



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:32 AM UTC

PDB ID : 9FN0 / pdb_00009fn0
Title : Succinyl-CoA:(R)-benzylsuccinate CoA-transferase (BbsEF)
Authors : Ermler, U.; Heider, J.; Demmer, U.
Deposited on : 2024-06-07
Resolution : 1.50 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

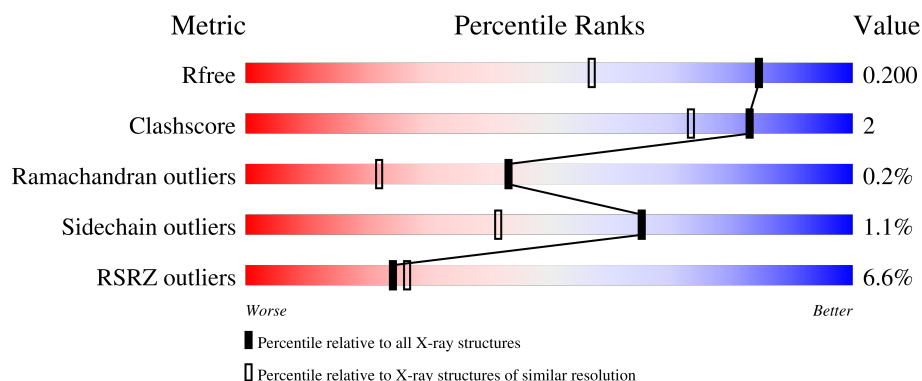
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	410	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
1	C	410	<div> <div>16%</div> <div>91%</div> <div>7% ..</div> </div>
2	B	409	<div> <div>6%</div> <div>94%</div> <div>5%</div> </div>
2	D	409	<div> <div>2%</div> <div>94%</div> <div>5% .</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 26038 atoms, of which 12326 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	407	Total	C	H	N	O	S	0	1	0
			6231	1999	3052	571	594	15			
1	C	407	Total	C	H	N	O	S	0	0	0
			6222	1997	3046	571	593	15			

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

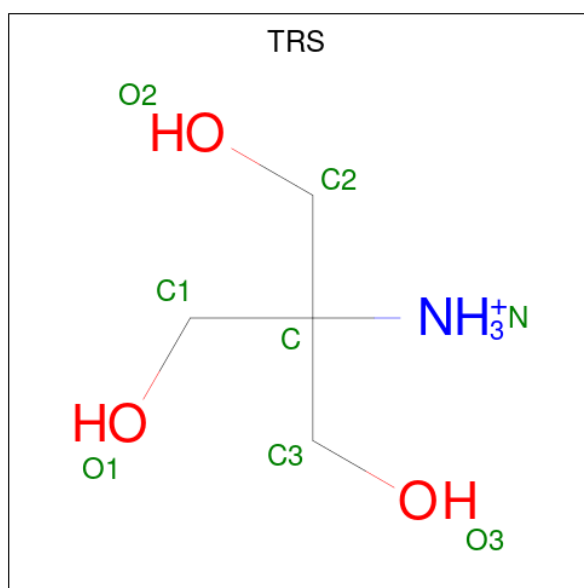
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	407	Total	C	H	N	O	S	0	2	0
			6220	1972	3077	567	587	17			
2	D	406	Total	C	H	N	O	S	0	2	0
			6206	1968	3071	565	585	17			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



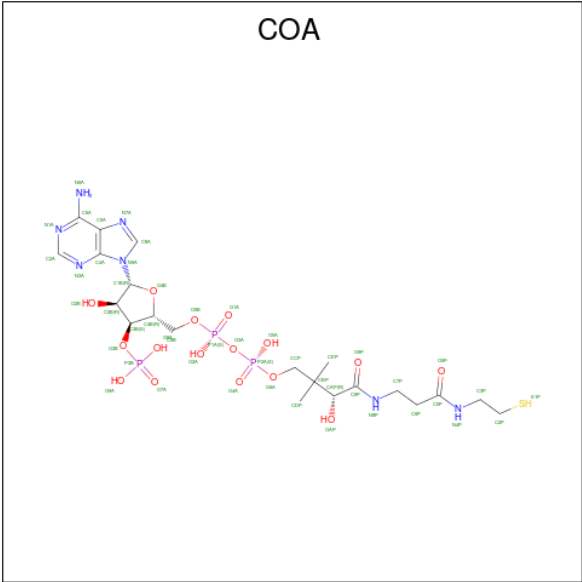
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H N O 20 4 12 1 3	0	0
4	D	1	Total C H N O 20 4 12 1 3	0	0

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	P	S	0	0
			80	21	32	7	16	3	1		

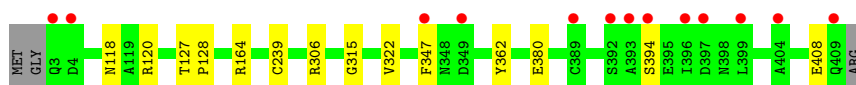
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total	O	0	0
			224	224		
6	B	225	Total	O	0	1
			226	226		
6	C	222	Total	O	0	0
			222	222		
6	D	310	Total	O	0	3
			313	313		

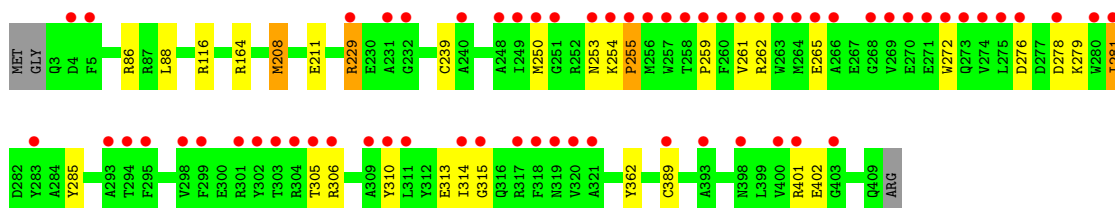
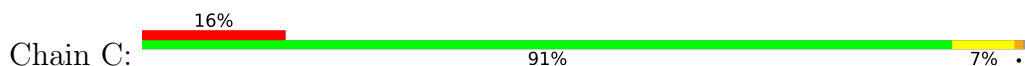
3 Residue-property plots [i](#)

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.

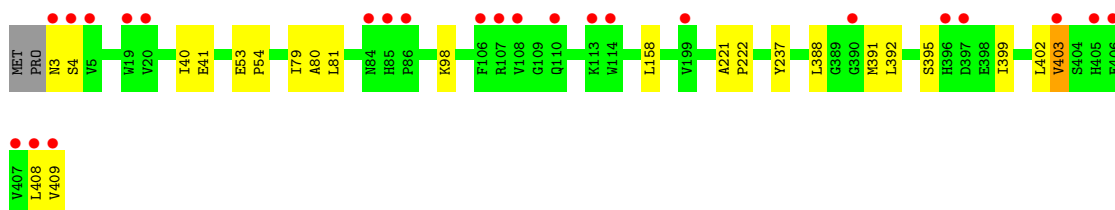
- Molecule 1: Subunit of Benzylsuccinate CoA-transferase



- 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, α , β , γ	92.40Å 101.30Å 192.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.50 48.98 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.98-1.50) 95.7 (48.98-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.50Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.175 , 0.197 (Not available) , 0.200	Depositor DCC
R_{free} test set	13817 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 32.6	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	0.97	EDS
Total number of atoms	26038	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.64% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.43	0/3259	0.59	0/4420
1	C	0.51	1/3253 (0.0%)	0.65	1/4412 (0.0%)
2	B	0.44	0/3220	0.61	0/4370
2	D	0.57	0/3212	0.66	1/4359 (0.0%)
All	All	0.49	1/12944 (0.0%)	0.63	2/17561 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	208	MET	SD-CE	-7.43	1.60	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	353	GLU	CA-CB-CG	-5.17	103.77	114.10
1	C	229	ARG	CD-NE-CZ	5.14	131.59	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3179	3052	3051	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3176	3046	3046	22	0
2	B	3143	3077	3076	17	0
2	D	3135	3071	3070	17	0
3	B	12	16	16	0	0
3	C	6	0	8	0	0
3	D	12	8	15	0	0
4	B	8	12	12	0	0
4	D	8	12	12	0	0
5	D	48	32	31	0	0
6	A	224	0	0	0	0
6	B	226	0	0	0	0
6	C	222	0	0	4	0
6	D	313	0	0	7	0
All	All	13712	12326	12337	59	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 2.

All (59) 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:402:LEU:HB3	2:B:408:LEU:HD12	1.73	0.71
2:D:38:ILE:CD1	2:D:391:MET:HE1	2.21	0.71
2:D:38:ILE:HD11	2:D:391:MET:HE1	1.74	0.68
1:C:259:PRO:HA	1:C:262:ARG:HD3	1.77	0.66
2:D:4:SER:O	2:D:4:SER:OG	2.13	0.63
2:D:138:THR:HG22	6:D:868:HOH:O	2.01	0.61
1:A:380:GLU:HA	1:A:408:GLU:HG2	1.85	0.58
2:B:402:LEU:HB3	2:B:408:LEU:CD1	2.34	0.57
1:C:254:LYS:HD2	1:C:254:LYS:O	2.04	0.57
2:D:25:ILE:CD1	6:D:841:HOH:O	2.51	0.57
2:D:372:GLU:HG3	6:D:754:HOH:O	2.04	0.56
1:C:88:LEU:HD23	1:C:389:CYS:SG	2.46	0.56
1:C:261:VAL:O	1:C:265:GLU:HG2	2.05	0.55
2:D:25:ILE:HD12	6:D:841:HOH:O	2.07	0.54
1:C:306:ARG:NH2	1:C:310:TYR:OH	2.41	0.53
1:A:315:GLY:HA3	1:A:322:VAL:HG11	1.91	0.52
1:C:208:MET:SD	2:D:363:PRO:HD3	2.49	0.52
2:B:81:LEU:HD21	2:B:408:LEU:HD21	1.92	0.52
2:D:41:GLU:O	2:D:80:ALA:HA	2.11	0.50
1:A:118:ASN:OD1	1:A:120:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ASP:O	1:C:281:ILE:HG22	2.12	0.49
2:D:48:THR:HG23	6:D:851:HOH:O	2.13	0.48
1:C:164:ARG:HG3	2:D:237:TYR:HA	1.96	0.47
2:B:388:LEU:HD23	2:B:392:LEU:HD12	1.97	0.46
1:C:86:ARG:NH2	1:C:116:ARG:HH21	2.13	0.46
2:B:403:VAL:HB	2:B:408:LEU:O	2.14	0.46
2:D:409:VAL:HG12	6:D:601:HOH:O	2.13	0.46
1:C:265:GLU:HB3	1:C:272:TRP:CE3	2.51	0.46
1:C:265:GLU:HG3	6:C:804:HOH:O	2.15	0.45
2:B:41:GLU:O	2:B:80:ALA:HA	2.17	0.45
1:C:261:VAL:HG13	6:C:802:HOH:O	2.16	0.45
1:C:314:ILE:HG23	1:C:315:GLY:N	2.32	0.45
1:C:306:ARG:HB3	1:C:310:TYR:CD2	2.51	0.45
2:D:148:TYR:HB3	6:D:602:HOH:O	2.15	0.45
2:B:40:ILE:HD12	2:B:79:ILE:HD11	1.99	0.45
1:C:305:THR:OG1	1:C:306:ARG:HD3	2.16	0.45
2:B:81:LEU:CD2	2:B:408:LEU:CD2	2.96	0.44
2:B:81:LEU:CD2	2:B:408:LEU:HD21	2.48	0.44
2:D:43:VAL:HG11	2:D:409:VAL:HG21	2.00	0.44
1:A:164:ARG:HG3	2:B:237:TYR:HA	1.99	0.44
2:D:80:ALA:O	2:D:408:LEU:HA	2.17	0.44
2:B:388:LEU:HD11	2:B:408:LEU:HD13	2.00	0.43
1:A:347:PHE:CE2	1:C:313:GLU:HG2	2.53	0.43
2:B:53:GLU:HB2	2:B:54:PRO:HA	2.00	0.43
1:C:239:CYS:HB2	1:C:306:ARG:O	2.18	0.42
2:D:158:LEU:C	2:D:158:LEU:HD23	2.44	0.42
1:A:239:CYS:HB2	1:A:306:ARG:O	2.19	0.42
1:C:279:LYS:O	1:C:285:TYR:CD2	2.72	0.42
2:B:158:LEU:C	2:B:158:LEU:HD23	2.44	0.42
2:B:98:LYS:HE2	2:B:391:MET:O	2.19	0.41
1:C:276:ASP:N	6:C:802:HOH:O	2.52	0.41
1:C:254:LYS:HA	6:C:851:HOH:O	2.20	0.41
2:B:221:ALA:HB3	2:B:222:PRO:HD3	2.02	0.41
1:C:265:GLU:HB3	1:C:272:TRP:CZ3	2.55	0.41
2:B:81:LEU:HD23	2:B:408:LEU:HG	2.03	0.40
2:D:134:SER:O	2:D:210:GLN:HG3	2.21	0.40
1:A:127:THR:HB	1:A:128:PRO:HD2	2.02	0.40
2:B:395:SER:O	2:B:399:ILE:HG13	2.21	0.40
1:C:253:ASN:C	1:C:255:PRO:HD2	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	406/410 (99%)	398 (98%)	8 (2%)	0	100	100
1	C	405/410 (99%)	390 (96%)	13 (3%)	2 (0%)	24	8
2	B	407/409 (100%)	401 (98%)	6 (2%)	0	100	100
2	D	406/409 (99%)	399 (98%)	6 (2%)	1 (0%)	43	22
All	All	1624/1638 (99%)	1588 (98%)	33 (2%)	3 (0%)	43	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	PRO
2	D	20	VAL
1	C	211	GLU

5.3.2 Protein sidechains

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	316/317 (100%)	314 (99%)	2 (1%)	78	62
1	C	315/317 (99%)	309 (98%)	6 (2%)	50	22
2	B	320/320 (100%)	316 (99%)	4 (1%)	61	35
2	D	319/320 (100%)	317 (99%)	2 (1%)	78	62
All	All	1270/1274 (100%)	1256 (99%)	14 (1%)	65	41

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	TYR
1	A	394	SER
2	B	3	ASN
2	B	4	SER
2	B	403	VAL
2	B	409	VAL
1	C	229	ARG
1	C	250	MET
1	C	281	ILE
1	C	362	TYR
1	C	401	ARG
1	C	402	GLU
2	D	5	VAL
2	D	138	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	344	GLN
1	A	368	GLN
1	C	61	GLN
1	C	123	GLN
1	C	253	ASN
1	C	339	HIS
1	C	344	GLN
1	C	354	ASN
1	C	368	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

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	B	502	-	7,7,7	1.12	1 (14%)	9,9,9	1.30	1 (11%)
3	GOL	D	504	-	5,5,5	0.83	0	5,5,5	1.30	0
3	GOL	D	501	-	5,5,5	0.67	0	5,5,5	0.96	0
3	GOL	C	701	-	5,5,5	0.68	0	5,5,5	1.17	1 (20%)
5	COA	D	502	-	47,50,50	2.95	13 (27%)	69,75,75	2.14	17 (24%)
3	GOL	B	503	-	5,5,5	0.57	0	5,5,5	1.26	0
4	TRS	D	503	-	7,7,7	1.17	1 (14%)	9,9,9	0.97	1 (11%)
3	GOL	B	501	-	5,5,5	0.68	0	5,5,5	0.84	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
4	TRS	B	502	-	-	0/9/9/9	-
3	GOL	D	504	-	-	0/4/4/4	-
3	GOL	D	501	-	-	1/4/4/4	-
3	GOL	C	701	-	-	0/4/4/4	-
5	COA	D	502	-	-	15/48/64/64	0/3/3/3
3	GOL	B	503	-	-	0/4/4/4	-
4	TRS	D	503	-	-	0/9/9/9	-
3	GOL	B	501	-	-	0/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	COA	C3B-C4B	-9.15	1.29	1.52
5	D	502	COA	O4B-C1B	7.43	1.59	1.42
5	D	502	COA	C2B-C1B	-7.23	1.30	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	COA	C2B-C3B	7.15	1.68	1.53
5	D	502	COA	C9P-N8P	5.47	1.46	1.33
5	D	502	COA	C5P-N4P	5.00	1.45	1.33
5	D	502	COA	P3B-O3B	4.17	1.66	1.59
5	D	502	COA	C6A-N6A	3.77	1.43	1.34
5	D	502	COA	O4B-C4B	3.42	1.52	1.45
4	B	502	TRS	C-N	2.86	1.58	1.49
5	D	502	COA	O9P-C9P	-2.83	1.18	1.23
4	D	503	TRS	C-N	2.74	1.58	1.49
5	D	502	COA	P2A-O6A	2.62	1.69	1.59
5	D	502	COA	C5B-C4B	2.29	1.58	1.51
5	D	502	COA	CCP-CBP	2.21	1.56	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502	COA	C6P-C7P-N8P	-6.82	97.48	112.00
5	D	502	COA	C5A-C4A-N3A	-4.85	120.04	126.72
5	D	502	COA	C7P-C6P-C5P	4.58	120.02	112.39
5	D	502	COA	O6A-CCP-CBP	4.47	117.74	110.55
5	D	502	COA	CEP-CBP-CCP	-4.36	101.03	108.22
5	D	502	COA	N3A-C2A-N1A	-4.02	122.50	128.58
5	D	502	COA	CDP-CBP-CCP	3.83	114.55	108.22
5	D	502	COA	CDP-CBP-CAP	3.74	115.15	108.77
5	D	502	COA	O3A-P1A-O1A	-3.61	99.84	110.70
5	D	502	COA	O6A-P2A-O4A	3.51	122.84	108.94
5	D	502	COA	O5A-P2A-O3A	-3.42	98.04	107.27
5	D	502	COA	N3A-C4A-N9A	3.18	132.58	127.17
5	D	502	COA	C2A-N3A-C4A	3.09	119.38	111.83
5	D	502	COA	O2A-P1A-O3A	2.70	114.58	107.27
5	D	502	COA	O5P-C5P-C6P	-2.57	117.36	122.02
5	D	502	COA	P2A-O6A-CCP	-2.56	107.19	121.12
5	D	502	COA	O3B-C3B-C2B	-2.36	103.22	111.68
4	D	503	TRS	C3-C-N	2.17	113.70	108.17
4	B	502	TRS	C2-C-N	2.11	113.56	108.17
3	C	701	GOL	C3-C2-C1	-2.06	104.23	111.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	COA	CCP-O6A-P2A-O3A

Continued on next page...

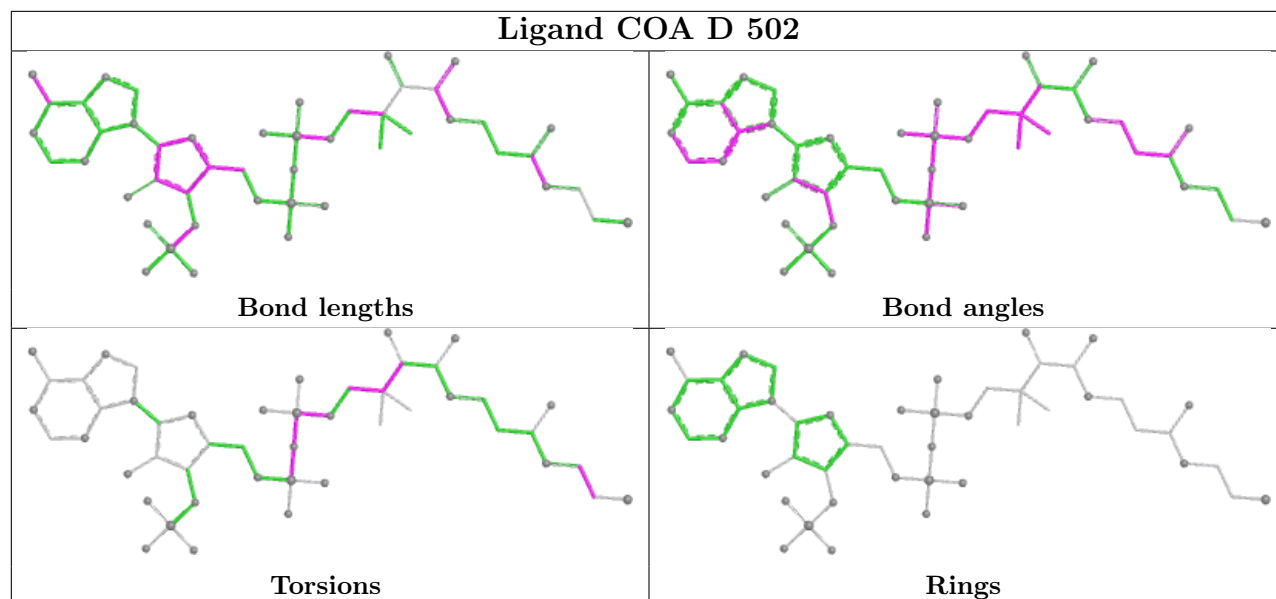
Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	502	COA	CCP-O6A-P2A-O4A
5	D	502	COA	CEP-CBP-CCP-O6A
5	D	502	COA	CAP-CBP-CCP-O6A
5	D	502	COA	OAP-CAP-CBP-CCP
5	D	502	COA	C9P-CAP-CBP-CCP
5	D	502	COA	S1P-C2P-C3P-N4P
5	D	502	COA	OAP-CAP-CBP-CDP
5	D	502	COA	OAP-CAP-CBP-CEP
5	D	502	COA	C9P-CAP-CBP-CEP
5	D	502	COA	CDP-CBP-CCP-O6A
5	D	502	COA	P2A-O3A-P1A-O2A
5	D	502	COA	P2A-O3A-P1A-O1A
5	D	502	COA	P1A-O3A-P2A-O4A
5	D	502	COA	P1A-O3A-P2A-O5A
3	D	501	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	407/410 (99%)	0.08	13 (3%) 50 54	12, 32, 65, 93	1 (0%)
1	C	407/410 (99%)	0.47	64 (15%) 5 5	18, 33, 75, 87	0
2	B	407/409 (99%)	0.19	24 (5%) 28 30	13, 32, 74, 124	2 (0%)
2	D	406/409 (99%)	-0.26	7 (1%) 69 72	11, 26, 40, 93	2 (0%)
All	All	1627/1638 (99%)	0.12	108 (6%) 24 26	11, 30, 68, 124	5 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	255	PRO	7.7
1	C	318	PHE	7.0
2	B	408	LEU	6.7
1	C	263	TRP	6.6
1	C	314	ILE	6.4
2	B	20	VAL	6.3
1	C	275	LEU	6.3
1	C	266	ALA	6.3
1	C	261	VAL	6.2
1	C	272	TRP	6.1
1	C	274	VAL	5.9
1	C	269	VAL	5.8
2	B	19	TRP	5.5
1	C	260	PHE	5.3
1	C	281	ILE	5.0
1	C	259	PRO	4.9
1	C	257	TRP	4.8
1	C	320	VAL	4.7
2	B	106	PHE	4.7
1	C	319	ASN	4.6
1	C	258	THR	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	114	TRP	4.4
1	C	310	TYR	4.3
1	C	302	TYR	4.2
1	C	280	TRP	4.1
1	C	298	VAL	3.9
2	B	409	VAL	3.9
2	B	5	VAL	3.7
1	C	262	ARG	3.5
1	C	299	PHE	3.5
2	B	403	VAL	3.5
1	C	315	GLY	3.4
2	B	407	VAL	3.3
1	C	268	GLY	3.3
1	A	389	CYS	3.3
1	A	393	ALA	3.3
1	A	394	SER	3.2
1	C	256	MET	3.2
1	C	248	ALA	3.2
1	C	254	LYS	3.1
2	D	145	TYR	3.1
2	B	86	PRO	3.1
1	C	317	ARG	3.1
2	B	3	ASN	3.0
1	A	409	GLN	3.0
1	C	253	ASN	2.9
1	C	295	PHE	2.9
1	C	264	MET	2.8
2	D	4	SER	2.8
2	D	305	TRP	2.8
1	A	349	ASP	2.8
1	C	303	THR	2.8
1	C	403	GLY	2.7
2	B	110	GLN	2.7
2	D	138	THR	2.7
1	C	389	CYS	2.7
2	B	108	VAL	2.7
2	B	405	HIS	2.7
1	C	271	GLU	2.7
1	C	398	ASN	2.6
1	C	294	THR	2.6
1	C	400	VAL	2.6
1	C	249	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	390	GLY	2.6
1	C	278	ASP	2.6
1	C	265	GLU	2.6
1	C	305	THR	2.6
1	C	293	ALA	2.5
1	C	304	ARG	2.5
2	D	144	ARG	2.5
2	B	396	HIS	2.5
1	C	251	GLY	2.5
2	B	113	LYS	2.4
1	C	401	ARG	2.4
1	C	276	ASP	2.4
1	C	301	ARG	2.4
2	B	107	ARG	2.4
1	C	240	ALA	2.4
1	A	3	GLN	2.4
2	B	85	HIS	2.3
1	C	4	ASP	2.3
1	C	270	GLU	2.3
1	C	311	LEU	2.3
1	A	397	ASP	2.2
1	C	273	GLN	2.2
1	A	392	SER	2.2
2	B	4	SER	2.2
1	A	4	ASP	2.2
1	A	396	ILE	2.2
2	B	406	GLU	2.2
1	A	404	ALA	2.2
1	C	283	TYR	2.2
1	C	309	ALA	2.2
1	C	232	GLY	2.2
1	C	250	MET	2.2
1	C	393	ALA	2.1
2	B	397	ASP	2.1
2	D	148	TYR	2.1
1	A	347	PHE	2.1
2	B	84	ASN	2.1
1	C	321	ALA	2.1
1	C	229	ARG	2.1
1	C	5	PHE	2.0
2	B	199	VAL	2.0
2	D	108	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	231	ALA	2.0
1	C	306	ARG	2.0
1	A	399	LEU	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](#)

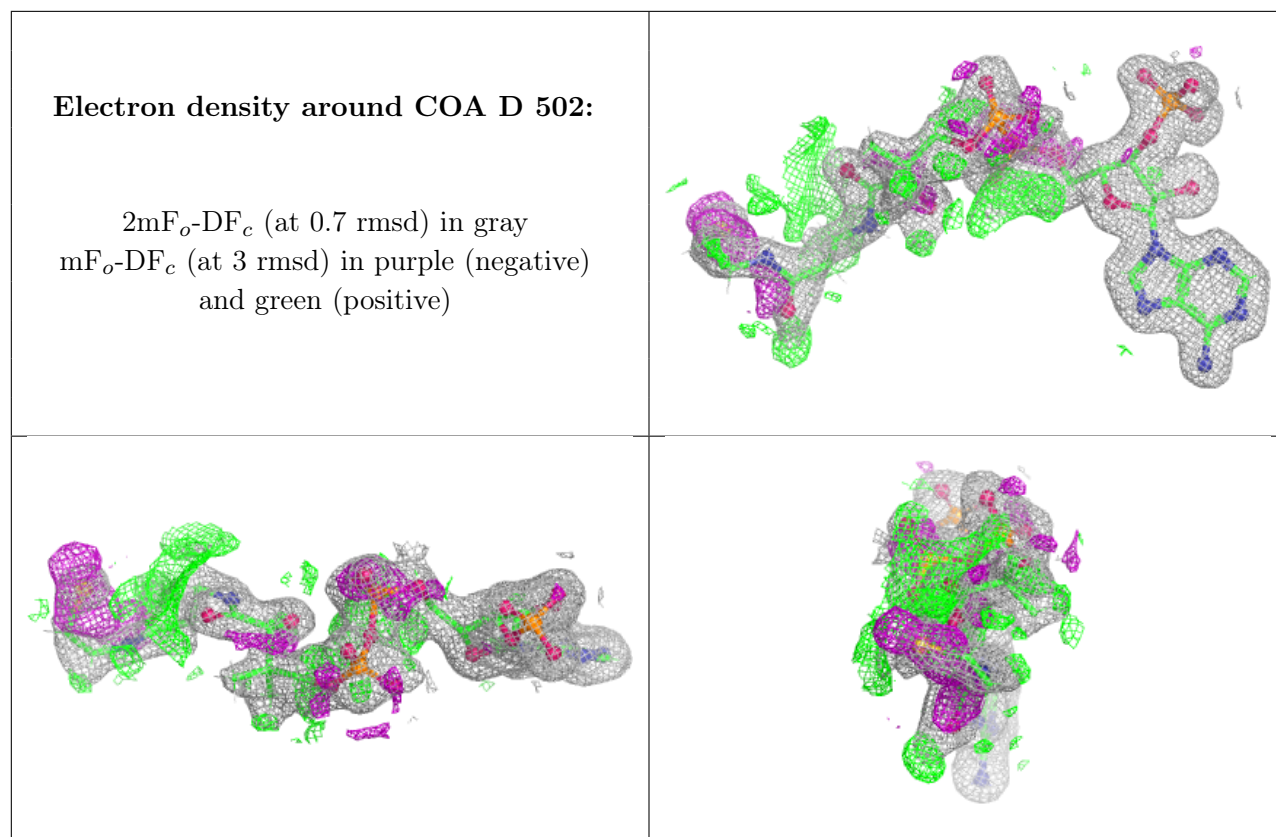
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	GOL	D	504	6/6	0.86	0.13	30,34,42,42	0
3	GOL	C	701	6/6	0.89	0.12	32,34,39,39	0
5	COA	D	502	48/48	0.91	0.11	22,35,53,54	0
3	GOL	B	503	6/6	0.92	0.09	29,35,42,44	0
3	GOL	D	501	6/6	0.94	0.08	22,28,34,34	0
4	TRS	D	503	8/8	0.95	0.07	19,26,31,35	0
4	TRS	B	502	8/8	0.96	0.06	18,24,31,32	0
3	GOL	B	501	6/6	0.97	0.07	25,31,35,38	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.