



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 AM UTC

PDB ID : 9FUN / pdb_00009fun
Title : Succinyl-CoA:(R)-benzylsuccinate CoA-transferase (BbsEF) + CoA + benzylsuccinate (weakly occupied)
Authors : Ermler, U.; Heider, J.; Demmer, U.
Deposited on : 2024-06-26
Resolution : 2.00 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

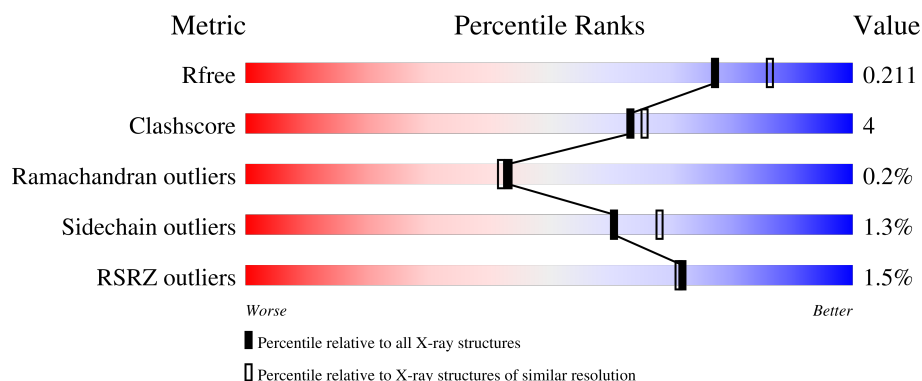
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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></div> <div>92%7% .</div> </div>
1	C	410	<div> <div>%</div> <div>91%9%</div> </div>
2	B	409	<div> <div>4%</div> <div>87%11% ..</div> </div>
2	D	409	<div> <div></div> <div>91%8% .</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	TRS	D	504	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 26024 atoms, of which 12484 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.

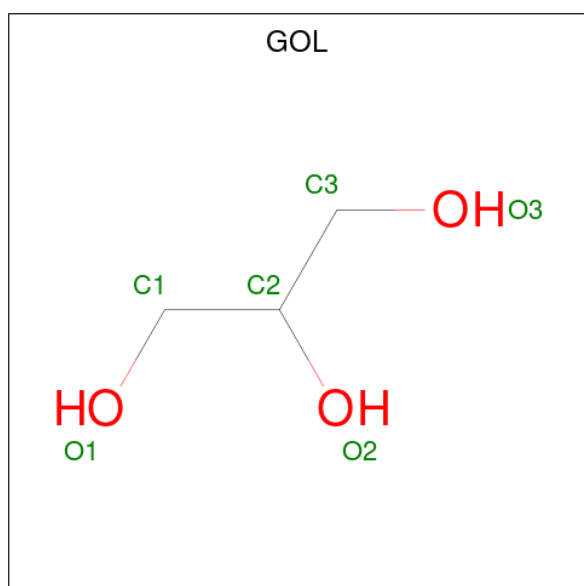
- Molecule 1 is a protein called Subunit of Benzylsuccinate CoA-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	H	N	O	S	0	6	0
			6294	2015	3089	579	596	15			
1	C	408	Total	C	H	N	O	S	0	5	0
			6280	2012	3081	576	596	15			

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

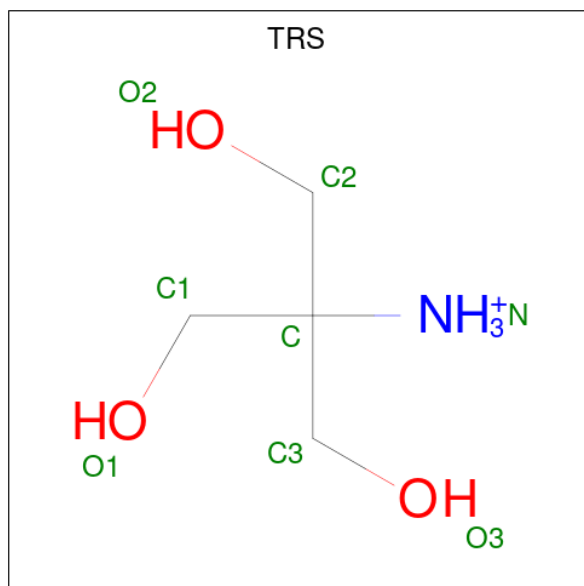
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	406	Total	C	H	N	O	S	0	2	0
			6206	1968	3071	565	585	17			
2	D	406	Total	C	H	N	O	S	0	3	0
			6221	1973	3077	566	588	17			

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



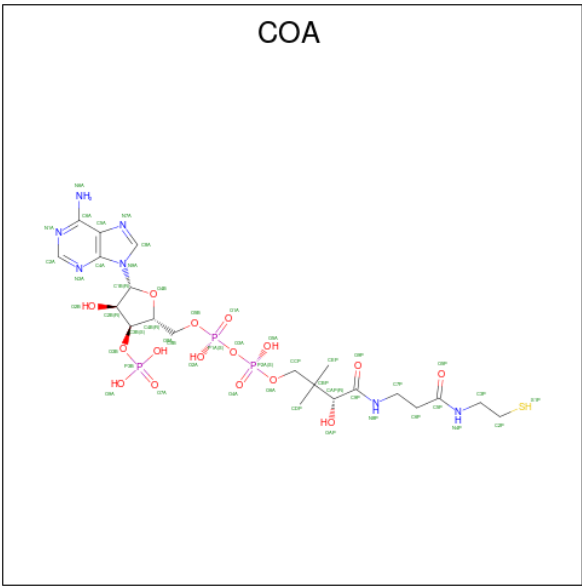
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



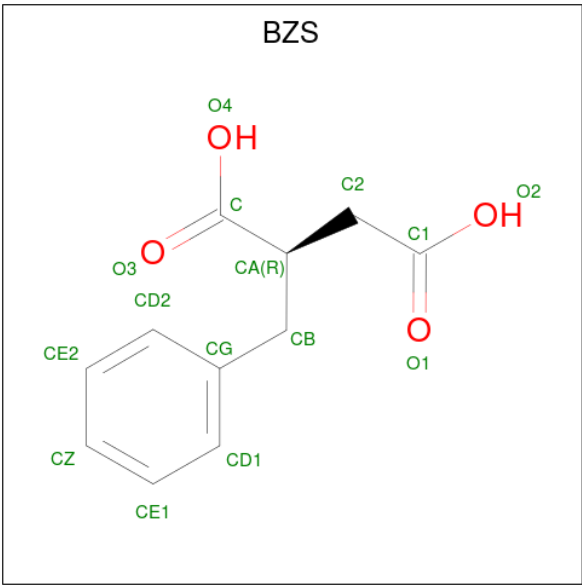
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0
			20	4	12	1	3	0
4	D	1	Total	C	H	N	O	0
			20	4	12	1	3	0

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



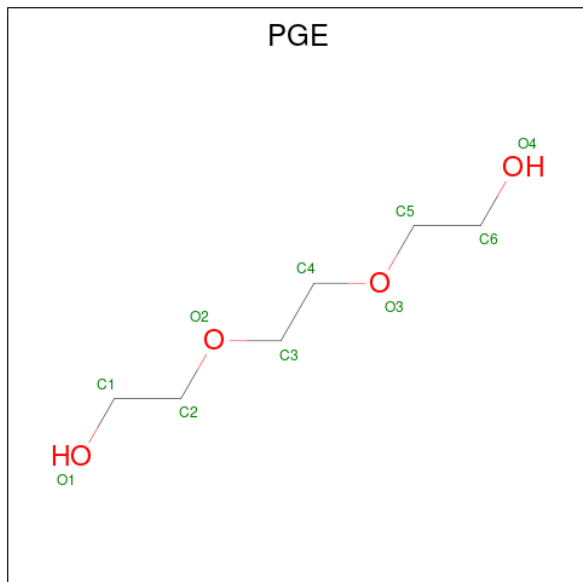
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
5	D	1	80	21	32	7	16	3	1	0	0

- Molecule 6 is L-BENZYLsuccinic ACID (CCD ID: BZS) (formula: C₁₁H₁₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	D	1	25	11	10	4	0	0

- Molecule 7 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
7	D	1	Total	C	H	O	0	0
			24	6	14	4		
7	D	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 8 is water.

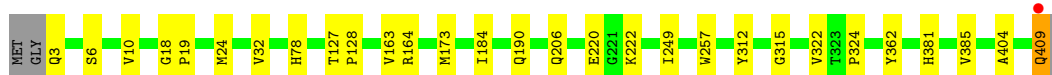
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	163	Total	O	0	0
			163	163		
8	B	153	Total	O	0	1
			154	154		
8	C	181	Total	O	0	3
			184	184		
8	D	203	Total	O	0	0
			203	203		

3 Residue-property plots

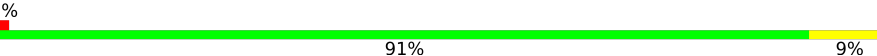
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A: 




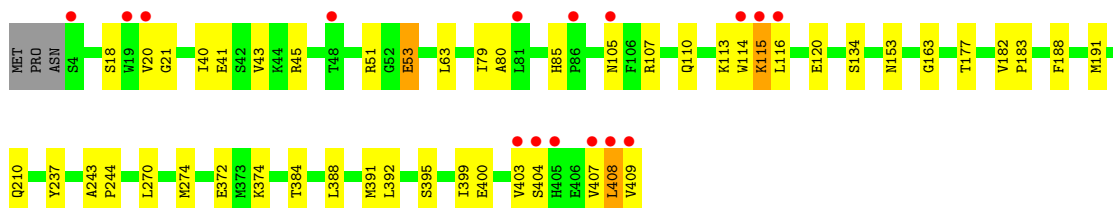
- Molecule 1: Subunit of Benzylsuccinate CoA-transferase

Chain C: 



- Molecule 2: Subunit of Benzylsuccinate CoA-transferase

Chain B: 



- Molecule 2: Subunit of Benzylsuccinate CoA-transferase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.30Å 101.29Å 192.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.00 48.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.98-2.00) 98.1 (48.98-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.178 , 0.210 0.179 , 0.211	Depositor DCC
R_{free} test set	5890 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26024	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.11% 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: COA, GOL, TRS, PGE, BZS

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	0.19	0/3303	0.42	0/4478
1	C	0.23	0/3297	0.46	0/4471
2	B	0.24	0/3212	0.48	4/4359 (0.1%)
2	D	0.21	0/3221	0.42	0/4371
All	All	0.22	0/13033	0.45	4/17679 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	LEU	CA-C-N	5.31	130.93	121.48
2	B	116	LEU	C-N-CA	5.31	130.93	121.48
2	B	114	TRP	CA-C-N	5.18	129.69	122.08
2	B	114	TRP	C-N-CA	5.18	129.69	122.08

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	3205	3089	3074	17	0
1	C	3199	3081	3067	27	0
2	B	3135	3071	3070	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3144	3077	3075	28	0
3	A	6	8	8	0	0
3	B	18	24	24	0	0
3	C	12	16	15	2	0
3	D	18	24	24	1	0
4	B	8	12	12	0	0
4	D	8	12	12	5	0
5	D	48	32	31	0	0
6	D	15	10	10	2	0
7	D	20	28	28	1	0
8	A	163	0	0	0	0
8	B	154	0	0	1	0
8	C	184	0	0	1	0
8	D	203	0	0	1	0
All	All	13540	12484	12450	101	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.

All (101) 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:115:LYS:O	2:B:120:GLU:HG3	1.51	1.07
2:B:384:THR:CG2	2:B:408:LEU:HD23	2.07	0.85
2:D:48:THR:HG21	8:D:655:HOH:O	1.83	0.78
2:B:384:THR:HG23	2:B:408:LEU:HD23	1.65	0.78
2:B:43:VAL:HG11	2:B:409:VAL:HG21	1.73	0.71
2:B:388:LEU:HD11	2:B:408:LEU:HD22	1.71	0.71
1:C:250:MET:HE2	1:C:256:MET:HE1	1.72	0.71
2:B:115:LYS:O	2:B:120:GLU:CG	2.36	0.70
1:C:173:MET:HG2	2:D:180:VAL:HG11	1.76	0.68
1:C:290:GLU:O	1:C:294:THR:HG23	1.94	0.67
2:B:153:ASN:OD1	2:B:177:THR:HG23	1.95	0.67
2:D:250:THR:O	4:D:504:TRS:H11	1.98	0.64
1:C:250:MET:SD	6:D:505:BZS:CG	2.87	0.63
2:B:51:ARG:HD3	2:B:63:LEU:CD2	2.29	0.62
2:D:38:ILE:CD1	2:D:391:MET:HE1	2.30	0.61
1:C:208:MET:HG3	2:D:363:PRO:HD3	1.81	0.61
2:B:107:ARG:HG2	2:B:110:GLN:HB2	1.84	0.60
2:D:252:GLY:O	4:D:504:TRS:H12	2.03	0.59
2:D:6:GLU:HG2	2:D:369:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ILE:HD11	2:D:391:MET:HE1	1.85	0.57
1:A:409:GLN:HE21	1:A:409:GLN:HA	1.69	0.57
2:B:43:VAL:CG1	2:B:409:VAL:HG21	2.34	0.57
2:B:45:ARG:NH2	8:B:603:HOH:O	2.37	0.57
1:A:164:ARG:HG3	2:B:237:TYR:HA	1.85	0.56
2:D:153:ASN:OD1	2:D:177:THR:HG23	2.06	0.56
2:B:51:ARG:HD3	2:B:63:LEU:HD23	1.89	0.55
2:D:41:GLU:O	2:D:80:ALA:HA	2.07	0.54
2:B:85:HIS:CD2	2:B:407:VAL:HG22	2.43	0.54
1:C:310:TYR:CD1	1:C:310:TYR:C	2.86	0.53
1:A:173:MET:HE3	1:A:206:GLN:HG2	1.91	0.53
2:B:270:LEU:HG	2:B:274:MET:HE2	1.91	0.52
3:C:601:GOL:O1	3:D:502:GOL:H11	2.09	0.52
2:B:40:ILE:CD1	2:B:79:ILE:HD11	2.40	0.51
1:C:164:ARG:HG3	2:D:237:TYR:HA	1.92	0.51
2:B:110:GLN:OE1	2:B:113:LYS:HD2	2.10	0.51
2:B:182:VAL:HB	2:B:183:PRO:HD3	1.93	0.51
1:A:163:VAL:HG11	2:B:163:GLY:HA2	1.93	0.51
2:D:249:THR:HB	4:D:504:TRS:N	2.27	0.50
2:B:110:GLN:OE1	2:B:113:LYS:CD	2.60	0.50
2:B:40:ILE:HD12	2:B:79:ILE:HD11	1.94	0.50
2:B:18:SER:HB2	2:B:105:ASN:OD1	2.12	0.50
1:C:208:MET:CG	2:D:363:PRO:HD3	2.43	0.49
1:C:222:LYS:NZ	8:C:705:HOH:O	2.45	0.49
1:A:409:GLN:HE21	1:A:409:GLN:CA	2.25	0.49
2:B:53:GLU:H	2:B:53:GLU:CD	2.22	0.48
1:A:184:ILE:HA	2:B:191:MET:HE2	1.94	0.48
1:C:4:ASP:N	1:C:4:ASP:OD1	2.44	0.48
1:C:127:THR:HB	1:C:128:PRO:HD2	1.95	0.48
1:C:290:GLU:OE2	1:C:294:THR:HG21	2.14	0.48
1:A:127:THR:HB	1:A:128:PRO:HD2	1.95	0.48
1:A:315:GLY:HA3	1:A:322[A]:VAL:HG11	1.96	0.48
1:C:250:MET:SD	6:D:505:BZS:CD1	3.02	0.47
1:A:220:GLU:HB3	1:A:222:LYS:HE3	1.95	0.47
1:C:315:GLY:HA3	1:C:322:VAL:HG11	1.97	0.47
2:D:43:VAL:HG11	2:D:409:VAL:HG21	1.96	0.47
2:B:51:ARG:CD	2:B:63:LEU:HD23	2.46	0.46
2:B:110:GLN:OE1	2:B:110:GLN:HA	2.16	0.45
2:B:41:GLU:O	2:B:80:ALA:HA	2.16	0.45
2:B:388:LEU:HD23	2:B:392:LEU:HD12	1.97	0.45
1:A:18:GLY:N	1:A:19:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:PRO:HD2	2:D:155:LEU:HD13	1.97	0.45
1:C:18:GLY:N	1:C:19:PRO:CD	2.79	0.45
2:D:80:ALA:O	2:D:408:LEU:HA	2.17	0.45
2:D:249:THR:HB	4:D:504:TRS:HN2	1.81	0.45
1:C:216:PHE:CZ	3:C:602:GOL:H32	2.52	0.45
2:B:399:ILE:O	2:B:403:VAL:HG22	2.17	0.44
1:A:78:HIS:CD2	1:A:404:ALA:HB2	2.53	0.44
1:A:24:MET:HE2	2:B:188:PHE:CG	2.52	0.44
1:C:409:GLN:OE1	1:C:409:GLN:HA	2.18	0.43
1:C:254:LYS:N	1:C:255:PRO:CD	2.80	0.43
2:B:372:GLU:HB2	2:B:374:LYS:HE3	1.99	0.43
2:D:38:ILE:HD13	2:D:391:MET:HE1	2.01	0.43
1:A:10:VAL:HB	1:A:32:VAL:HG22	2.01	0.43
2:B:388:LEU:HD11	2:B:408:LEU:CD2	2.45	0.43
2:B:391:MET:HG2	2:B:392:LEU:HG	2.01	0.43
2:D:18:SER:HB2	2:D:23:GLY:HA3	2.00	0.43
1:C:88:LEU:HD23	1:C:389:CYS:SG	2.60	0.42
1:C:9:ARG:HG2	1:C:92:ALA:HA	2.02	0.42
1:C:296:CYS:O	1:C:300:GLU:HB2	2.18	0.42
2:B:134:SER:O	2:B:210:GLN:HG3	2.20	0.42
2:D:45:ARG:HD2	2:D:45:ARG:HA	1.89	0.42
2:B:395:SER:O	2:B:399:ILE:HD12	2.20	0.42
1:C:250:MET:HE1	2:D:148:TYR:CE1	2.55	0.41
1:C:342:PHE:CD1	2:D:212:GLU:HG2	2.55	0.41
2:D:53:GLU:H	2:D:53:GLU:CD	2.27	0.41
2:D:158:LEU:C	2:D:158:LEU:HD23	2.45	0.41
2:D:250:THR:O	4:D:504:TRS:H31	2.19	0.41
2:D:310:TYR:H	7:D:506:PGE:H6	1.85	0.41
2:B:384:THR:HG21	2:B:408:LEU:HD23	1.95	0.41
1:C:310:TYR:O	1:C:314:ILE:HG22	2.19	0.41
2:D:293:ARG:HE	2:D:293:ARG:HB2	1.65	0.41
1:A:381:HIS:O	1:A:385:VAL:HG23	2.20	0.41
1:C:310:TYR:C	1:C:310:TYR:HD1	2.29	0.41
1:A:312:TYR:CG	1:A:324:PRO:HD3	2.54	0.41
1:A:3:GLN:OE1	1:A:3:GLN:N	2.54	0.41
2:B:243:ALA:HA	2:B:244:PRO:C	2.46	0.41
2:B:400:GLU:O	2:B:404:SER:HB3	2.21	0.41
1:C:281:ILE:HG22	1:C:281:ILE:O	2.21	0.41
2:D:79:ILE:HG22	2:D:384:THR:HA	2.02	0.40
2:B:115:LYS:HB3	2:B:115:LYS:HE3	1.83	0.40
1:A:249:ILE:HD12	1:A:257:TRP:HB2	2.04	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	411/410 (100%)	398 (97%)	13 (3%)	0	100	100
1	C	411/410 (100%)	403 (98%)	7 (2%)	1 (0%)	43	42
2	B	406/409 (99%)	397 (98%)	7 (2%)	2 (0%)	24	21
2	D	407/409 (100%)	397 (98%)	9 (2%)	1 (0%)	43	42
All	All	1635/1638 (100%)	1595 (98%)	36 (2%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	211	GLU
2	D	20	VAL
2	B	20	VAL
2	B	21	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	321/317 (101%)	317 (99%)	4 (1%)	63	70
1	C	320/317 (101%)	316 (99%)	4 (1%)	61	68
2	B	319/320 (100%)	316 (99%)	3 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	320/320 (100%)	315 (98%)	5 (2%)	55	62
All	All	1280/1274 (100%)	1264 (99%)	16 (1%)	61	68

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	190	GLN
1	A	362	TYR
1	A	409	GLN
2	B	53	GLU
2	B	115	LYS
2	B	408	LEU
1	C	3	GLN
1	C	5	PHE
1	C	362	TYR
1	C	394	SER
2	D	4	SER
2	D	5	VAL
2	D	39	ARG
2	D	48	THR
2	D	404	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	346	GLN
1	A	409	GLN
1	C	123	GLN
1	C	344	GLN
1	C	346	GLN
1	C	354	ASN
2	D	235	GLN
2	D	276	ASN

5.3.3 RNA ⓘ

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](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	504	-	5,5,5	0.91	0	5,5,5	1.13	0
3	GOL	D	502	-	5,5,5	0.96	0	5,5,5	0.80	0
3	GOL	D	508	-	5,5,5	0.95	0	5,5,5	0.67	0
3	GOL	A	801	-	5,5,5	0.83	0	5,5,5	1.23	0
4	TRS	B	502	-	7,7,7	0.15	0	9,9,9	0.21	0
6	BZS	D	505	-	15,15,15	0.81	0	19,19,19	1.09	1 (5%)
4	TRS	D	504	-	7,7,7	1.75	1 (14%)	9,9,9	2.82	6 (66%)
5	COA	D	503	-	47,50,50	3.45	16 (34%)	69,75,75	1.76	16 (23%)
7	PGE	D	507	-	9,9,9	0.53	0	8,8,8	0.64	0
3	GOL	C	601	-	5,5,5	1.46	1 (20%)	5,5,5	1.56	1 (20%)
3	GOL	D	501	-	5,5,5	1.12	0	5,5,5	1.05	1 (20%)
3	GOL	C	602	-	5,5,5	1.33	1 (20%)	5,5,5	1.25	1 (20%)
3	GOL	B	501	-	5,5,5	1.00	0	5,5,5	1.00	0
3	GOL	B	503	-	5,5,5	1.17	0	5,5,5	1.22	0
7	PGE	D	506	-	9,9,9	0.51	0	8,8,8	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	508	-	-	2/4/4/4	-
3	GOL	A	801	-	-	0/4/4/4	-
4	TRS	B	502	-	-	5/9/9/9	-
6	BZS	D	505	-	-	6/12/12/12	0/1/1/1
4	TRS	D	504	-	-	8/9/9/9	-
5	COA	D	503	-	-	4/48/64/64	0/3/3/3
7	PGE	D	507	-	-	4/7/7/7	-
3	GOL	C	601	-	-	0/4/4/4	-
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	C	602	-	-	3/4/4/4	-
3	GOL	B	501	-	-	0/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
7	PGE	D	506	-	-	4/7/7/7	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	COA	C3B-C4B	-9.38	1.28	1.52
5	D	503	COA	C2B-C1B	-9.11	1.24	1.53
5	D	503	COA	O4B-C1B	8.84	1.62	1.42
5	D	503	COA	C2B-C3B	7.58	1.69	1.53
5	D	503	COA	P1A-O3A	7.08	1.67	1.59
5	D	503	COA	P2A-O3A	6.33	1.66	1.59
5	D	503	COA	C9P-N8P	5.29	1.46	1.33
5	D	503	COA	P3B-O3B	4.62	1.67	1.59
5	D	503	COA	C5P-N4P	4.49	1.44	1.33
5	D	503	COA	C6A-N6A	4.15	1.44	1.34
5	D	503	COA	O4B-C4B	3.97	1.53	1.45
4	D	504	TRS	C-N	3.96	1.62	1.49
5	D	503	COA	O9P-C9P	-2.75	1.18	1.23
5	D	503	COA	C8A-N9A	-2.70	1.33	1.37
5	D	503	COA	CCP-CBP	2.40	1.56	1.52
5	D	503	COA	C5B-C4B	2.25	1.58	1.51
3	C	601	GOL	O2-C2	-2.24	1.36	1.43
3	C	602	GOL	O2-C2	-2.17	1.37	1.43
5	D	503	COA	P2A-O6A	2.09	1.67	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503	COA	C5A-C4A-N3A	-5.74	118.81	126.72
4	D	504	TRS	C2-C-N	5.09	121.14	108.17
5	D	503	COA	N3A-C2A-N1A	-4.85	121.25	128.58
5	D	503	COA	N3A-C4A-N9A	4.40	134.65	127.17
5	D	503	COA	C2A-N3A-C4A	3.70	120.88	111.83
5	D	503	COA	C2B-C1B-N9A	-3.61	104.34	113.30
4	D	504	TRS	C3-C-C2	-3.61	101.05	110.66
4	D	504	TRS	C3-C-C1	-3.28	101.91	110.66
3	C	601	GOL	C3-C2-C1	-3.04	100.67	111.80
5	D	503	COA	N9A-C8A-N7A	-2.96	109.74	113.94
4	D	504	TRS	C3-C-N	2.70	115.05	108.17
5	D	503	COA	C5A-N7A-C8A	2.65	107.61	103.45
5	D	503	COA	C2P-C3P-N4P	-2.53	106.56	112.31
5	D	503	COA	O2B-C2B-C1B	2.51	118.75	110.10
4	D	504	TRS	O3-C3-C	2.46	117.73	110.88
5	D	503	COA	C4A-N9A-C8A	2.38	108.24	105.74
5	D	503	COA	C4A-C5A-N7A	-2.37	107.87	110.58
3	C	602	GOL	C3-C2-C1	-2.32	103.27	111.80
6	D	505	BZS	O4-C-CA	2.31	120.14	114.16
4	D	504	TRS	C2-C-C1	-2.27	104.60	110.66
5	D	503	COA	CAP-C9P-N8P	2.26	120.78	116.48
5	D	503	COA	O4B-C1B-N9A	2.26	112.43	108.09
5	D	503	COA	C2A-N1A-C6A	2.07	122.13	118.73
5	D	503	COA	OAP-CAP-CBP	-2.03	105.47	110.18
3	D	501	GOL	C3-C2-C1	-2.03	104.37	111.80
5	D	503	COA	C2B-C3B-C4B	2.02	106.78	103.24

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-C3
3	B	504	GOL	C1-C2-C3-O3
3	B	504	GOL	O2-C2-C3-O3
3	C	602	GOL	O1-C1-C2-C3
3	D	501	GOL	C1-C2-C3-O3
3	D	502	GOL	O1-C1-C2-C3
4	D	504	TRS	C2-C-C3-O3
5	D	503	COA	S1P-C2P-C3P-N4P
6	D	505	BZS	C1-C2-CA-C
7	D	507	PGE	O2-C3-C4-O3
3	D	508	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	D	505	BZS	C2-CA-CB-CG
3	C	602	GOL	O1-C1-C2-O2
3	D	501	GOL	O2-C2-C3-O3
3	D	502	GOL	O1-C1-C2-O2
6	D	505	BZS	C-CA-CB-CG
7	D	507	PGE	O3-C5-C6-O4
4	B	502	TRS	C3-C-C2-O2
4	B	502	TRS	N-C-C2-O2
4	D	504	TRS	N-C-C3-O3
7	D	506	PGE	C4-C3-O2-C2
7	D	507	PGE	C4-C3-O2-C2
4	D	504	TRS	C2-C-C1-O1
4	D	504	TRS	C1-C-C3-O3
6	D	505	BZS	O3-C-CA-C2
6	D	505	BZS	O4-C-CA-C2
7	D	506	PGE	C6-C5-O3-C4
7	D	506	PGE	O2-C3-C4-O3
4	D	504	TRS	C3-C-C1-O1
4	D	504	TRS	C3-C-C2-O2
3	C	602	GOL	C1-C2-C3-O3
3	D	508	GOL	O2-C2-C3-O3
7	D	507	PGE	C6-C5-O3-C4
7	D	506	PGE	C1-C2-O2-C3
5	D	503	COA	C5P-C6P-C7P-N8P
5	D	503	COA	C4B-C5B-O5B-P1A
4	B	502	TRS	C3-C-C1-O1
4	B	502	TRS	C1-C-C2-O2
6	D	505	BZS	C1-C2-CA-CB
5	D	503	COA	O4B-C4B-C5B-O5B
4	B	502	TRS	C2-C-C1-O1
4	D	504	TRS	N-C-C1-O1
4	D	504	TRS	N-C-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

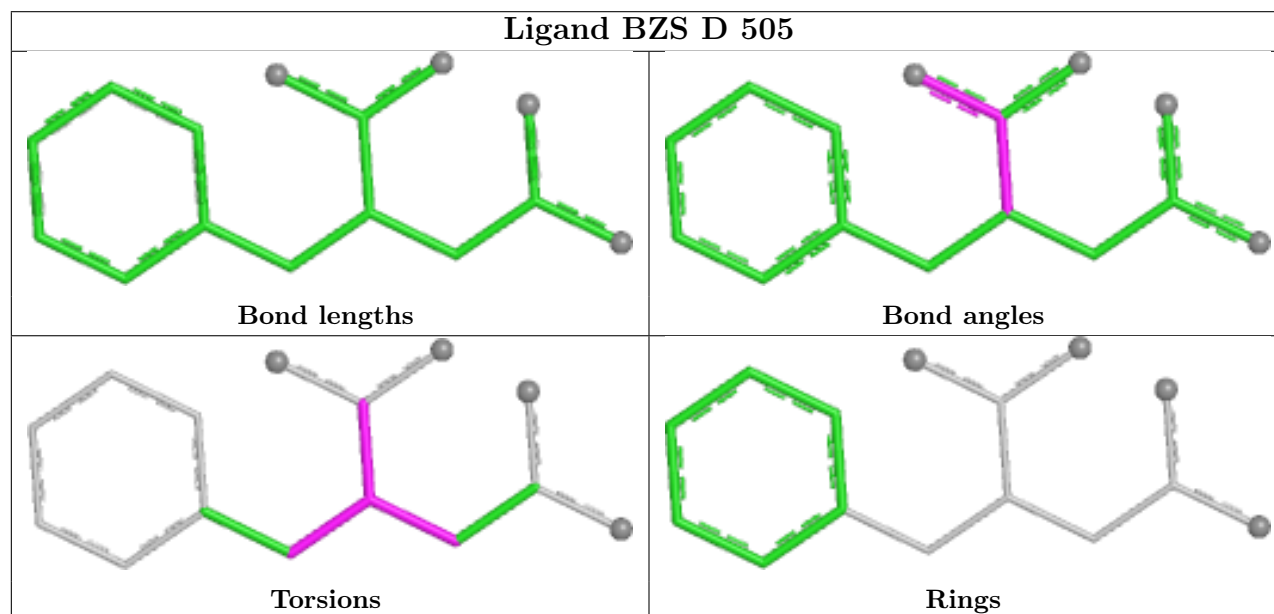
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	GOL	1	0
6	D	505	BZS	2	0
4	D	504	TRS	5	0
3	C	601	GOL	1	0
3	C	602	GOL	1	0

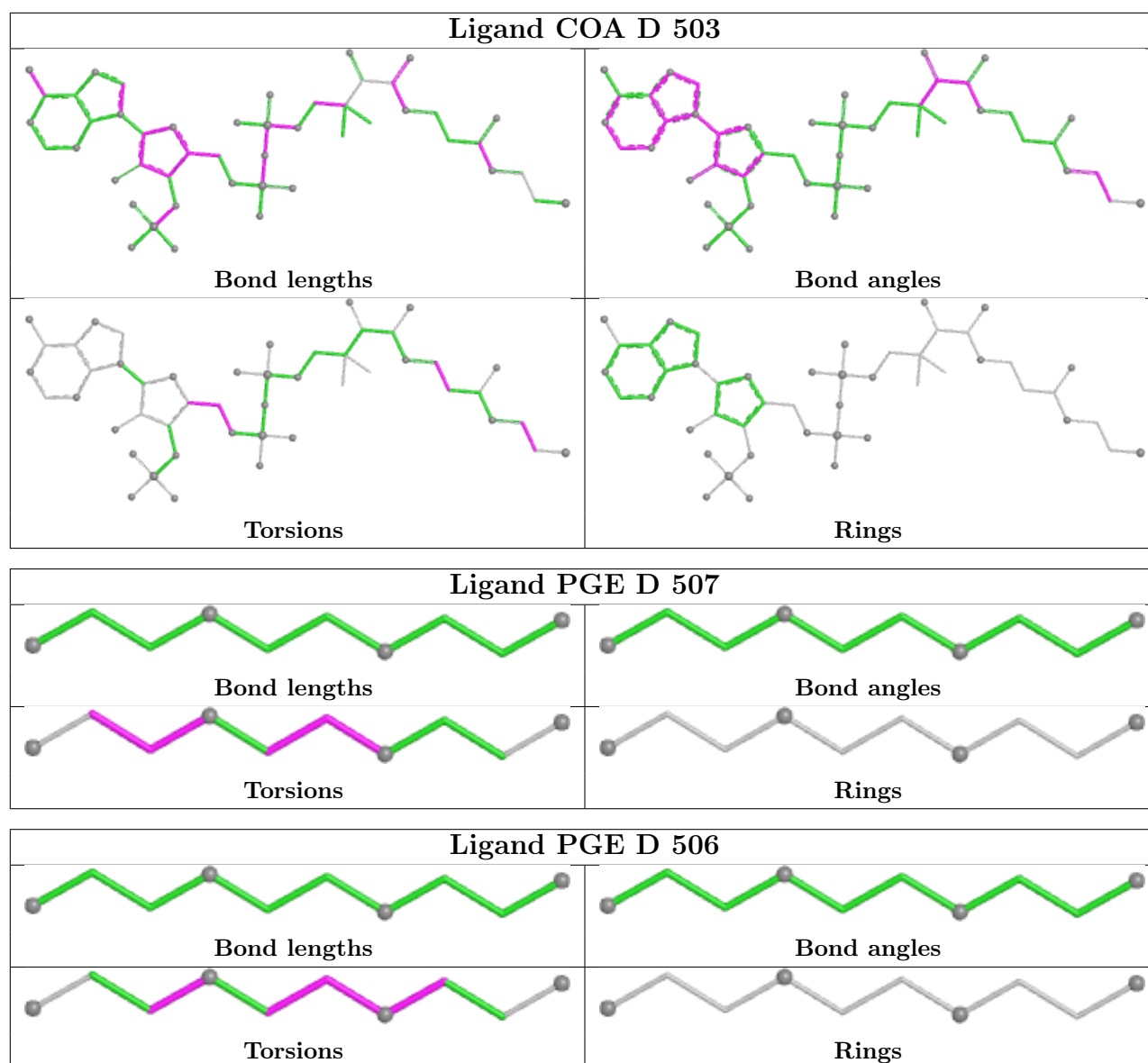
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	506	PGE	1	0

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	407/410 (99%)	-0.14	1 (0%) 91 90	16, 41, 75, 119	4 (0%)
1	C	408/410 (99%)	-0.10	5 (1%) 76 76	21, 40, 69, 122	3 (0%)
2	B	406/409 (99%)	0.18	16 (3%) 43 42	16, 43, 90, 113	2 (0%)
2	D	406/409 (99%)	-0.35	2 (0%) 87 87	14, 35, 55, 98	3 (0%)
All	All	1627/1638 (99%)	-0.10	24 (1%) 72 71	14, 39, 77, 122	12 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	408	LEU	5.2
2	B	20	VAL	4.2
2	B	116	LEU	4.1
1	C	2	GLY	3.8
2	B	19	TRP	3.1
1	C	4	ASP	3.0
1	A	409	GLN	2.8
1	C	3	GLN	2.6
2	B	405	HIS	2.6
2	B	4	SER	2.6
2	B	407	VAL	2.5
2	B	409	VAL	2.5
2	D	4	SER	2.4
2	B	403	VAL	2.3
2	B	115	LYS	2.2
2	B	48	THR	2.2
2	B	86	PRO	2.2
2	B	404	SER	2.2
2	B	114	TRP	2.2
1	C	409	GLN	2.1
2	B	105	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	283	TYR	2.1
2	D	5	VAL	2.1
2	B	81	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](#)

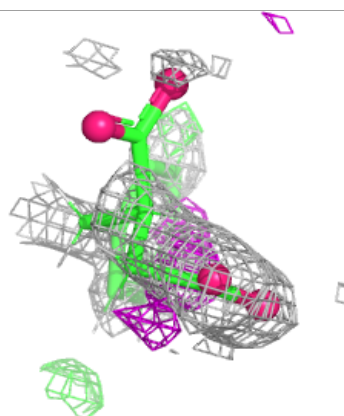
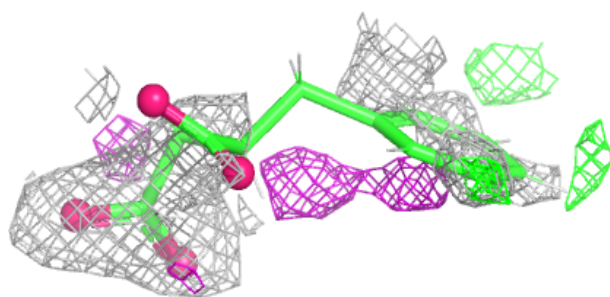
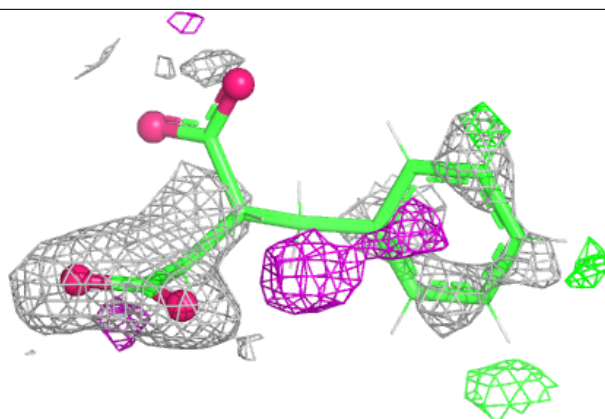
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TRS	D	504	8/8	0.65	0.26	33,49,70,70	0
3	GOL	A	801	6/6	0.76	0.23	49,77,88,105	0
3	GOL	C	602	6/6	0.78	0.16	49,65,78,85	0
3	GOL	D	502	6/6	0.80	0.22	49,100,120,132	0
6	BZS	D	505	15/15	0.83	0.26	46,109,150,150	0
3	GOL	D	508	6/6	0.85	0.17	59,74,88,92	0
7	PGE	D	506	10/10	0.85	0.13	41,57,66,79	0
3	GOL	B	503	6/6	0.86	0.10	41,55,66,66	0
3	GOL	C	601	6/6	0.86	0.12	43,57,72,76	0
3	GOL	B	501	6/6	0.89	0.13	42,55,69,69	0
3	GOL	B	504	6/6	0.90	0.11	40,52,65,65	0
4	TRS	B	502	8/8	0.91	0.08	28,36,48,54	0
7	PGE	D	507	10/10	0.91	0.11	37,51,70,80	0
3	GOL	D	501	6/6	0.93	0.10	36,46,55,55	0
5	COA	D	503	48/48	0.95	0.07	29,40,64,74	0

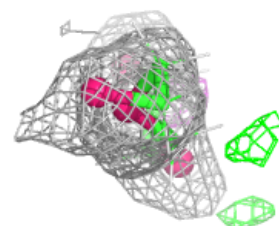
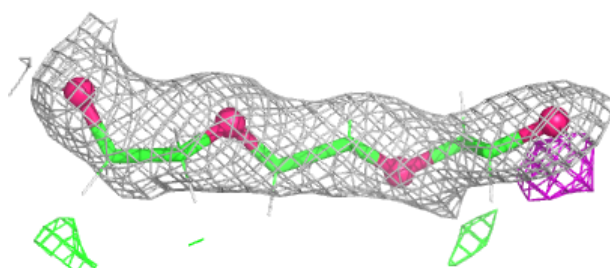
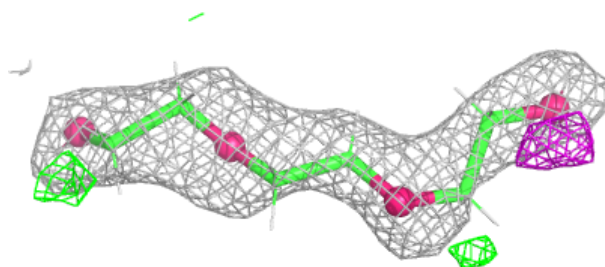
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BZS 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)

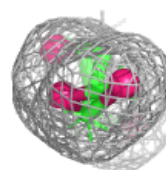
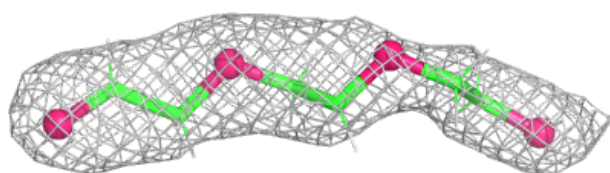
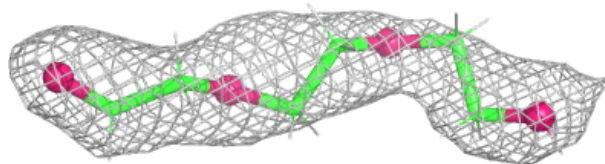
**Electron density around PGE D 506:**

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

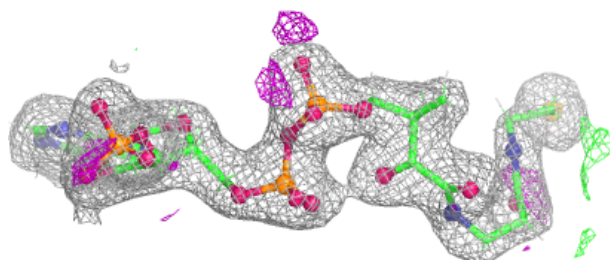
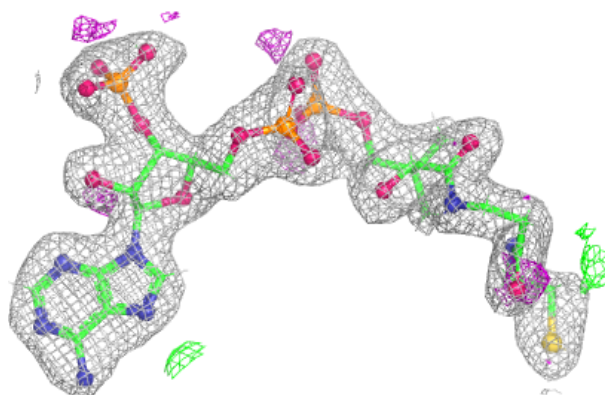


Electron density around PGE D 507:

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

**Electron density around COA D 503:**

$2mF_o-DF_c$ (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.