



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:15 AM UTC

PDB ID : 6Y1E / pdb_00006y1e
Title : Crystal structure of human glutathione transferase P1-1 (hGSTP1-1) that was co-crystallised in the presence of indanyloxyacetic acid-94 (IAA-94)
Authors : Pandian, R.; Worth, R.; Thangaraj, V.; Sayed, Y.; Dirr, H.W.
Deposited on : 2020-02-12
Resolution : 1.40 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

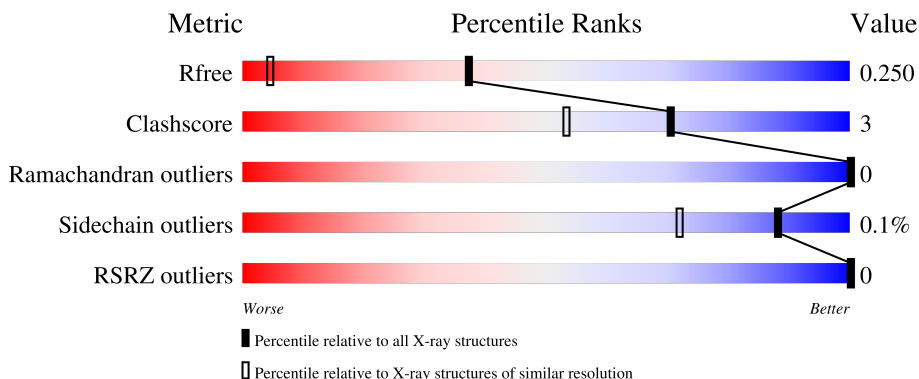
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

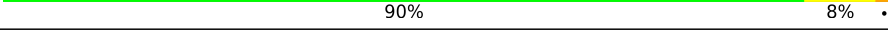
The reported resolution of this entry is 1.40 Å.

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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	210	
1	B	210	
1	C	210	
1	D	210	

2 Entry composition [i](#)

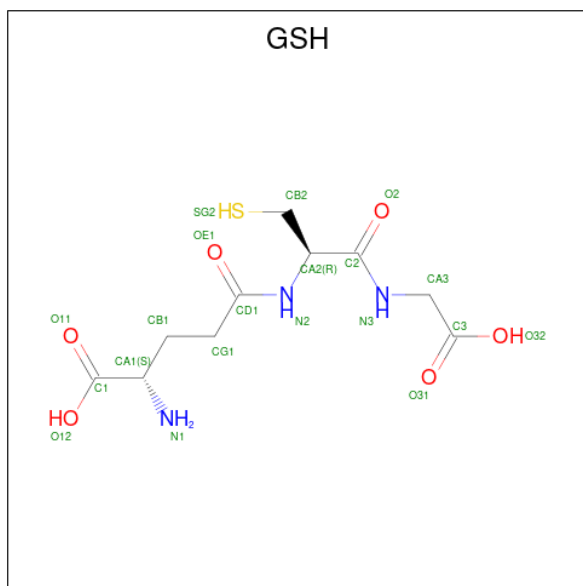
There are 6 unique types of molecules in this entry. The entry contains 7649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutathione S-transferase P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	2	0
			1652	1060	274	310	8			
1	B	208	Total	C	N	O	S	0	4	0
			1659	1064	275	312	8			
1	C	209	Total	C	N	O	S	0	2	0
			1652	1060	274	310	8			
1	D	209	Total	C	N	O	S	0	3	0
			1658	1063	275	312	8			

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



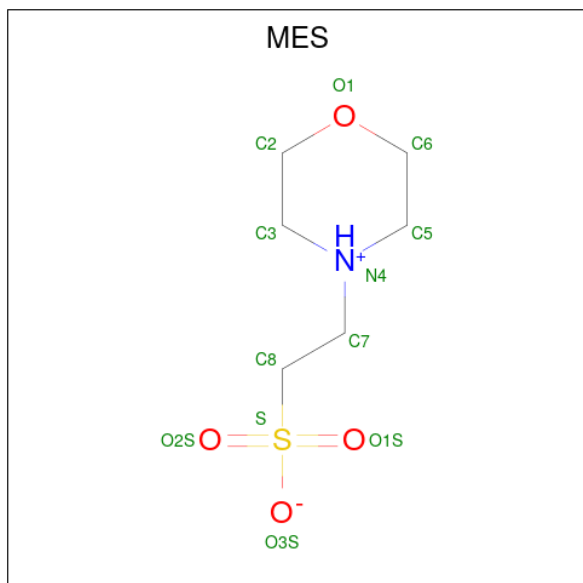
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

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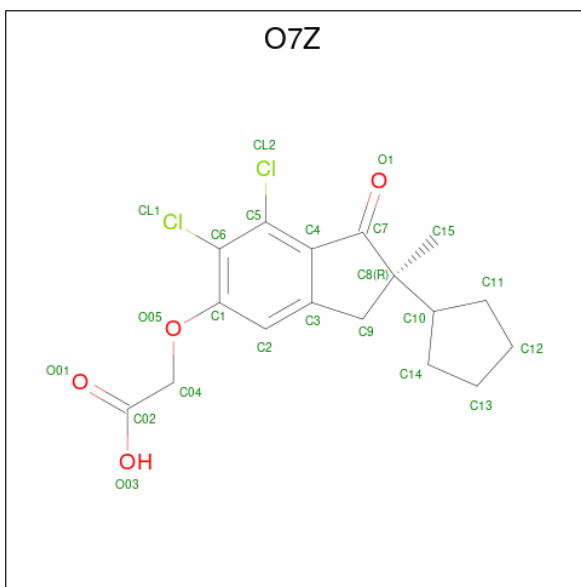
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



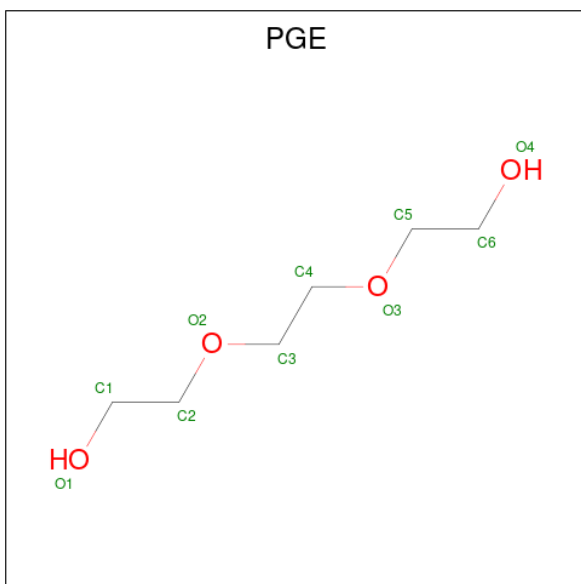
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is 2-[[6,7-bis(chloranyl)-2-cyclopentyl-2-methyl-1-oxidanylidene-3 {H}-inden-5-yl]oxy]ethanoic acid (CCD ID: O7Z) (formula: $C_{17}H_{18}Cl_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	2	3		
4	B	1	Total	C	O	0	0
			5	2	3		
4	D	1	Total	C	O	0	0
			5	2	3		

- Molecule 5 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
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	206	Total	O	0	0
			206	206		
6	B	212	Total	O	0	0
			212	212		
6	C	207	Total	O	0	0
			207	207		
6	D	216	Total	O	0	0
			216	216		

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.

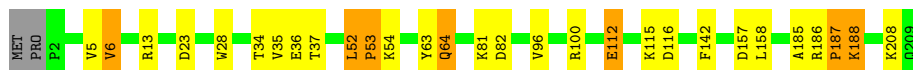
- Molecule 1: Glutathione S-transferase P

Chain A: 



- Molecule 1: Glutathione S-transferase P

Chain B: 



- Molecule 1: Glutathione S-transferase P

Chain C: 



- Molecule 1: Glutathione S-transferase P

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.64Å 72.18Å 88.62Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	55.97 – 1.40 55.97 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (55.97-1.40) 94.4 (55.97-1.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.217 , 0.251 0.220 , 0.250	Depositor DCC
R_{free} test set	7891 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l 0.000 for k,h,-l 0.179 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8230e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PGE, GSH, O7Z, MES

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	1.19	11/1687 (0.7%)	1.12	15/2287 (0.7%)
1	B	1.49	17/1693 (1.0%)	1.25	24/2294 (1.0%)
1	C	1.17	11/1687 (0.7%)	0.90	5/2287 (0.2%)
1	D	1.41	10/1693 (0.6%)	0.80	5/2295 (0.2%)
All	All	1.32	49/6760 (0.7%)	1.03	49/9163 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	ASP	C-N	-32.07	0.91	1.33
1	D	35	VAL	C-N	-32.01	0.88	1.33
1	C	115	LYS	C-N	-29.72	0.92	1.33
1	D	34	THR	C-N	-27.32	1.01	1.33
1	A	196	PRO	C-N	-23.73	1.04	1.33
1	B	34	THR	C-N	-21.45	1.07	1.33
1	D	36	GLU	C-N	-16.87	1.11	1.34
1	B	187	PRO	N-CA	16.05	1.69	1.47
1	A	196	PRO	N-CA	15.78	1.67	1.47
1	C	196	PRO	N-CA	14.83	1.67	1.47
1	B	157	ASP	C-N	-14.41	1.15	1.33
1	C	58	GLY	C-N	-12.31	1.14	1.33
1	B	52	LEU	C-N	-12.24	1.10	1.34
1	B	81	LYS	C-N	-11.75	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PRO	C-N	-11.56	1.19	1.34
1	B	63	TYR	C-N	10.61	1.48	1.33
1	D	100	ARG	C-N	-10.26	1.20	1.33
1	A	197	GLU	C-N	-10.13	1.19	1.33
1	B	53	PRO	N-CA	10.07	1.64	1.47
1	C	1	PRO	C-N	9.80	1.48	1.33
1	A	83	GLN	C-N	-9.73	1.21	1.33
1	A	39	GLN	C-N	-9.63	1.20	1.33
1	C	116	ASP	C-N	-9.32	1.21	1.33
1	A	84	GLN	C-N	-8.37	1.23	1.33
1	B	36	GLU	C-N	-8.24	1.22	1.33
1	C	2	PRO	C-O	-8.15	1.13	1.24
1	C	100	ARG	C-N	-8.13	1.23	1.33
1	A	100	ARG	C-N	-7.67	1.23	1.33
1	C	59	ASP	C-N	-7.65	1.22	1.33
1	B	188	LYS	C-N	-7.49	1.23	1.33
1	B	6	VAL	C-N	-7.26	1.24	1.33
1	B	35	VAL	C-N	7.23	1.44	1.34
1	A	91	MET	C-N	-7.01	1.25	1.33
1	D	132	LEU	C-O	-6.84	1.16	1.24
1	B	115	LYS	C-N	-6.68	1.25	1.33
1	D	1	PRO	N-CD	-6.64	1.38	1.47
1	C	196	PRO	C-O	-6.57	1.15	1.24
1	B	5	VAL	C-N	-6.51	1.24	1.33
1	D	64	GLN	C-O	-6.21	1.16	1.24
1	A	196	PRO	C-O	-6.19	1.16	1.24
1	B	100	ARG	C-N	-5.75	1.26	1.33
1	D	187	PRO	C-O	-5.73	1.16	1.24
1	B	64	GLN	C-O	-5.61	1.17	1.24
1	B	187	PRO	C-O	-5.60	1.16	1.24
1	C	177	SER	C-N	5.51	1.41	1.34
1	C	195	SER	C-N	5.37	1.42	1.33
1	D	186	ARG	C-O	-5.26	1.17	1.24
1	A	104	ILE	C-O	-5.25	1.18	1.24
1	A	174	PRO	C-O	-5.01	1.17	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ARG	CA-C-N	19.30	139.04	118.97
1	B	186	ARG	C-N-CA	19.30	139.04	118.97
1	A	195	SER	CA-C-N	14.09	137.46	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	SER	C-N-CA	14.09	137.46	119.84
1	A	28	TRP	CA-C-N	13.47	141.31	122.72
1	A	28	TRP	C-N-CA	13.47	141.31	122.72
1	C	195	SER	CA-C-N	12.87	134.00	119.32
1	C	195	SER	C-N-CA	12.87	134.00	119.32
1	A	29	LYS	O-C-N	11.49	136.26	123.27
1	C	1	PRO	CA-C-N	11.43	132.35	119.32
1	C	1	PRO	C-N-CA	11.43	132.35	119.32
1	A	196	PRO	O-C-N	11.10	137.63	122.64
1	B	112	GLU	O-C-N	10.99	133.39	122.07
1	A	195	SER	O-C-N	-10.46	109.81	121.53
1	B	35	VAL	O-C-N	9.81	135.26	121.82
1	B	36	GLU	O-C-N	-9.10	111.08	122.27
1	B	186	ARG	O-C-N	-8.93	112.10	121.30
1	B	116	ASP	O-C-N	8.90	131.56	122.12
1	B	112	GLU	CA-C-N	-8.52	106.20	120.68
1	B	112	GLU	C-N-CA	-8.52	106.20	120.68
1	B	82	ASP	O-C-N	-8.29	114.56	123.26
1	A	59	ASP	CA-CB-CG	8.15	120.75	112.60
1	B	52	LEU	C-N-CD	7.20	136.44	120.60
1	B	36	GLU	CA-C-N	7.04	130.29	120.29
1	B	36	GLU	C-N-CA	7.04	130.29	120.29
1	D	1	PRO	O-C-N	-6.92	111.92	123.00
1	B	187	PRO	N-CA-C	-6.70	103.89	113.47
1	B	185	ALA	CA-C-N	-6.65	111.14	120.39
1	B	185	ALA	C-N-CA	-6.65	111.14	120.39
1	A	29	LYS	CA-C-N	-6.60	113.99	122.77
1	A	29	LYS	C-N-CA	-6.60	113.99	122.77
1	A	39	GLN	CA-C-N	6.24	129.15	120.29
1	A	39	GLN	C-N-CA	6.24	129.15	120.29
1	C	196	PRO	N-CA-C	-6.19	104.53	113.75
1	B	35	VAL	CA-C-N	-5.90	111.34	120.31
1	B	35	VAL	C-N-CA	-5.90	111.34	120.31
1	B	100	ARG	CA-C-O	-5.86	114.34	120.55
1	B	53	PRO	CA-N-CD	-5.83	103.34	111.50
1	A	28	TRP	O-C-N	-5.66	116.80	123.25
1	B	187	PRO	CA-N-CD	-5.64	104.11	112.00
1	A	100	ARG	CA-C-O	-5.62	114.60	120.55
1	D	35	VAL	CA-C-N	5.60	132.24	121.54
1	D	35	VAL	C-N-CA	5.60	132.24	121.54
1	D	141	THR	CB-CA-C	5.58	121.52	110.42
1	B	100	ARG	O-C-N	5.55	128.01	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	ARG	CA-C-O	-5.55	114.67	120.55
1	A	196	PRO	N-CA-C	-5.35	101.46	112.47
1	B	6	VAL	O-C-N	-5.22	116.04	122.88
1	B	142	PHE	N-CA-CB	5.04	119.53	111.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLU	Mainchain

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	1652	0	1654	14	0
1	B	1659	0	1658	10	0
1	C	1652	0	1653	9	0
1	D	1658	0	1656	13	0
2	A	20	0	15	0	0
2	B	20	0	15	0	0
2	C	20	0	15	1	0
2	D	20	0	15	0	0
3	A	12	0	12	0	0
3	B	24	0	24	1	0
3	C	12	0	12	1	0
3	D	24	0	24	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	2	0
5	C	10	0	14	1	0
5	D	10	0	14	2	0
6	A	206	0	0	1	0
6	B	212	0	0	2	0
6	C	207	0	0	2	0
6	D	216	0	0	1	0
All	All	7649	0	6781	46	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 (46) 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)
1:B:187:PRO:N	1:B:187:PRO:CA	1.69	1.42
1:C:196:PRO:N	1:C:196:PRO:CA	1.67	1.35
1:A:196:PRO:N	1:A:196:PRO:CA	1.67	1.29
2:C:301:GSH:SG2	6:C:557:HOH:O	2.35	0.83
1:D:1:PRO:H2	1:D:2:PRO:HD2	1.46	0.80
1:A:196:PRO:N	1:A:197:GLU:N	2.30	0.80
1:A:147:GLN:NE2	1:D:187:PRO:HD2	2.01	0.76
1:D:99:LEU:HD23	1:D:158:LEU:HD21	1.72	0.71
1:A:99:LEU:HD23	1:A:158:LEU:HD21	1.72	0.71
1:A:196:PRO:N	1:A:196:PRO:C	2.48	0.70
1:D:54:LYS:NZ	5:D:304:PGE:H6	2.07	0.70
1:A:147:GLN:HE22	1:D:187:PRO:HD2	1.59	0.67
1:A:84:GLN:NE2	6:A:402:HOH:O	2.29	0.66
1:D:135:GLN:HA	1:D:135:GLN:OE1	1.95	0.66
1:B:187:PRO:N	1:B:187:PRO:C	2.54	0.65
1:D:54:LYS:HZ3	5:D:304:PGE:H6	1.62	0.65
1:A:19[B]:MET:HE1	1:A:157:ASP:HB2	1.82	0.62
1:C:196:PRO:N	1:C:196:PRO:C	2.54	0.62
1:B:52:LEU:HB3	1:B:53:PRO:HA	1.82	0.61
1:A:19[B]:MET:HG2	1:A:189:LEU:HD11	1.89	0.54
1:C:99:LEU:HD23	1:C:158:LEU:HD21	1.89	0.54
1:C:84:GLN:NE2	6:C:401:HOH:O	2.24	0.54
1:D:1:PRO:H2	1:D:2:PRO:CD	2.21	0.52
1:D:4:THR:HB	1:D:56:GLN:HB2	1.94	0.50
3:D:303:MES:O1S	4:D:305:O7Z:O05	2.29	0.50
1:D:6:VAL:HB	1:D:54:LYS:HB3	1.94	0.49
1:B:13:ARG:NH1	6:B:407:HOH:O	2.45	0.49
1:B:23:ASP:O	1:B:188:LYS:HE2	2.13	0.48
1:D:92:VAL:HG22	1:D:132:LEU:HD13	1.96	0.47
1:C:59:ASP:OD1	1:C:60:LEU:N	2.49	0.45
1:B:112:GLU:OE2	1:B:208:LYS:NZ	2.45	0.45
1:A:1:PRO:H2	1:A:2:PRO:HA	1.82	0.44
1:D:137:GLN:NE2	1:D:141:THR:HG21	2.32	0.43
1:C:6:VAL:HB	1:C:54:LYS:HB3	2.00	0.43
1:A:19[B]:MET:CE	1:A:157:ASP:HB2	2.48	0.43
1:D:27:SER:HA	6:D:530:HOH:O	2.19	0.43
1:C:28:TRP:O	3:C:302:MES:H21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HB3	1:C:53:PRO:HA	2.01	0.42
1:B:28:TRP:CH2	3:B:302:MES:H81	2.56	0.41
1:A:94:ASP:HB2	1:B:64:GLN:HG3	2.02	0.41
1:A:70:ARG:HD2	6:B:466:HOH:O	2.21	0.41
1:B:6:VAL:HB	1:B:54:LYS:HB3	2.03	0.41
1:B:96:VAL:HG13	1:B:158:LEU:HD22	2.02	0.41
1:A:156:LEU:HD22	1:A:183:LEU:HB3	2.04	0.40
1:C:56:GLN:OE1	5:C:303:PGE:H42	2.22	0.40
3:D:303:MES:S	4:D:305:O7Z:O05	2.79	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	209/210 (100%)	205 (98%)	4 (2%)	0	100	100
1	B	210/210 (100%)	205 (98%)	5 (2%)	0	100	100
1	C	209/210 (100%)	203 (97%)	6 (3%)	0	100	100
1	D	210/210 (100%)	205 (98%)	5 (2%)	0	100	100
All	All	838/840 (100%)	818 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	178/177 (101%)	178 (100%)	0	100	100
1	B	179/177 (101%)	178 (99%)	1 (1%)	78	56
1	C	178/177 (101%)	178 (100%)	0	100	100
1	D	179/177 (101%)	179 (100%)	0	100	100
All	All	714/708 (101%)	713 (100%)	1 (0%)	88	72

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	51	GLN
1	A	147	GLN
1	A	204	ASN
1	B	24	GLN
1	B	147	GLN
1	B	204	ASN
1	C	51	GLN
1	C	204	ASN
1	D	24	GLN
1	D	51	GLN
1	D	137	GLN

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

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
2	GSH	D	301	-	18,19,19	1.93	3 (16%)	21,24,24	1.35	3 (14%)
2	GSH	B	301	-	18,19,19	1.97	4 (22%)	21,24,24	1.37	3 (14%)
2	GSH	C	301	-	18,19,19	1.86	2 (11%)	21,24,24	1.17	1 (4%)
3	MES	D	303	-	12,12,12	4.38	6 (50%)	15,16,16	1.23	2 (13%)
3	MES	C	302	-	12,12,12	4.33	7 (58%)	15,16,16	1.74	4 (26%)
4	O7Z	A	303	-	4,4,25	1.07	0	4,4,38	2.63	1 (25%)
4	O7Z	D	305	-	4,4,25	1.04	0	4,4,38	2.49	1 (25%)
5	PGE	C	303	-	9,9,9	0.54	0	8,8,8	0.38	0
5	PGE	D	304	-	9,9,9	0.51	0	8,8,8	0.34	0
3	MES	A	302	-	12,12,12	4.37	7 (58%)	15,16,16	1.92	4 (26%)
4	O7Z	B	304	-	4,4,25	0.95	0	4,4,38	2.82	1 (25%)
3	MES	D	302	-	12,12,12	4.35	7 (58%)	15,16,16	1.37	2 (13%)
2	GSH	A	301	-	18,19,19	1.83	3 (16%)	21,24,24	1.43	2 (9%)
3	MES	B	303	-	12,12,12	4.49	6 (50%)	15,16,16	1.49	5 (33%)
3	MES	B	302	-	12,12,12	4.34	7 (58%)	15,16,16	1.37	3 (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
2	GSH	D	301	-	-	0/24/24/24	-
2	GSH	B	301	-	-	1/24/24/24	-
2	GSH	C	301	-	-	2/24/24/24	-
3	MES	D	303	-	-	1/6/14/14	0/1/1/1
3	MES	C	302	-	-	0/6/14/14	0/1/1/1
4	O7Z	A	303	-	-	2/2/2/33	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	O7Z	D	305	-	-	2/2/2/33	-
5	PGE	C	303	-	-	3/7/7/7	-
5	PGE	D	304	-	-	2/7/7/7	-
3	MES	A	302	-	-	2/6/14/14	0/1/1/1
4	O7Z	B	304	-	-	2/2/2/33	-
3	MES	D	302	-	-	2/6/14/14	0/1/1/1
2	GSH	A	301	-	-	0/24/24/24	-
3	MES	B	303	-	-	6/6/14/14	0/1/1/1
3	MES	B	302	-	-	5/6/14/14	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	MES	C7-N4	-8.89	1.27	1.47
3	D	303	MES	C7-N4	-8.82	1.27	1.47
3	D	302	MES	C7-N4	-8.63	1.27	1.47
3	B	302	MES	C7-N4	-8.59	1.27	1.47
3	C	302	MES	C7-N4	-8.48	1.28	1.47
3	B	303	MES	O2S-S	8.24	1.68	1.45
3	A	302	MES	C7-N4	-8.21	1.28	1.47
3	A	302	MES	O1S-S	7.99	1.67	1.45
3	D	302	MES	O2S-S	7.33	1.65	1.45
3	B	302	MES	O2S-S	7.33	1.65	1.45
3	D	303	MES	O2S-S	7.31	1.65	1.45
3	C	302	MES	O2S-S	7.23	1.65	1.45
3	A	302	MES	O2S-S	7.14	1.65	1.45
3	D	303	MES	O1S-S	6.74	1.64	1.45
3	B	303	MES	O1S-S	6.74	1.64	1.45
3	D	302	MES	O1S-S	6.73	1.64	1.45
3	C	302	MES	O1S-S	6.69	1.64	1.45
3	B	302	MES	O1S-S	6.60	1.63	1.45
3	B	302	MES	O3S-S	5.55	1.68	1.47
3	D	302	MES	O3S-S	5.52	1.68	1.47
3	D	303	MES	O3S-S	5.47	1.67	1.47
3	C	302	MES	O3S-S	5.46	1.67	1.47
2	B	301	GSH	CD1-N2	5.14	1.44	1.34
3	B	303	MES	O3S-S	5.01	1.66	1.47
2	D	301	GSH	C2-N3	5.00	1.45	1.33
2	C	301	GSH	CD1-N2	4.99	1.44	1.34
2	B	301	GSH	C2-N3	4.88	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	GSH	CD1-N2	4.84	1.44	1.34
2	A	301	GSH	C2-N3	4.73	1.44	1.33
2	C	301	GSH	C2-N3	4.66	1.44	1.33
2	A	301	GSH	CD1-N2	4.48	1.43	1.34
3	A	302	MES	O3S-S	4.31	1.63	1.47
3	B	303	MES	C3-N4	-2.99	1.38	1.46
3	B	302	MES	C3-N4	-2.92	1.39	1.46
3	A	302	MES	C5-N4	-2.87	1.39	1.46
3	D	302	MES	C5-N4	-2.87	1.39	1.46
3	B	303	MES	C5-N4	-2.81	1.39	1.46
3	A	302	MES	C3-N4	-2.79	1.39	1.46
3	D	303	MES	C3-N4	-2.77	1.39	1.46
3	D	303	MES	C5-N4	-2.77	1.39	1.46
3	C	302	MES	C8-S	2.74	1.81	1.77
3	C	302	MES	C3-N4	-2.73	1.39	1.46
3	A	302	MES	C8-S	2.70	1.81	1.77
3	D	302	MES	C3-N4	-2.61	1.39	1.46
3	B	302	MES	C5-N4	-2.61	1.39	1.46
3	C	302	MES	C5-N4	-2.52	1.40	1.46
2	D	301	GSH	O2-C2	-2.35	1.18	1.23
2	B	301	GSH	OE1-CD1	-2.33	1.18	1.23
3	B	302	MES	C8-S	2.19	1.80	1.77
2	A	301	GSH	O2-C2	-2.17	1.19	1.23
3	D	302	MES	C8-S	2.02	1.80	1.77
2	B	301	GSH	O2-C2	-2.01	1.19	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	304	O7Z	O03-C02-C04	4.94	120.87	111.90
4	A	303	O7Z	O03-C02-C04	4.81	120.65	111.90
4	D	305	O7Z	O03-C02-C04	4.31	119.73	111.90
2	B	301	GSH	CA2-CB2-SG2	-4.03	109.62	114.16
2	A	301	GSH	CB2-CA2-N2	-3.91	105.71	111.28
3	A	302	MES	C5-N4-C3	3.88	117.20	108.84
2	D	301	GSH	CB2-CA2-N2	-3.71	105.99	111.28
3	A	302	MES	C6-C5-N4	3.52	115.47	110.12
2	C	301	GSH	CA2-CB2-SG2	-3.40	110.33	114.16
3	C	302	MES	C6-C5-N4	3.39	115.27	110.12
2	A	301	GSH	CA2-CB2-SG2	-3.31	110.43	114.16
3	C	302	MES	C2-C3-N4	3.11	114.84	110.12
3	A	302	MES	C2-C3-N4	2.87	114.47	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	MES	C6-C5-N4	2.72	114.25	110.12
3	D	303	MES	O3S-S-C8	2.67	111.23	106.00
2	B	301	GSH	CB2-CA2-N2	-2.52	107.69	111.28
3	C	302	MES	C5-N4-C3	2.51	114.26	108.84
2	D	301	GSH	CA2-CB2-SG2	-2.41	111.44	114.16
3	A	302	MES	O2S-S-C8	2.40	110.36	106.73
3	D	303	MES	O2S-S-C8	2.33	110.25	106.73
2	D	301	GSH	O32-C3-CA3	2.29	121.52	112.81
3	B	303	MES	C5-N4-C3	2.28	113.76	108.84
3	B	303	MES	C6-C5-N4	2.28	113.59	110.12
3	D	302	MES	O1S-S-C8	2.27	110.16	106.73
3	B	302	MES	O1S-S-C8	2.23	110.09	106.73
3	B	302	MES	C2-C3-N4	2.22	113.49	110.12
3	B	303	MES	O1S-S-C8	2.18	110.02	106.73
3	B	302	MES	C6-C5-N4	2.17	113.42	110.12
3	B	303	MES	O2S-S-C8	2.10	109.89	106.73
2	B	301	GSH	O32-C3-CA3	2.06	120.64	112.81
3	C	302	MES	O3S-S-C8	2.06	110.03	106.00
3	B	303	MES	C2-C3-N4	2.04	113.22	110.12

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	MES	C7-C8-S-O2S
3	B	302	MES	C7-C8-S-O3S
3	B	303	MES	N4-C7-C8-S
3	B	303	MES	C7-C8-S-O2S
3	D	303	MES	N4-C7-C8-S
4	A	303	O7Z	O01-C02-C04-O05
4	A	303	O7Z	O03-C02-C04-O05
4	B	304	O7Z	O01-C02-C04-O05
4	B	304	O7Z	O03-C02-C04-O05
4	D	305	O7Z	O01-C02-C04-O05
4	D	305	O7Z	O03-C02-C04-O05
5	D	304	PGE	O2-C3-C4-O3
5	C	303	PGE	O1-C1-C2-O2
5	C	303	PGE	O3-C5-C6-O4
5	C	303	PGE	O2-C3-C4-O3
5	D	304	PGE	O3-C5-C6-O4
3	B	302	MES	C8-C7-N4-C3
3	B	303	MES	C8-C7-N4-C3

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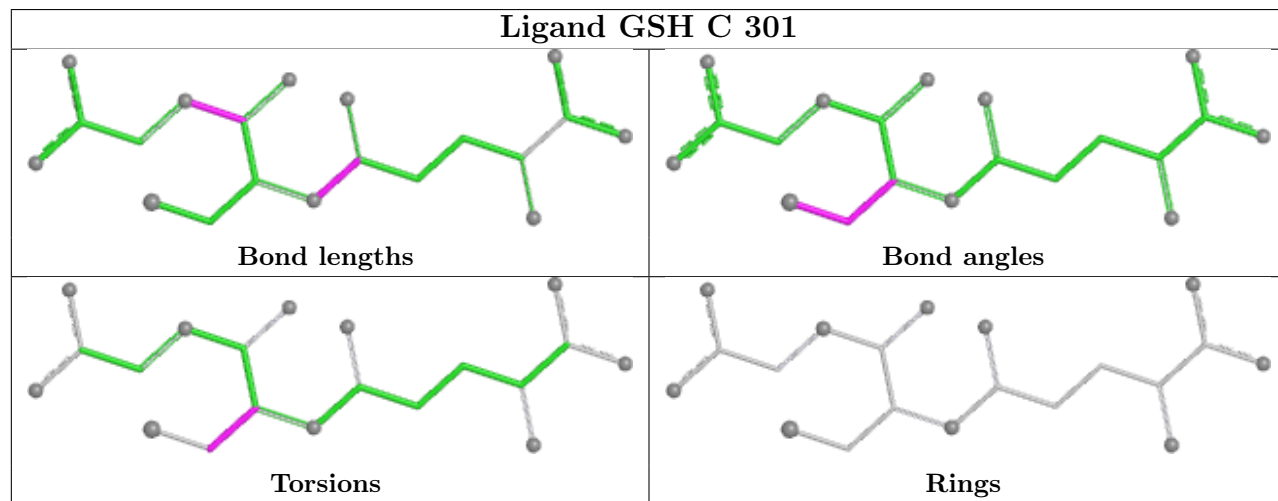
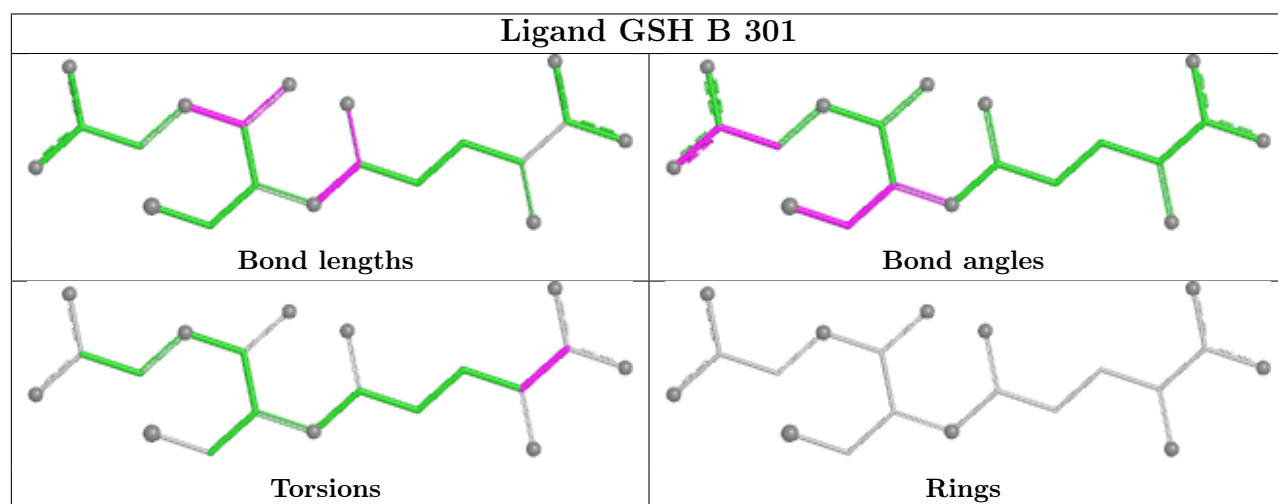
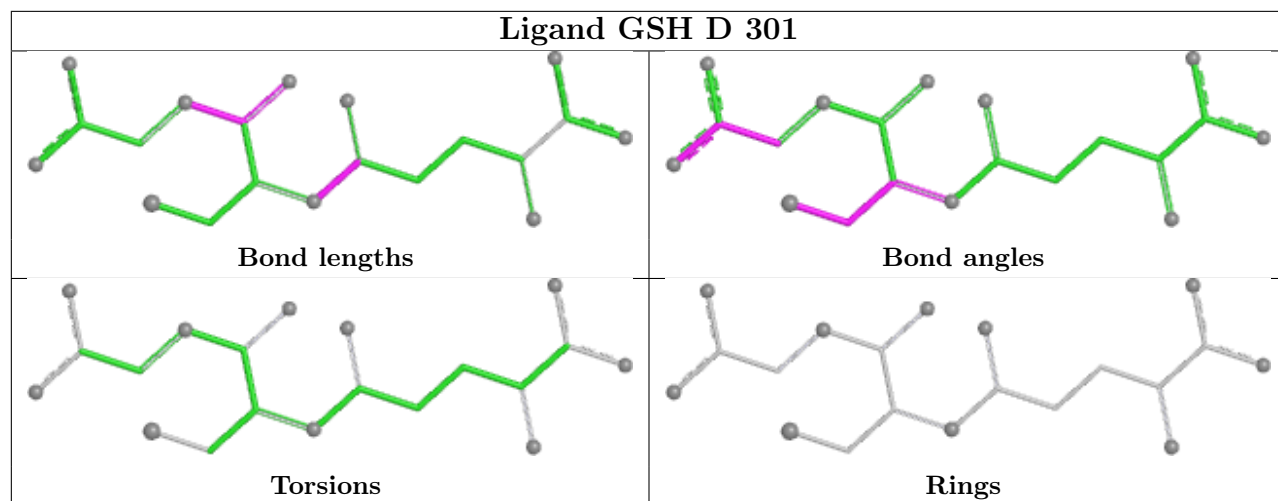
Mol	Chain	Res	Type	Atoms
3	D	302	MES	C8-C7-N4-C3
3	D	302	MES	C8-C7-N4-C5
3	A	302	MES	C7-C8-S-O2S
3	B	302	MES	C7-C8-S-O1S
3	B	303	MES	C7-C8-S-O1S
3	A	302	MES	C7-C8-S-O3S
2	C	301	GSH	N2-CA2-CB2-SG2
3	B	302	MES	C8-C7-N4-C5
3	B	303	MES	C8-C7-N4-C5
2	C	301	GSH	C2-CA2-CB2-SG2
3	B	303	MES	C7-C8-S-O3S
2	B	301	GSH	O12-C1-CA1-N1

There are no ring outliers.

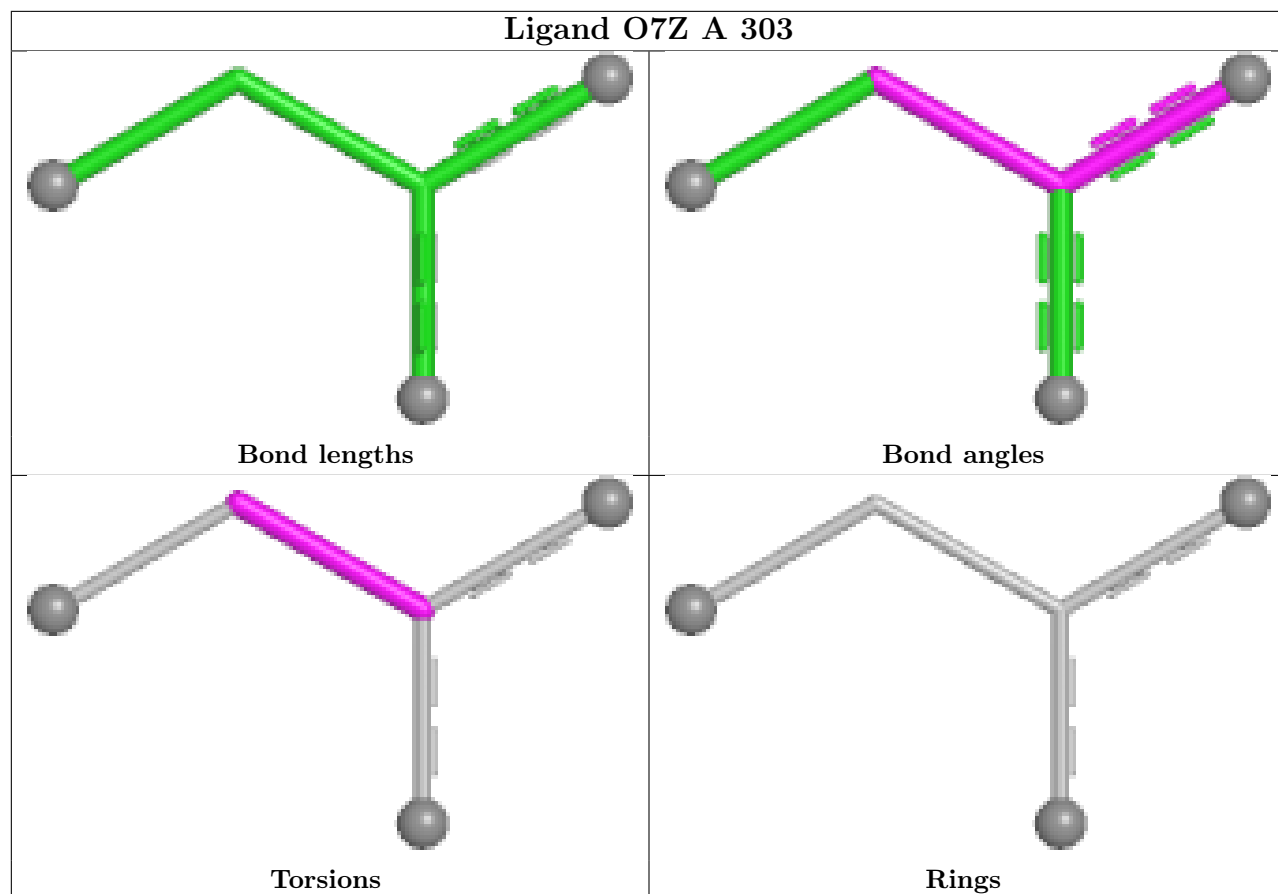
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	GSH	1	0
3	D	303	MES	2	0
3	C	302	MES	1	0
4	D	305	O7Z	2	0
5	C	303	PGE	1	0
5	D	304	PGE	2	0
3	B	302	MES	1	0

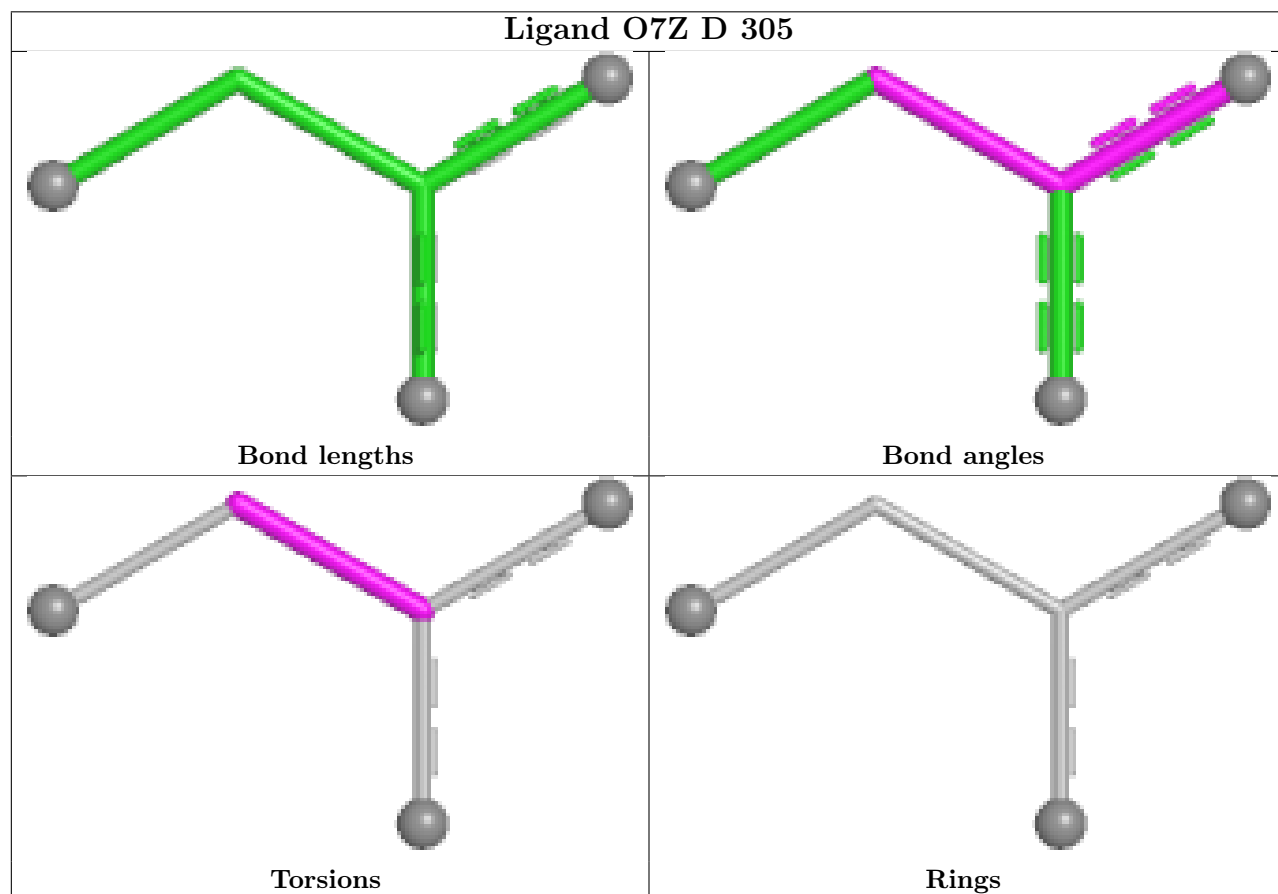
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

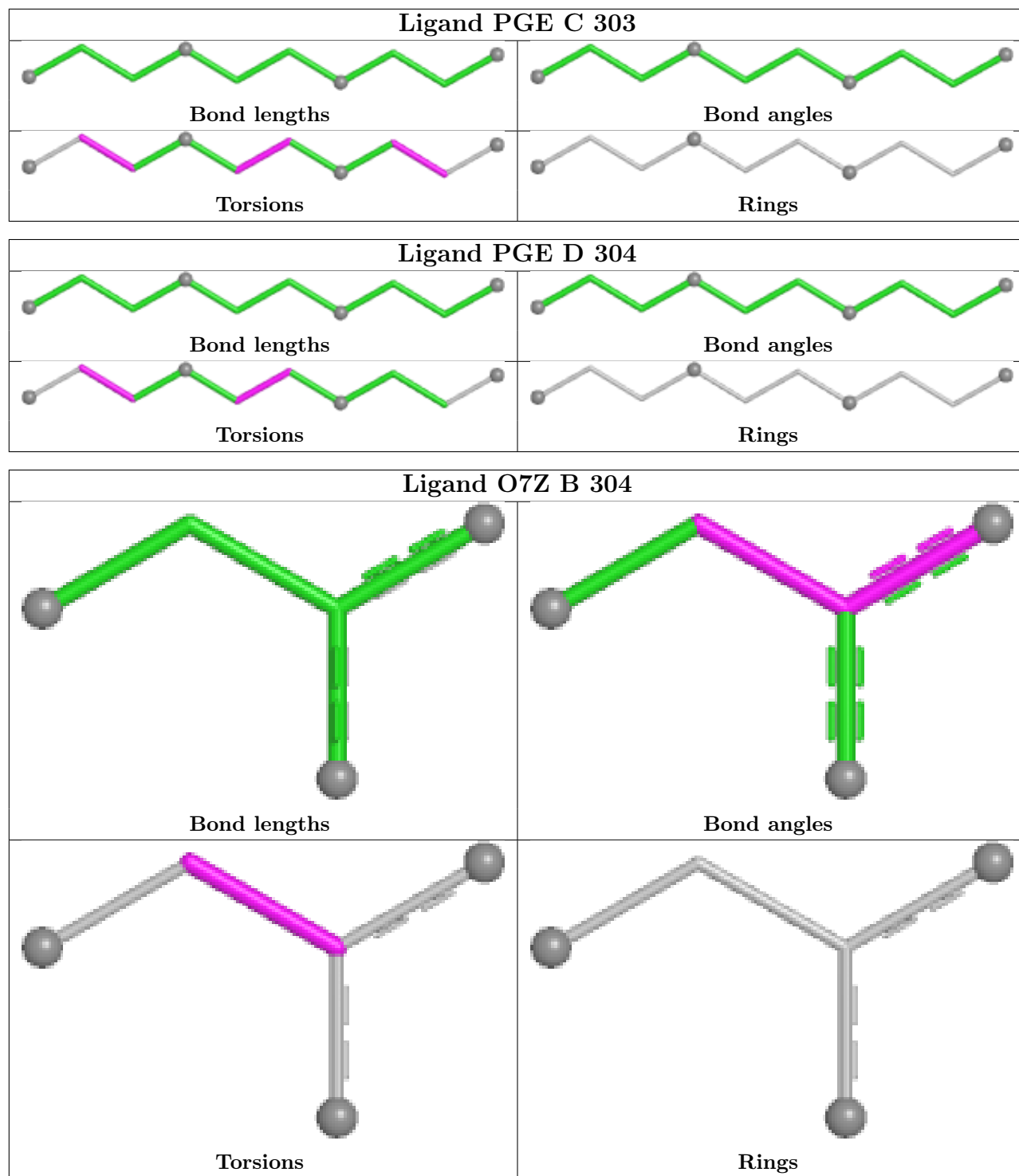


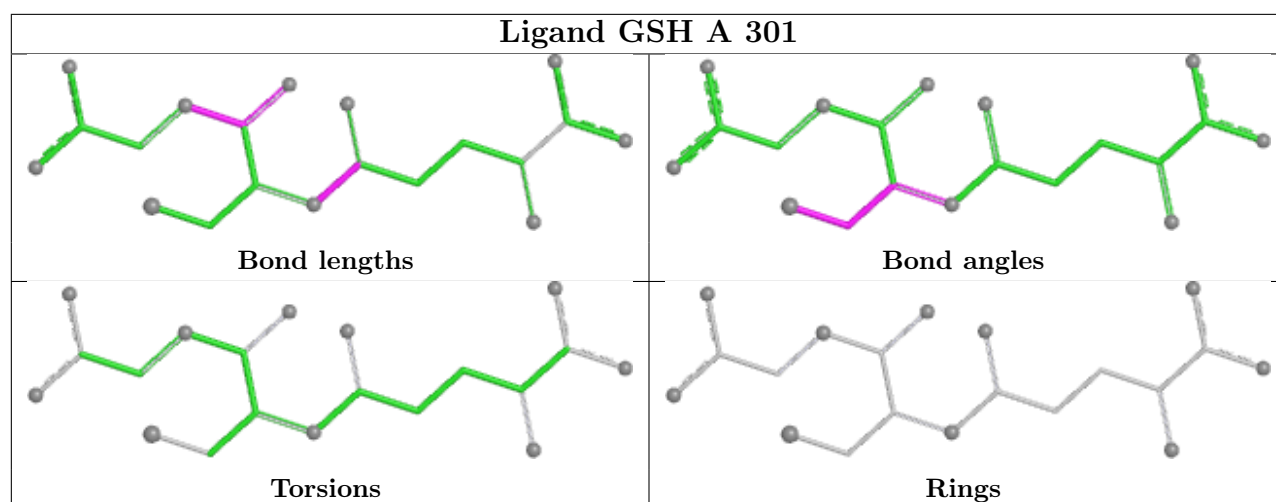
Ligand O7Z A 303



Ligand O7Z D 305







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	5
1	B	5
1	A	2
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	100:ARG	C	101[B]:CYS	N	1.20
1	A	197:GLU	C	198:TYR	N	1.19
1	D	1:PRO	C	2:PRO	N	1.19
1	B	81:LYS	C	82:ASP	N	1.18
1	B	157:ASP	C	158:LEU	N	1.15
1	C	58:GLY	C	59:ASP	N	1.14
1	B	52:LEU	C	53:PRO	N	1.11
1	D	36:GLU	C	37:THR	N	1.11
1	B	34:THR	C	35:VAL	N	1.07
1	A	196:PRO	C	197:GLU	N	1.04
1	D	34:THR	C	35:VAL	N	1.01
1	B	116:ASP	C	117:ASP	N	0.91
1	C	115:LYS	C	116:ASP	N	0.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	35:VAL	C	36:GLU	N	0.88

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	209/210 (99%)	-0.87	0 100 100	8, 19, 31, 44	2 (0%)
1	B	208/210 (99%)	-0.79	0 100 100	8, 20, 36, 47	4 (1%)
1	C	209/210 (99%)	-0.86	0 100 100	8, 20, 33, 41	2 (0%)
1	D	209/210 (99%)	-0.86	0 100 100	7, 19, 32, 39	3 (1%)
All	All	835/840 (99%)	-0.85	0 100 100	7, 19, 32, 47	11 (1%)

There are no RSRZ outliers to report.

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	MES	B	302	12/12	0.97	0.07	20,27,37,38	0
3	MES	B	303	12/12	0.97	0.06	28,39,45,52	0
3	MES	D	303	12/12	0.97	0.06	30,38,44,51	0
4	O7Z	A	303	5/23	0.97	0.07	23,31,36,44	0

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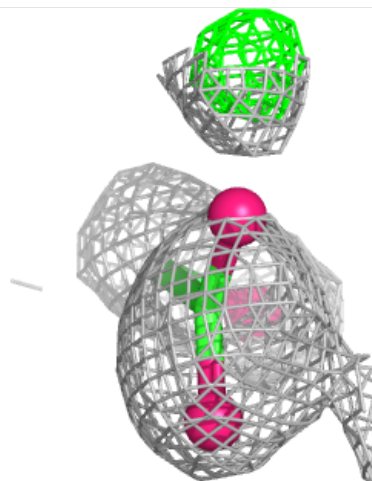
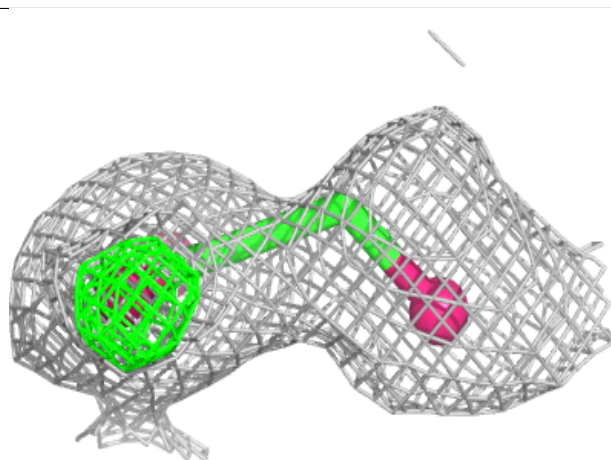
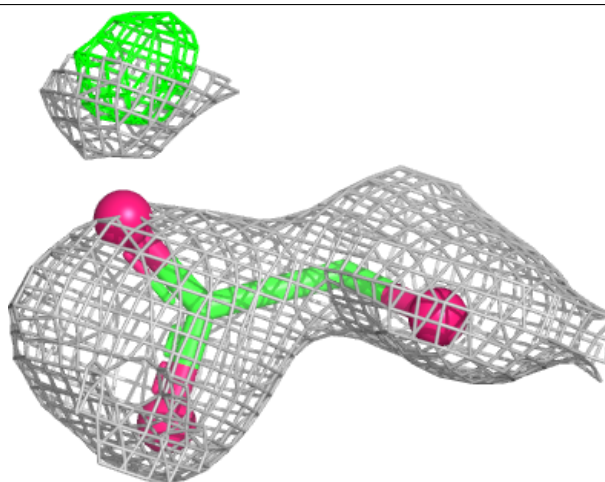
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	O7Z	D	305	5/23	0.97	0.05	29,30,39,42	0
5	PGE	C	303	10/10	0.97	0.06	33,39,47,49	0
3	MES	A	302	12/12	0.98	0.05	20,27,37,39	0
2	GSH	A	301	20/20	0.98	0.04	12,17,25,30	0
4	O7Z	B	304	5/23	0.98	0.04	27,30,38,47	0
2	GSH	C	301	20/20	0.98	0.04	11,18,24,32	0
3	MES	D	302	12/12	0.98	0.06	18,27,40,41	0
5	PGE	D	304	10/10	0.98	0.06	32,38,45,45	0
2	GSH	B	301	20/20	0.99	0.04	14,19,31,32	0
3	MES	C	302	12/12	0.99	0.05	22,26,40,43	0
2	GSH	D	301	20/20	0.99	0.04	14,18,26,32	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.

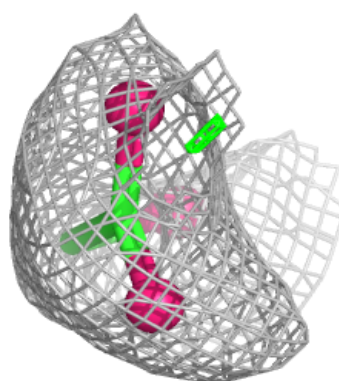
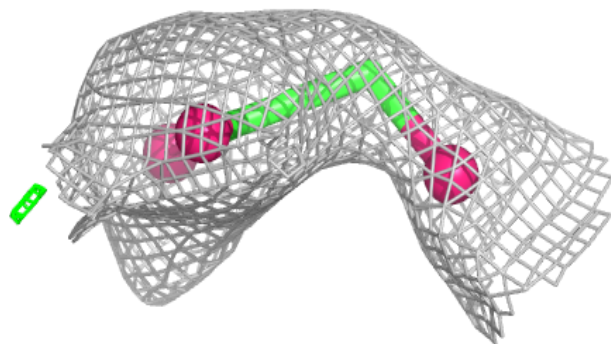
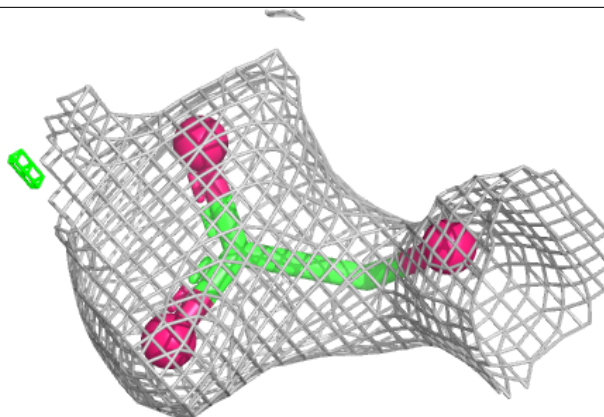
Electron density around O7Z A 303:

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

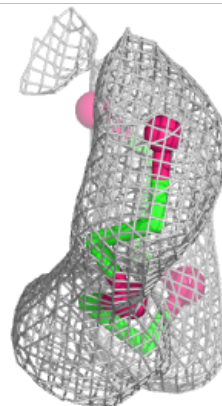
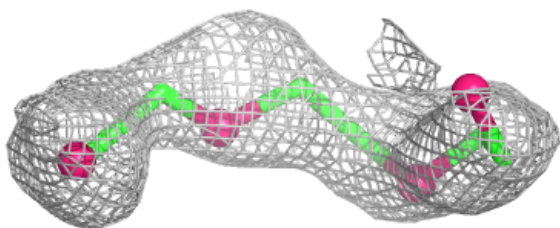
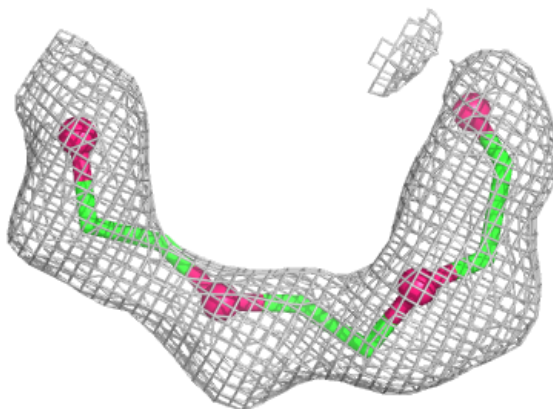


Electron density around O7Z D 305:

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

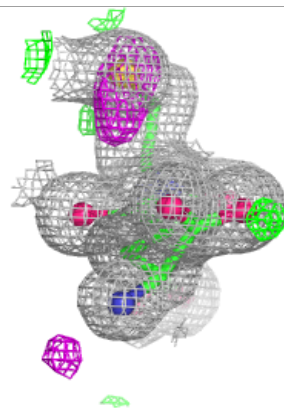
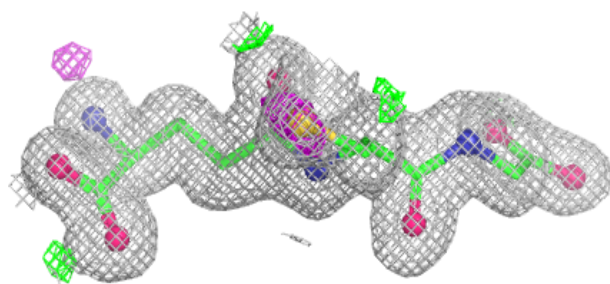
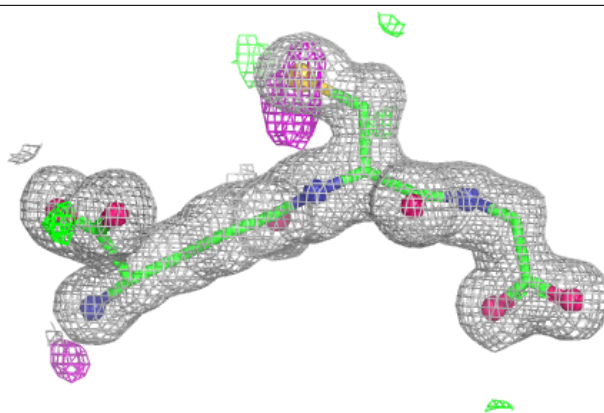
**Electron density around PGE C 303:**

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



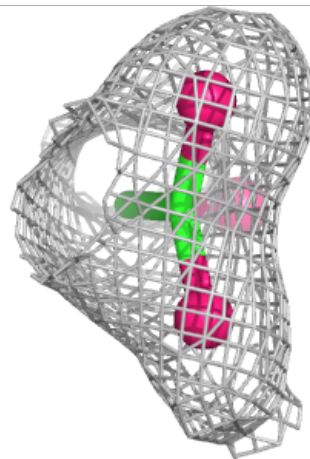
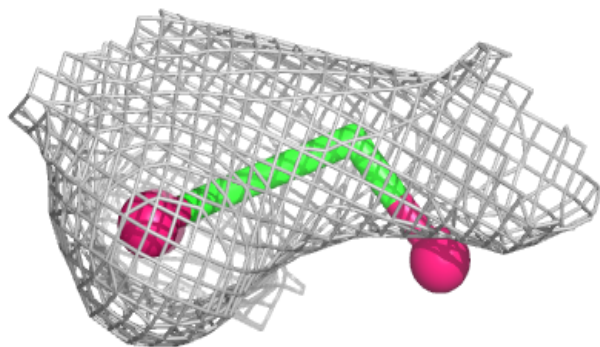
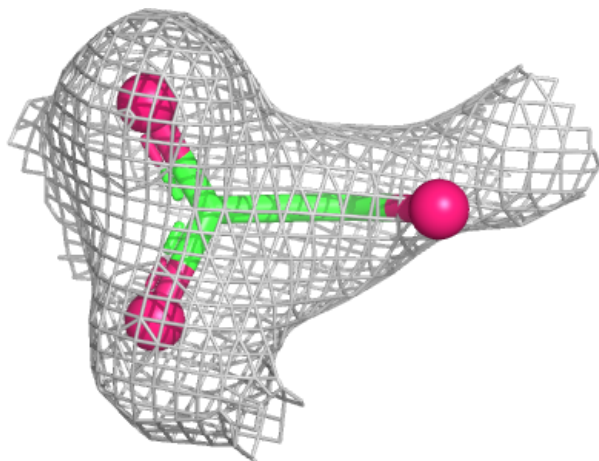
Electron density around GSH A 301:

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



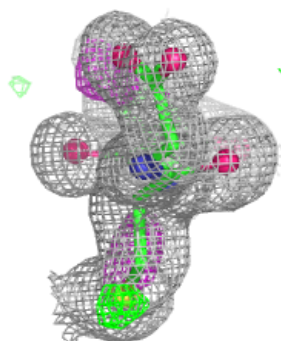
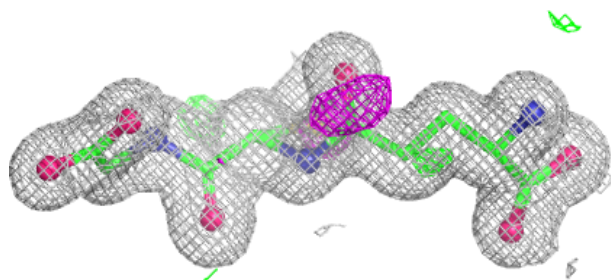
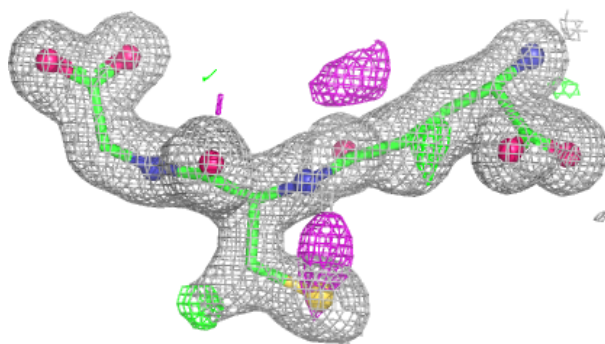
Electron density around O7Z B 304:

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

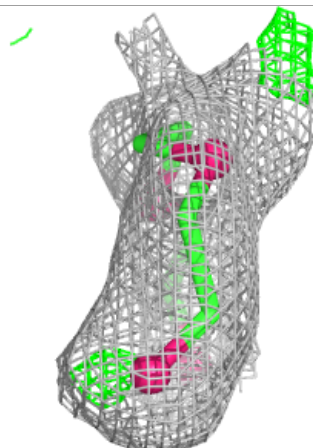
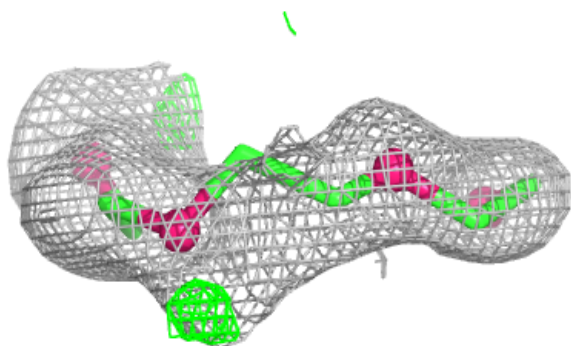
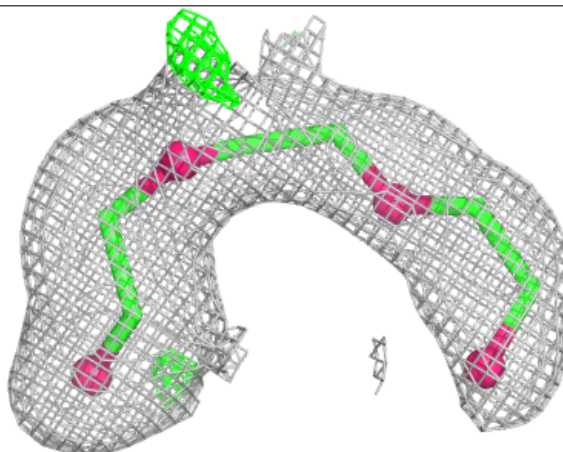


Electron density around GSH C 301:

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

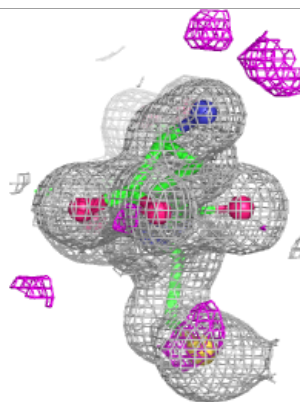
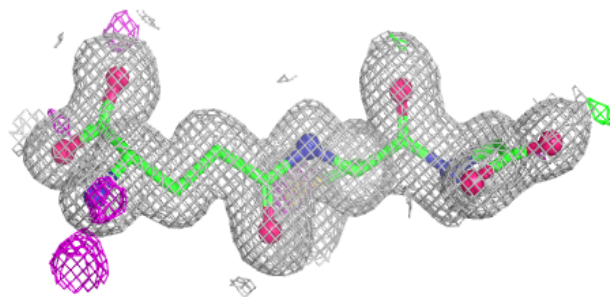
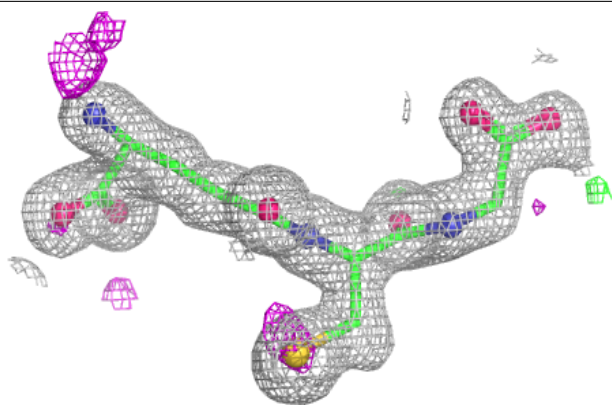
**Electron density around PGE D 304:**

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

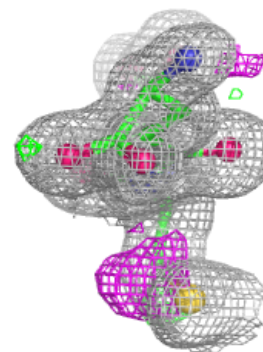
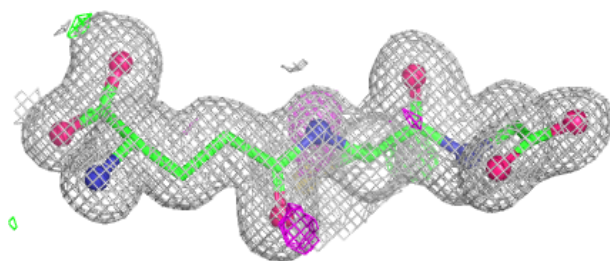
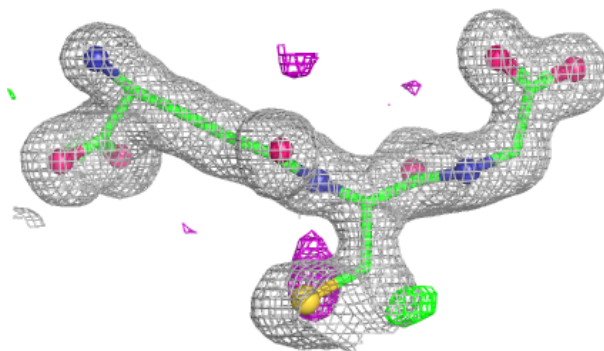


Electron density around GSH B 301:

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

**Electron density around GSH D 301:**

$2mF_o-DF_c$ (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.