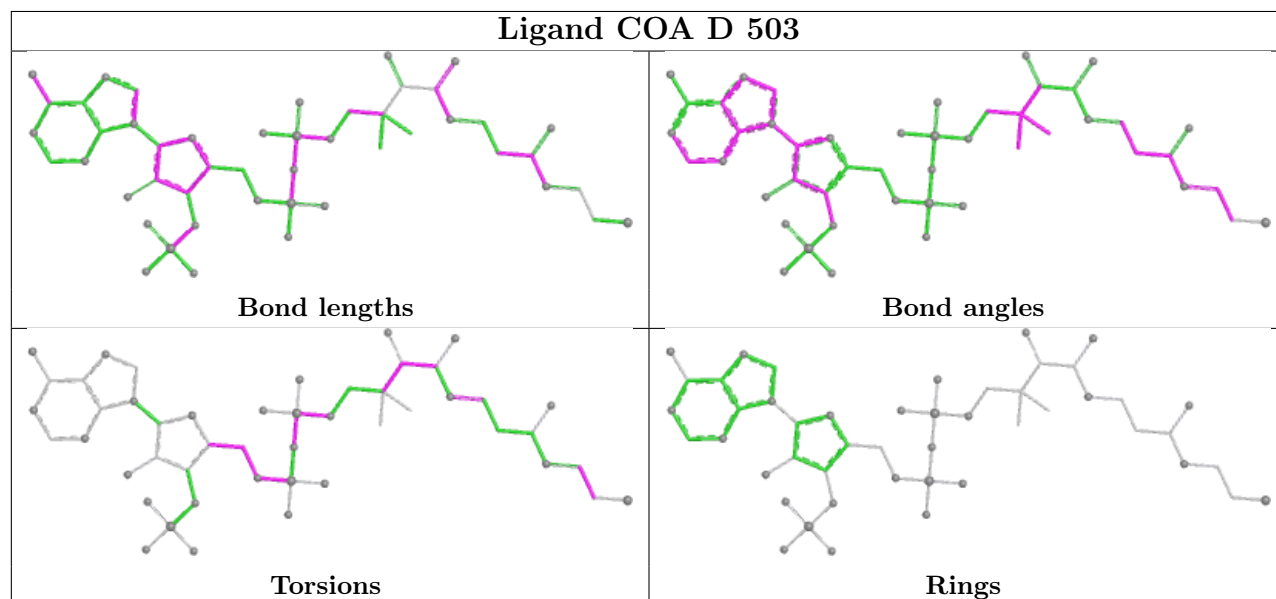
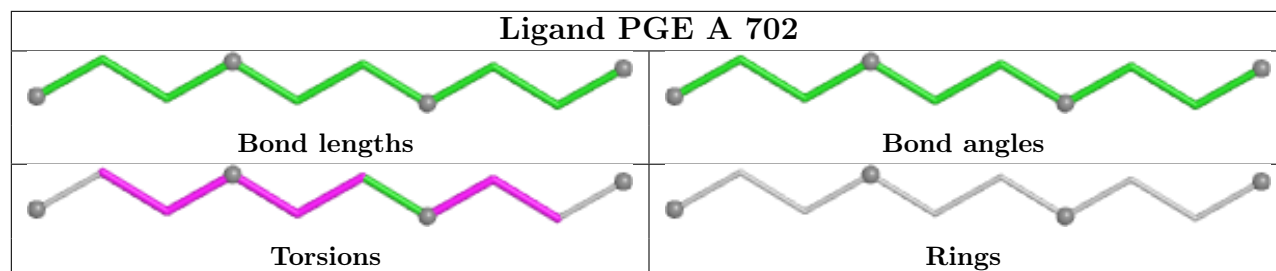
There are no ring outliers.

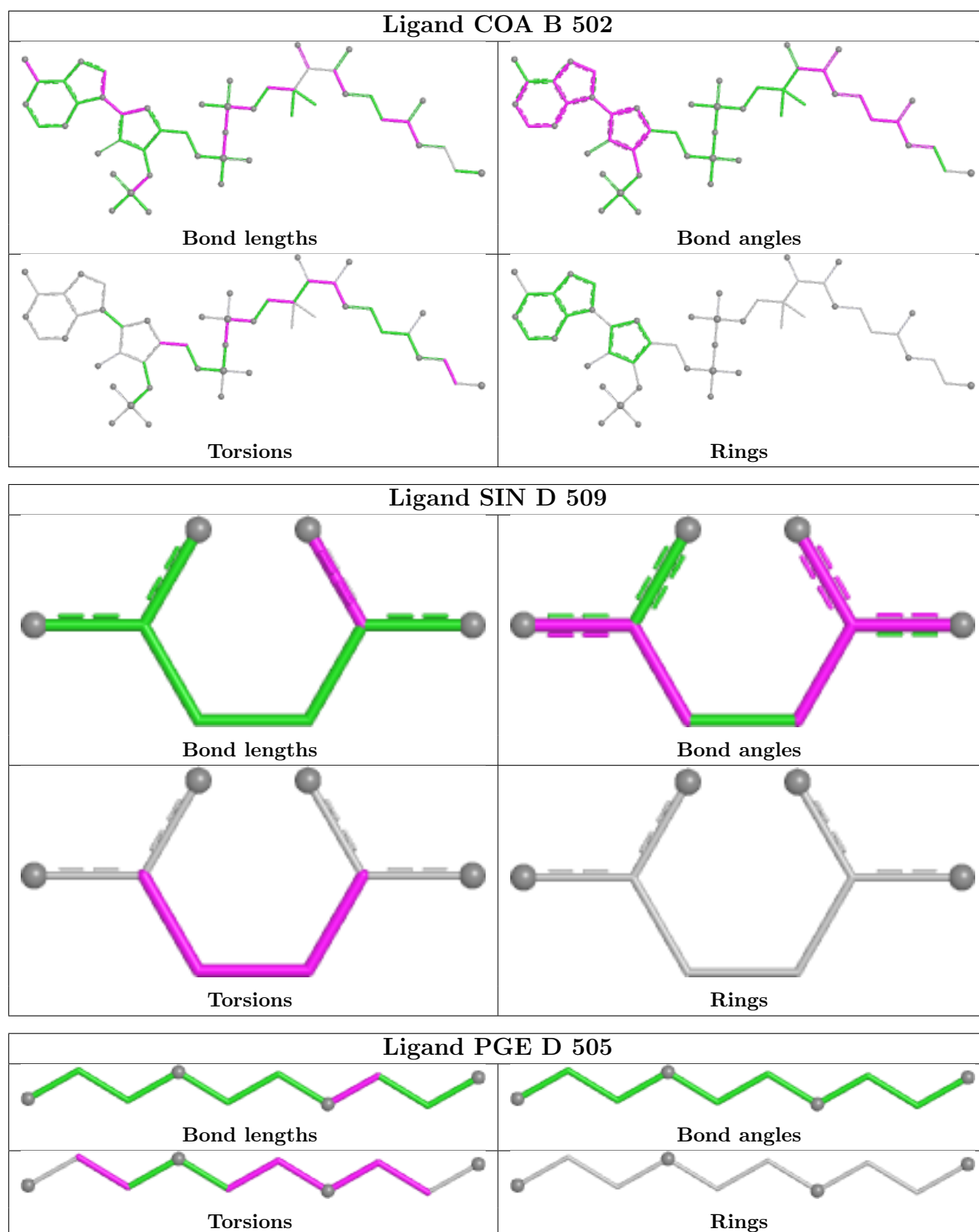
9 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	GOL	3	0
4	C	601	PGE	5	0
5	D	503	COA	5	0
4	B	505	PGE	3	0
4	C	602	PGE	4	0
5	B	502	COA	6	0
7	D	509	SIN	1	0
3	D	508	GOL	1	0
3	D	502	GOL	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	405/410 (98%)	0.16	7 (1%) 69 69	15, 34, 61, 75	6 (1%)
1	C	408/410 (99%)	0.54	52 (12%) 8 6	16, 35, 72, 94	5 (1%)
2	B	406/409 (99%)	0.42	29 (7%) 22 20	14, 34, 70, 87	4 (0%)
2	D	405/409 (99%)	0.02	11 (2%) 56 56	14, 30, 46, 63	7 (1%)
All	All	1624/1638 (99%)	0.28	99 (6%) 27 25	14, 33, 66, 94	22 (1%)

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	VAL	6.5
1	C	255	PRO	6.4
2	B	409	VAL	6.3
1	C	249	ILE	5.3
1	C	314	ILE	5.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

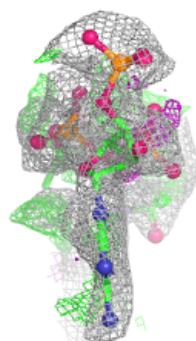
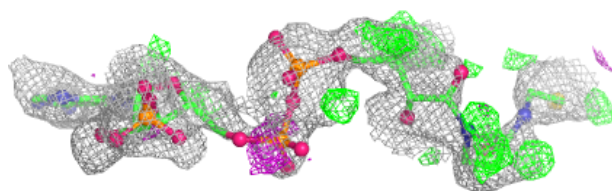
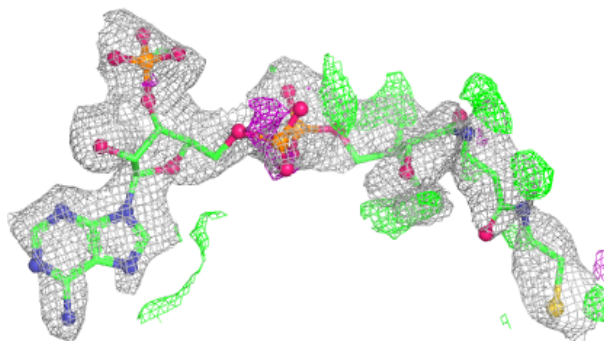
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
5	COA	B	502	48/48	0.69	0.19	44,65,79,88	48
4	PGE	A	702	10/10	0.74	0.20	37,49,69,75	0
7	SIN	D	509	8/8	0.74	0.21	35,45,50,54	0
4	PGE	C	602	10/10	0.75	0.22	43,56,66,67	0
4	PGE	C	601	10/10	0.76	0.19	28,44,53,56	0
4	PGE	B	505	10/10	0.79	0.19	40,51,63,70	0
3	GOL	B	504	6/6	0.80	0.14	43,48,50,55	0
3	GOL	C	604	6/6	0.80	0.12	39,44,46,53	0
3	GOL	D	502	6/6	0.80	0.16	42,47,53,61	0
3	GOL	D	508	6/6	0.80	0.13	52,55,56,66	0
3	GOL	A	703	6/6	0.80	0.14	29,35,36,45	0
4	PGE	D	505	10/10	0.81	0.15	41,50,55,56	0
3	GOL	C	605	6/6	0.82	0.14	40,45,50,52	0
3	GOL	A	701	6/6	0.84	0.14	48,52,55,58	0
4	PGE	D	506	10/10	0.85	0.13	30,44,49,54	0
5	COA	D	503	48/48	0.88	0.12	33,42,52,54	0
6	TRS	B	503	8/8	0.89	0.12	27,29,38,47	0
3	GOL	C	603	6/6	0.90	0.13	38,40,45,56	0
6	TRS	D	504	8/8	0.91	0.10	27,32,39,43	0
3	GOL	D	501	6/6	0.94	0.08	32,33,36,36	0
3	GOL	B	501	6/6	0.94	0.08	34,37,39,43	0
3	GOL	D	507	6/6	0.94	0.09	24,27,34,38	0

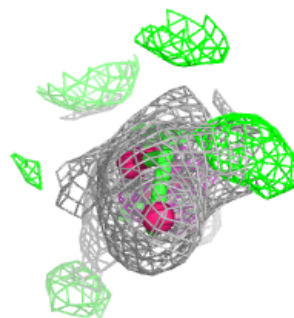
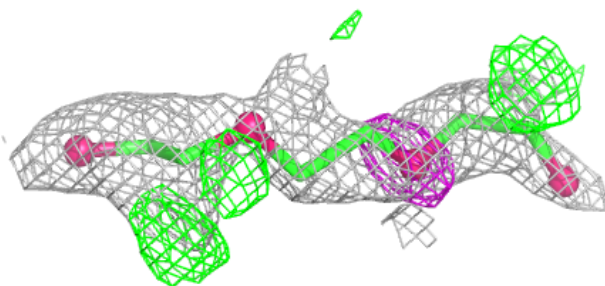
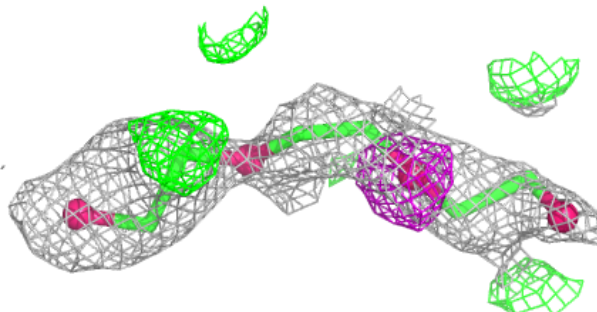
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around COA B 502:**

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

**Electron density around PGE A 702:**

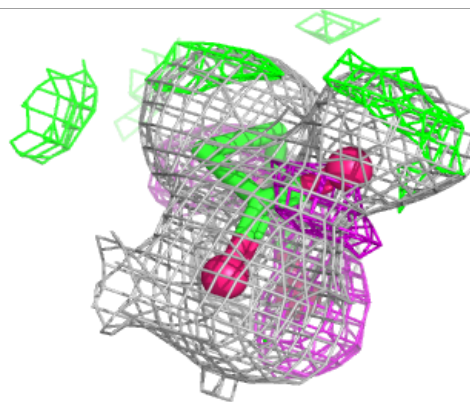
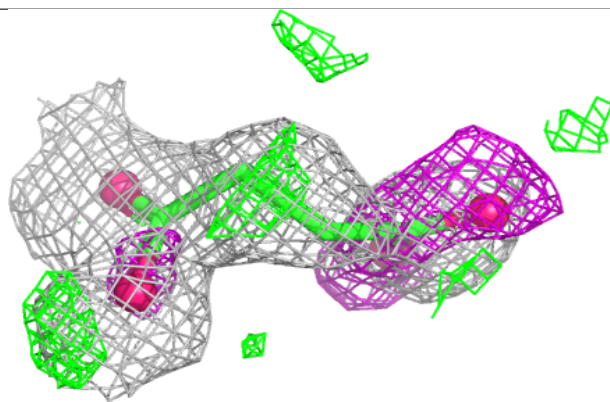
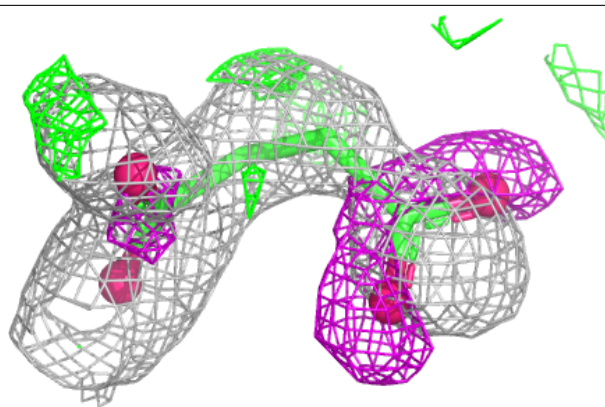
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



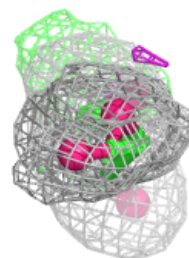
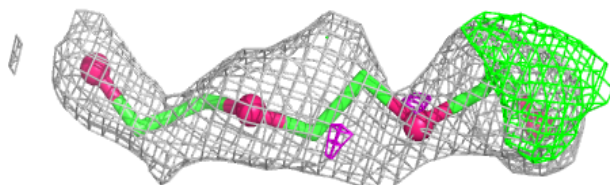
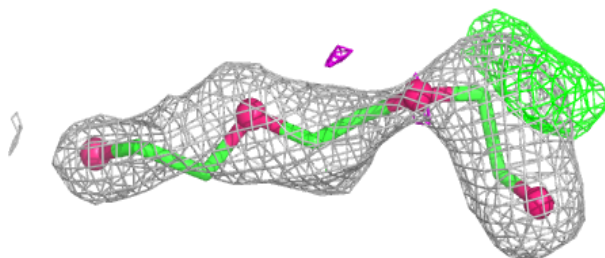


**Electron density around SIN D 509:**

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

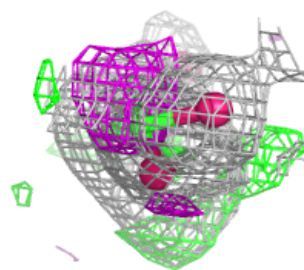
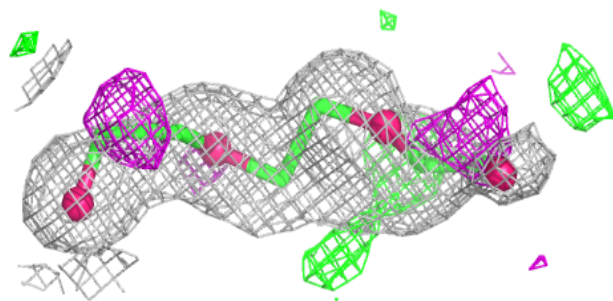
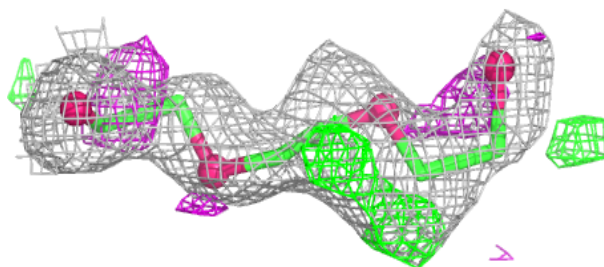
**Electron density around PGE C 602:**

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

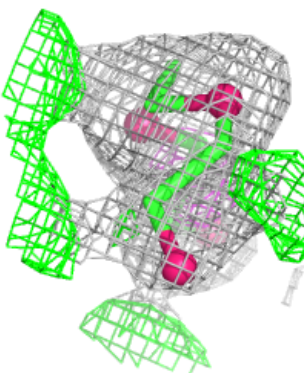
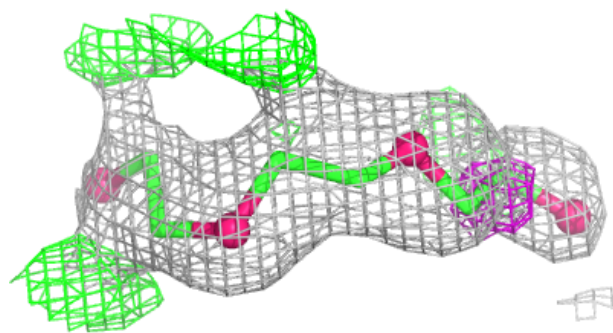
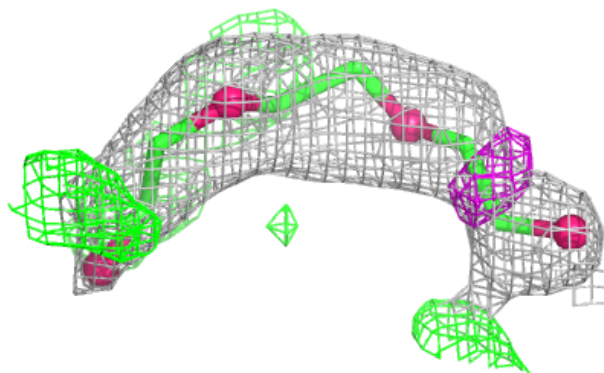


**Electron density around PGE C 601:**

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

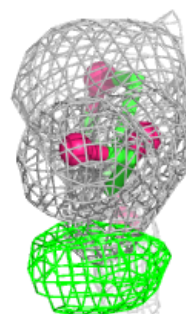
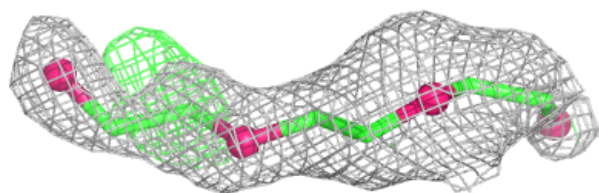
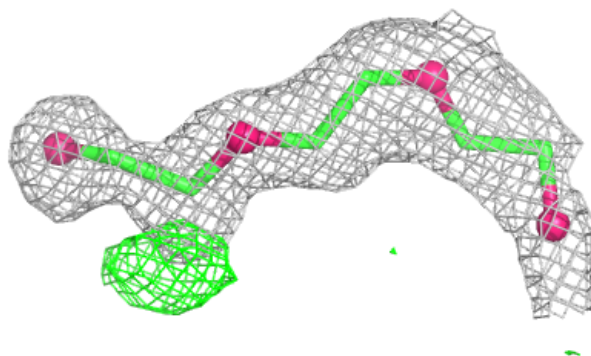
**Electron density around PGE B 505:**

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

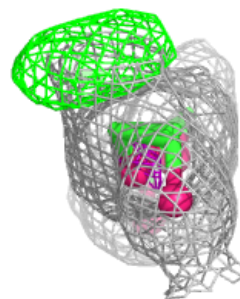
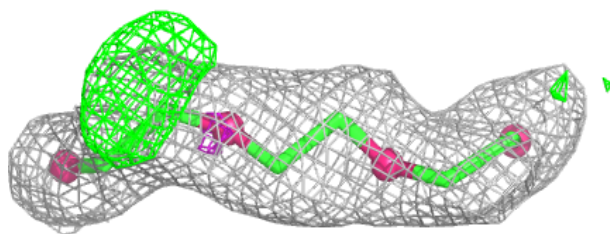
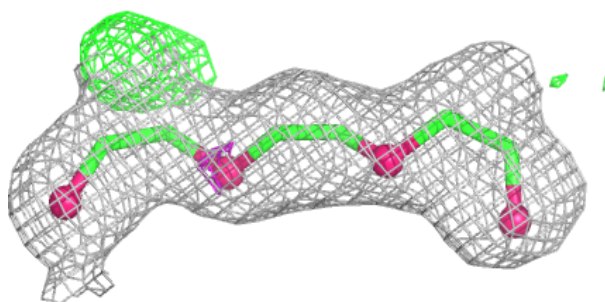


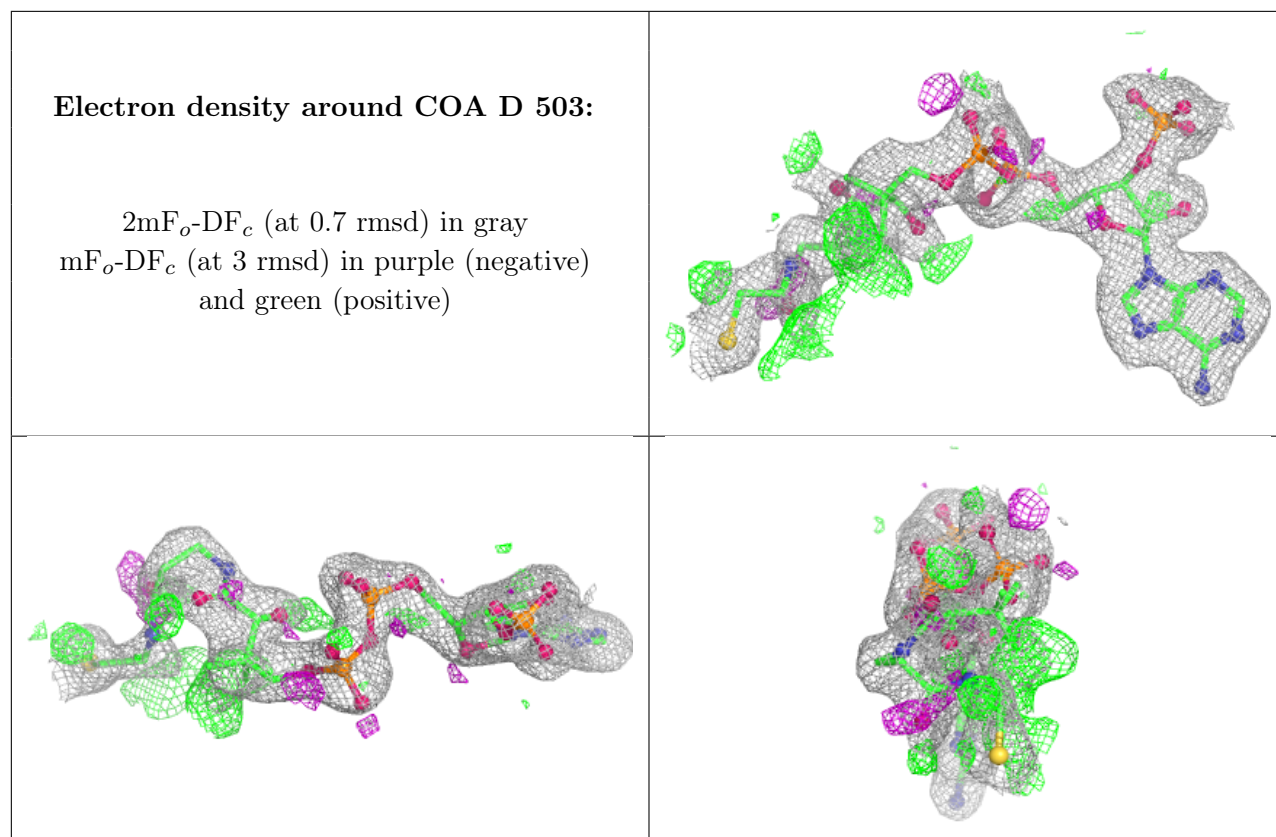
**Electron density around PGE D 505:**

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

**Electron density around PGE D 506:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.