



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:10 AM UTC

PDB ID : 1OYJ / pdb_00001oyj
Title : Crystal structure solution of Rice GST1 (OsGSTU1) in complex with glutathione.
Authors : Dixon, D.P.; McEwen, A.G.; Lapthorn, A.J.; Edwards, R.
Deposited on : 2003-04-04
Resolution : 1.95 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

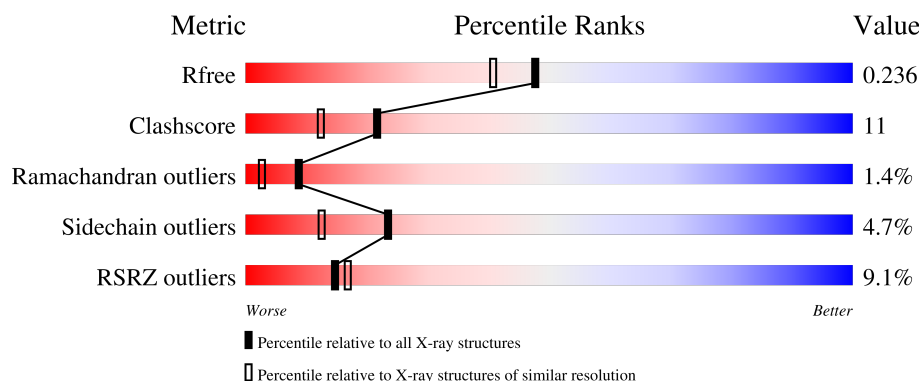
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	231	7% 79% 18% ..
1	B	231	11% 79% 13% ...
1	C	231	7% 84% 12% ...
1	D	231	10% 73% 18% 5% .

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
3	CL	B	831	-	-	X	-
4	GSH	A	800	X	-	-	-
4	GSH	B	801	X	-	-	-
4	GSH	C	802	X	-	-	-
4	GSH	C	803	X	-	-	-
4	GSH	C	804	X	X	-	-
4	GSH	D	805	X	-	-	-
5	GOL	A	814	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7954 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	3	0
			1807	1156	319	326	6			
1	B	224	Total	C	N	O	S	2	4	0
			1778	1140	314	318	6			
1	C	227	Total	C	N	O	S	2	0	0
			1784	1143	317	318	6			
1	D	223	Total	C	N	O	S	0	3	0
			1757	1127	309	315	6			

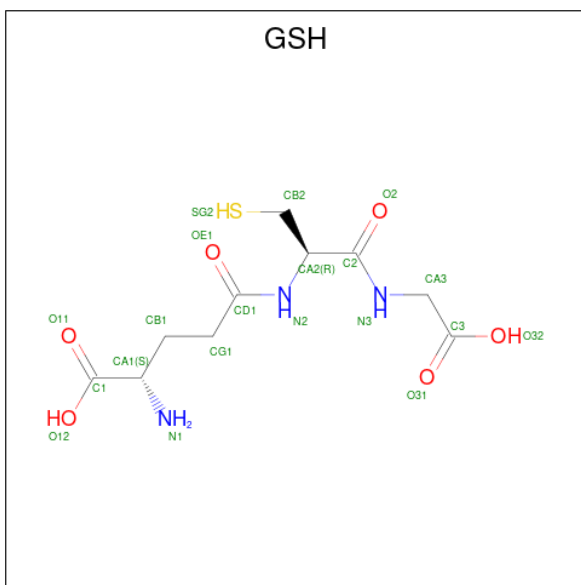
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	Cl	0	0
			7	7		
3	B	3	Total	Cl	0	0
			3	3		
3	C	6	Total	Cl	0	0
			6	6		
3	D	4	Total	Cl	0	0
			4	4		

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	109	Total	O	0	0
			109	109		
6	C	224	Total	O	0	0
			224	224		

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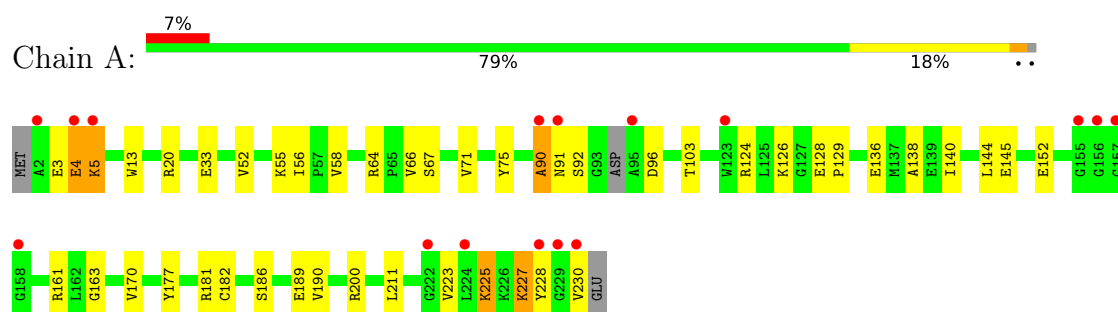
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	138	Total 138	O 138	0	0

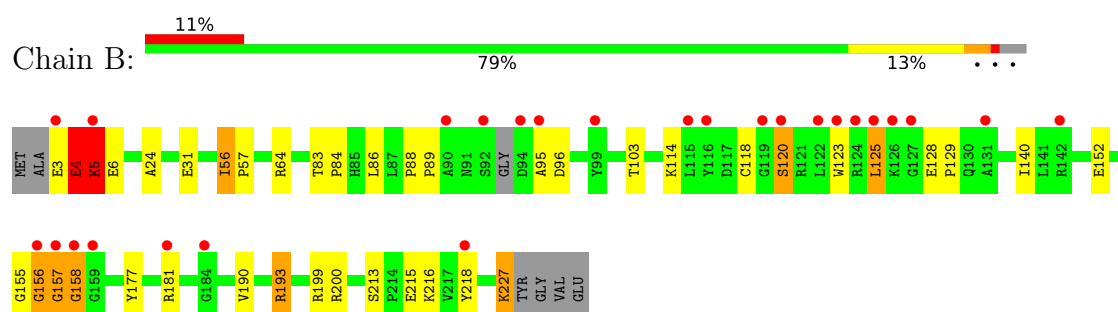
3 Residue-property plots

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.

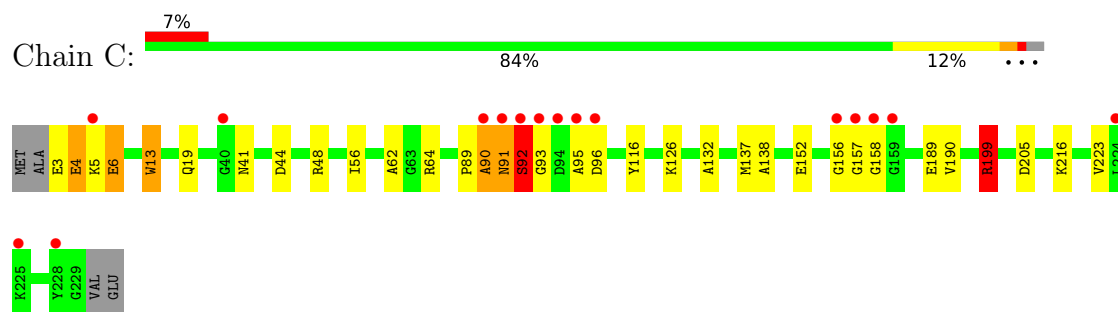
- Molecule 1: glutathione s-transferase



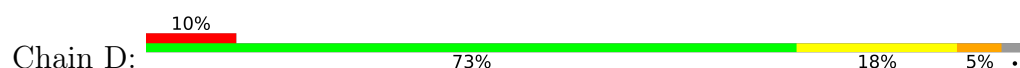
- Molecule 1: glutathione s-transferase



- Molecule 1: glutathione s-transferase



- Molecule 1: glutathione s-transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.83Å 91.13Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 40.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	84.5 (40.00-1.95) 84.5 (40.00-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.178 , 0.227 0.190 , 0.236	Depositor DCC
R_{free} test set	3635 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.104	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7954	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.87 % 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 6.3776e-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: GOL, MG, CL, GSH

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	1.48	13/1868 (0.7%)	1.23	3/2528 (0.1%)
1	B	1.35	3/1843 (0.2%)	1.27	8/2494 (0.3%)
1	C	1.38	5/1830 (0.3%)	1.26	9/2476 (0.4%)
1	D	1.25	1/1819 (0.1%)	1.26	7/2463 (0.3%)
All	All	1.37	22/7360 (0.3%)	1.25	27/9961 (0.3%)

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	C	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	LYS	CD-CE	13.20	1.92	1.52
1	C	19	GLN	N-CA	-6.63	1.38	1.46
1	A	58	VAL	CA-CB	6.60	1.63	1.54
1	A	140	ILE	CA-C	6.08	1.60	1.52
1	B	24	ALA	CA-CB	-6.04	1.44	1.53
1	B	56	ILE	CA-C	-5.94	1.46	1.52
1	A	20	ARG	N-CA	-5.93	1.39	1.46
1	A	170	VAL	CA-CB	-5.93	1.49	1.53
1	C	13	TRP	C-O	-5.84	1.17	1.24
1	A	71	VAL	CA-CB	5.61	1.61	1.54
1	C	199	ARG	CD-NE	-5.60	1.38	1.46
1	A	138	ALA	CA-CB	-5.57	1.44	1.53
1	A	163	GLY	C-O	5.54	1.29	1.23
1	A	211	LEU	CA-CB	-5.48	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	VAL	CA-CB	5.48	1.60	1.54
1	C	137	MET	SD-CE	-5.47	1.65	1.79
1	C	138	ALA	CA-CB	-5.42	1.44	1.53
1	A	103	THR	CA-CB	5.26	1.61	1.53
1	D	223	VAL	CA-CB	-5.23	1.48	1.54
1	A	58	VAL	CA-C	-5.17	1.46	1.52
1	A	144	LEU	C-O	5.17	1.30	1.24
1	A	145	GLU	C-O	5.14	1.30	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	NE-CZ-NH1	-13.11	108.39	121.50
1	C	199	ARG	NE-CZ-NH2	9.97	128.17	119.20
1	D	91	ASN	N-CA-C	-9.49	101.28	112.86
1	B	95	ALA	N-CA-C	-8.77	102.73	112.72
1	C	199	ARG	CD-NE-CZ	7.99	135.59	124.40
1	C	158	GLY	N-CA-C	-7.62	103.17	114.90
1	D	96	ASP	N-CA-C	-7.59	104.00	112.57
1	C	13	TRP	N-CA-C	6.63	119.35	111.33
1	B	199	ARG	NE-CZ-NH2	6.18	124.76	119.20
1	C	90	ALA	N-CA-C	-6.13	105.80	113.28
1	C	93	GLY	N-CA-C	-5.88	102.12	112.77
1	C	199	ARG	CG-CD-NE	-5.83	99.18	112.00
1	D	160	GLY	N-CA-C	-5.82	106.96	115.63
1	D	114	LYS	N-CA-C	5.69	120.72	113.55
1	B	199	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	B	5[A]	LYS	CA-C-N	5.58	128.03	120.38
1	B	5[A]	LYS	C-N-CA	5.58	128.03	120.38
1	B	5[B]	LYS	CA-C-N	5.58	128.03	120.38
1	B	5[B]	LYS	C-N-CA	5.58	128.03	120.38
1	D	226	LYS	N-CA-C	-5.53	99.02	110.80
1	A	90	ALA	N-CA-C	-5.49	106.55	113.20
1	B	157	GLY	N-CA-C	-5.47	100.21	113.18
1	D	199	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	A	136	GLU	N-CA-C	-5.37	105.51	111.36
1	A	13	TRP	N-CA-C	5.23	117.39	111.11
1	D	199	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	C	132	ALA	N-CA-C	-5.04	105.86	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	199	ARG	Sidechain

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	1807	0	1765	30	0
1	B	1778	0	1743	43	0
1	C	1784	0	1753	37	0
1	D	1757	0	1709	51	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
3	A	7	0	0	2	0
3	B	3	0	0	3	0
3	C	6	0	0	0	0
3	D	4	0	0	1	0
4	A	40	0	29	2	0
4	B	20	0	15	0	0
4	C	60	0	41	3	0
4	D	20	0	15	2	0
5	A	12	0	16	5	0
5	B	6	0	8	1	0
5	C	24	0	32	4	0
5	D	12	0	16	1	0
6	A	140	0	0	7	0
6	B	109	0	0	5	1
6	C	224	0	0	10	1
6	D	138	0	0	7	0
All	All	7954	0	7142	157	1

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 11.

All (157) 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:157:GLY:HA2	3:B:831:CL:CL	1.85	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HA	5:A:814:GOL:H31	1.16	1.12
1:B:157:GLY:CA	3:B:831:CL:CL	2.40	1.06
1:A:182:CYS:SG	6:A:975:HOH:O	2.13	1.05
1:C:6:GLU:OE1	1:C:6:GLU:HA	1.56	1.02
1:B:193:ARG:HH11	1:B:193:ARG:HG3	1.23	1.01
4:C:802:GSH:SG2	6:C:965:HOH:O	2.23	0.96
1:A:66:VAL:HA	5:A:814:GOL:C3	1.97	0.95
1:B:118:CYS:SG	6:B:940:HOH:O	2.27	0.91
1:B:5[B]:LYS:HG3	6:B:885:HOH:O	1.71	0.89
1:D:182:CYS:SG	6:D:931:HOH:O	2.31	0.88
1:C:116:TYR:OH	6:C:1014:HOH:O	1.93	0.86
1:C:5:LYS:HG2	1:C:6:GLU:H	1.41	0.84
1:C:91:ASN:O	1:C:92:SER:HB2	1.76	0.83
1:B:157:GLY:HA3	3:B:831:CL:CL	2.15	0.82
1:A:225:LYS:O	6:A:948:HOH:O	1.96	0.82
1:D:125:LEU:O	1:D:130:GLN:HB2	1.82	0.80
1:C:205:ASP:OD2	6:C:896:HOH:O	2.00	0.79
1:A:33:GLU:OE1	6:A:886:HOH:O	2.01	0.78
1:B:218:TYR:OH	1:C:152:GLU:OE2	2.02	0.78
1:D:147:GLU:OE1	6:D:855:HOH:O	2.01	0.77
1:C:6:GLU:OE1	1:C:6:GLU:CA	2.30	0.77
1:B:181:ARG:HH11	1:C:152:GLU:CD	1.94	0.76
1:C:189:GLU:HG2	6:C:948:HOH:O	1.86	0.73
1:B:157:GLY:O	1:B:158:GLY:O	2.07	0.73
1:D:222:GLY:O	1:D:225:LYS:N	2.21	0.72
1:D:155:GLY:O	1:D:156:GLY:C	2.32	0.71
1:D:9:LEU:CD1	1:D:11:ASP:HB2	2.20	0.71
1:B:177:TYR:OH	1:B:181:ARG:NH2	2.24	0.70
1:C:216:LYS:NZ	5:C:812:GOL:H32	2.08	0.69
1:D:157:GLY:O	1:D:159:GLY:N	2.26	0.69
1:D:147:GLU:O	6:D:929:HOH:O	2.09	0.69
1:D:152:GLU:HG2	1:D:200:ARG:HD3	1.74	0.69
1:D:128:GLU:N	1:D:129:PRO:CD	2.56	0.69
4:C:803:GSH:O12	6:C:901:HOH:O	2.11	0.68
1:C:44:ASP:O	1:C:48:ARG:HG3	1.95	0.67
1:C:189:GLU:HB3	6:C:948:HOH:O	1.95	0.66
1:A:4:GLU:O	1:A:5:LYS:CB	2.44	0.66
1:D:9:LEU:C	1:D:9:LEU:HD13	2.22	0.65
1:A:66:VAL:HG13	5:A:814:GOL:H32	1.78	0.65
1:B:120:SER:HA	1:B:123:TRP:CZ2	2.32	0.65
1:D:155:GLY:O	1:D:157:GLY:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:HH11	1:B:193:ARG:CG	2.05	0.64
1:A:56:ILE:C	1:A:56:ILE:HD12	2.22	0.64
1:C:216:LYS:HZ3	5:C:812:GOL:H32	1.63	0.63
1:C:6:GLU:CG	1:C:62:ALA:HA	2.29	0.62
1:D:186:SER:HB3	1:D:189:GLU:HG2	1.82	0.62
1:C:64:ARG:NH2	1:D:96:ASP:OD1	2.25	0.61
1:D:186:SER:HB3	1:D:189:GLU:CG	2.30	0.61
1:B:4:GLU:CD	1:B:4:GLU:C	2.70	0.60
1:A:227:LYS:C	1:A:228:TYR:HD1	2.09	0.60
1:B:193:ARG:HG3	1:B:193:ARG:NH1	2.02	0.60
1:B:125:LEU:N	1:B:125:LEU:HD13	2.17	0.59
1:C:96:ASP:OD1	1:D:64:ARG:NH1	2.26	0.59
1:D:126:LYS:O	1:D:129:PRO:HD2	2.03	0.59
1:D:128:GLU:N	1:D:129:PRO:HD2	2.17	0.59
1:B:125:LEU:N	1:B:125:LEU:CD1	2.66	0.59
1:D:39:LEU:HD13	4:D:805:GSH:HA32	1.84	0.59
1:D:9:LEU:HD12	1:D:11:ASP:HB2	1.83	0.59
1:A:64:ARG:NH2	1:B:96:ASP:OD1	2.22	0.58
1:A:96:ASP:OD1	1:B:64[A]:ARG:NH2	2.30	0.58
1:B:114:LYS:HB3	1:B:140:ILE:HD13	1.86	0.58
1:A:75:TYR:HA	6:A:865:HOH:O	2.04	0.57
1:D:156:GLY:CA	6:D:861:HOH:O	2.50	0.57
5:C:810:GOL:H32	6:C:912:HOH:O	2.03	0.57
1:D:120:SER:HA	1:D:123:TRP:CZ2	2.39	0.57
1:B:155:GLY:O	1:B:156:GLY:C	2.47	0.57
1:C:189:GLU:CG	6:C:948:HOH:O	2.46	0.57
1:D:156:GLY:N	6:D:861:HOH:O	2.30	0.57
1:A:126:LYS:O	1:A:129:PRO:HD2	2.04	0.56
1:C:6:GLU:HG3	1:C:62:ALA:HA	1.87	0.56
1:B:152:GLU:CG	1:B:200:ARG:HD3	2.35	0.56
1:D:222:GLY:O	1:D:225:LYS:HB2	2.05	0.56
5:A:814:GOL:H2	1:B:103:THR:HA	1.88	0.55
1:C:56:ILE:C	1:C:56:ILE:HD12	2.31	0.55
1:D:32:PHE:O	5:D:807:GOL:H31	2.06	0.55
1:D:90:ALA:C	1:D:92:SER:N	2.60	0.55
1:B:152:GLU:HG3	1:B:200:ARG:HD3	1.90	0.54
1:A:152:GLU:CG	1:A:200:ARG:HD3	2.37	0.54
1:D:111:VAL:HG13	1:D:115:LEU:HD13	1.90	0.54
1:B:215:GLU:H	1:B:215:GLU:CD	2.16	0.53
1:A:152:GLU:HG2	1:A:200:ARG:HD3	1.91	0.53
1:D:47:LEU:HD22	1:D:54:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:OD1	1:C:91:ASN:N	2.29	0.53
1:B:120:SER:HA	1:B:123:TRP:CE2	2.45	0.52
1:D:56:ILE:C	1:D:56:ILE:HD12	2.36	0.51
1:D:223:VAL:C	1:D:225:LYS:H	2.18	0.51
1:A:126:LYS:HG2	3:A:826:CL:CL	2.47	0.51
1:C:13:TRP:CE2	5:C:812:GOL:H2	2.46	0.51
1:C:189:GLU:CB	6:C:948:HOH:O	2.57	0.51
1:B:5[A]:LYS:NZ	6:B:872:HOH:O	2.30	0.50
1:C:156:GLY:O	1:C:157:GLY:C	2.55	0.50
1:D:9:LEU:CD1	1:D:9:LEU:C	2.85	0.50
1:B:181:ARG:NE	1:C:152:GLU:OE1	2.43	0.49
1:C:6:GLU:HG2	1:C:62:ALA:HA	1.94	0.49
1:D:114:LYS:HB3	1:D:140:ILE:HD13	1.93	0.49
1:B:213:SER:HB2	1:B:215:GLU:OE2	2.13	0.49
1:C:90:ALA:C	1:C:92:SER:H	2.20	0.49
1:A:67:SER:N	5:A:814:GOL:O3	2.33	0.49
1:D:157:GLY:HA2	3:D:832:CL:CL	2.50	0.48
1:D:152:GLU:CG	1:D:200:ARG:HD3	2.42	0.48
1:A:161:ARG:HB2	6:A:895:HOH:O	2.14	0.48
1:C:199:ARG:HD2	6:C:1004:HOH:O	2.13	0.48
1:D:91:ASN:C	1:D:91:ASN:OD1	2.57	0.48
1:B:128:GLU:N	1:B:129:PRO:CD	2.77	0.47
1:D:223:VAL:C	1:D:225:LYS:N	2.72	0.47
1:C:3:GLU:O	1:C:4:GLU:O	2.32	0.47
1:D:90:ALA:C	1:D:92:SER:H	2.21	0.47
1:D:186:SER:HB3	1:D:189:GLU:HG3	1.97	0.47
1:D:9:LEU:HD13	1:D:10:LEU:N	2.29	0.47
1:C:56:ILE:HD11	4:C:802:GSH:HB23	1.97	0.47
1:C:91:ASN:O	1:C:92:SER:CB	2.53	0.46
1:D:109:ASP:OD2	1:D:113:ARG:HD2	2.15	0.46
1:D:222:GLY:O	1:D:223:VAL:C	2.56	0.46
1:B:3:GLU:HA	6:B:939:HOH:O	2.15	0.46
1:A:177:TYR:CZ	1:A:181:ARG:HD2	2.51	0.46
1:A:124:ARG:NH1	6:A:924:HOH:O	2.48	0.46
1:A:124:ARG:NE	1:A:228:TYR:HE2	2.14	0.45
1:A:56:ILE:HD12	1:A:56:ILE:O	2.17	0.45
1:B:4:GLU:HA	1:B:4:GLU:OE1	2.15	0.45
1:C:6:GLU:HG3	1:C:6:GLU:O	2.17	0.45
1:D:125:LEU:O	1:D:130:GLN:CB	2.60	0.45
1:A:189:GLU:HG2	3:A:836:CL:CL	2.54	0.45
1:D:100:ALA:O	6:D:844:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HG2	4:A:799:GSH:N3	2.31	0.45
1:C:5:LYS:HG2	1:C:6:GLU:N	2.20	0.45
1:D:226:LYS:O	1:D:227:LYS:CB	2.65	0.44
1:B:5[B]:LYS:CD	1:B:6:GLU:H	2.30	0.44
1:A:128:GLU:HB3	1:A:129:PRO:HD3	1.98	0.44
1:B:86:LEU:HD21	6:B:846:HOH:O	2.18	0.44
1:D:68:GLU:OE1	4:D:805:GSH:N1	2.46	0.44
1:B:4:GLU:OE1	1:B:4:GLU:CA	2.65	0.44
1:C:56:ILE:HD12	1:C:56:ILE:O	2.18	0.44
1:A:90:ALA:C	1:A:92:SER:H	2.26	0.44
1:B:227:LYS:HD2	1:B:227:LYS:HA	1.65	0.44
1:B:5[B]:LYS:HG3	1:B:6:GLU:N	2.34	0.43
6:A:949:HOH:O	5:B:806:GOL:H12	2.19	0.43
1:B:56:ILE:HD12	1:B:56:ILE:C	2.44	0.43
1:B:83:THR:HB	1:B:84:PRO:HD2	2.01	0.43
1:C:89:PRO:CB	1:C:91:ASN:OD1	2.67	0.42
1:D:91:ASN:OD1	1:D:91:ASN:O	2.37	0.42
1:A:56:ILE:C	1:A:56:ILE:CD1	2.93	0.42
1:B:5[B]:LYS:HD2	1:B:6:GLU:H	1.85	0.42
1:D:83:THR:HB	1:D:84:PRO:HD2	2.02	0.42
1:A:124:ARG:CZ	1:A:228:TYR:HE2	2.33	0.42
1:A:152:GLU:HG2	1:A:200:ARG:CD	2.48	0.42
1:D:67:SER:O	1:D:68:GLU:HB2	2.20	0.42
1:D:64:ARG:HD2	6:D:953:HOH:O	2.20	0.41
1:D:225:LYS:O	1:D:226:LYS:HG3	2.20	0.41
1:A:56:ILE:HD11	4:A:799:GSH:HB23	2.02	0.41
1:D:123:TRP:HB2	1:D:225:LYS:HE3	2.02	0.41
1:B:181:ARG:NH1	1:C:152:GLU:OE1	2.52	0.41
1:B:88:PRO:HA	1:B:89:PRO:HD3	1.98	0.41
1:B:157:GLY:O	1:B:158:GLY:C	2.61	0.41
1:C:6:GLU:HG3	1:C:62:ALA:H	1.85	0.41
1:C:3:GLU:HB3	1:C:4:GLU:H	1.71	0.40
1:B:56:ILE:HB	1:B:57:PRO:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:858:HOH:O	6:C:1032:HOH:O[4_456]	1.98	0.22

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	227/231 (98%)	220 (97%)	5 (2%)	2 (1%)	14	6
1	B	224/231 (97%)	218 (97%)	3 (1%)	3 (1%)	9	3
1	C	225/231 (97%)	215 (96%)	7 (3%)	3 (1%)	9	3
1	D	222/231 (96%)	210 (95%)	7 (3%)	5 (2%)	5	1
All	All	898/924 (97%)	863 (96%)	22 (2%)	13 (1%)	9	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLY
1	C	4	GLU
1	C	92	SER
1	D	156	GLY
1	D	158	GLY
1	D	159	GLY
1	B	158	GLY
1	A	5	LYS
1	A	227	LYS
1	C	95	ALA
1	D	4[A]	GLU
1	D	4[B]	GLU
1	B	4	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	183/185 (99%)	175 (96%)	8 (4%)	25	15
1	B	180/185 (97%)	170 (94%)	10 (6%)	19	8
1	C	179/185 (97%)	172 (96%)	7 (4%)	28	18
1	D	177/185 (96%)	165 (93%)	12 (7%)	14	5
All	All	719/740 (97%)	682 (95%)	37 (5%)	23	10

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	GLU
1	A	91	ASN
1	A	186	SER
1	A	190	VAL
1	A	223	VAL
1	A	225	LYS
1	A	230	VAL
1	B	4	GLU
1	B	5[A]	LYS
1	B	5[B]	LYS
1	B	31[A]	GLU
1	B	31[B]	GLU
1	B	120	SER
1	B	125	LEU
1	B	190	VAL
1	B	193	ARG
1	B	227	LYS
1	C	6	GLU
1	C	41	ASN
1	C	91	ASN
1	C	92	SER
1	C	126	LYS
1	C	190	VAL
1	C	223	VAL
1	D	4[A]	GLU
1	D	4[B]	GLU
1	D	6	GLU
1	D	9	LEU
1	D	91	ASN
1	D	115	LEU
1	D	117	ASP
1	D	128	GLU

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Mol	Chain	Res	Type
1	D	200	ARG
1	D	216[A]	LYS
1	D	216[B]	LYS
1	D	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	130	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 [i](#)

Of 39 ligands modelled in this entry, 23 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	D	809	-	5,5,5	0.41	0	5,5,5	0.65	0
5	GOL	D	807	-	5,5,5	0.70	0	5,5,5	1.52	1 (20%)
4	GSH	C	803	2	18,19,19	1.35	2 (11%)	21,24,24	1.04	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GSH	A	800	2	18,19,19	1.23	2 (11%)	21,24,24	1.59	3 (14%)
4	GSH	C	804	-	18,19,19	1.23	4 (22%)	21,24,24	4.81	13 (61%)
4	GSH	C	802	-	18,19,19	1.12	1 (5%)	21,24,24	1.62	3 (14%)
5	GOL	A	814	-	5,5,5	0.31	0	5,5,5	0.81	0
5	GOL	C	808	-	5,5,5	0.49	0	5,5,5	0.86	0
5	GOL	C	813	-	5,5,5	0.44	0	5,5,5	1.05	0
4	GSH	D	805	-	18,19,19	1.38	4 (22%)	21,24,24	2.43	5 (23%)
5	GOL	B	806	-	5,5,5	0.43	0	5,5,5	0.86	0
4	GSH	A	799	-	18,19,19	1.20	2 (11%)	21,24,24	2.40	12 (57%)
5	GOL	C	812	-	5,5,5	0.53	0	5,5,5	1.19	0
5	GOL	A	811	-	5,5,5	0.32	0	5,5,5	0.34	0
5	GOL	C	810	-	5,5,5	0.45	0	5,5,5	1.13	1 (20%)
4	GSH	B	801	-	18,19,19	1.29	2 (11%)	21,24,24	1.80	7 (33%)

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
5	GOL	D	809	-	-	1/4/4/4	-
5	GOL	D	807	-	-	1/4/4/4	-
4	GSH	C	803	2	1/1/6/8	1/24/24/24	-
4	GSH	A	800	2	1/1/6/8	2/24/24/24	-
4	GSH	C	804	-	1/1/6/8	10/24/24/24	-
4	GSH	C	802	-	1/1/6/8	3/24/24/24	-
5	GOL	A	814	-	-	2/4/4/4	-
5	GOL	C	808	-	-	2/4/4/4	-
5	GOL	C	813	-	-	4/4/4/4	-
4	GSH	D	805	-	1/1/6/8	9/24/24/24	-
5	GOL	B	806	-	-	4/4/4/4	-
4	GSH	A	799	-	-	8/24/24/24	-
5	GOL	C	812	-	-	1/4/4/4	-
5	GOL	A	811	-	-	2/4/4/4	-
5	GOL	C	810	-	-	2/4/4/4	-
4	GSH	B	801	-	1/1/6/8	5/24/24/24	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	805	GSH	O12-C1	-3.28	1.20	1.30
4	B	801	GSH	O12-C1	-3.16	1.20	1.30
4	D	805	GSH	O2-C2	-2.88	1.17	1.23
4	A	799	GSH	O12-C1	-2.82	1.21	1.30
4	A	800	GSH	O12-C1	-2.72	1.22	1.30
4	C	803	GSH	CB2-CA2	-2.70	1.50	1.53
4	C	804	GSH	O12-C1	-2.68	1.22	1.30
4	D	805	GSH	O32-C3	-2.60	1.22	1.30
4	A	799	GSH	O32-C3	-2.49	1.22	1.30
4	C	803	GSH	O32-C3	-2.42	1.22	1.30
4	C	802	GSH	O32-C3	-2.39	1.22	1.30
4	C	804	GSH	O32-C3	-2.37	1.23	1.30
4	D	805	GSH	CG1-CD1	2.36	1.56	1.51
4	C	804	GSH	CA2-N2	2.26	1.50	1.45
4	B	801	GSH	CB2-CA2	2.16	1.55	1.53
4	C	804	GSH	CB2-SG2	-2.12	1.77	1.81
4	A	800	GSH	CB1-CA1	2.12	1.57	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	804	GSH	CB2-CA2-C2	-10.25	87.20	109.50
4	C	804	GSH	CA2-C2-N3	8.70	135.21	116.54
4	C	804	GSH	CA2-CB2-SG2	7.41	122.52	114.16
4	C	804	GSH	CB2-CA2-N2	6.68	120.82	111.28
4	D	805	GSH	CA3-N3-C2	-6.44	105.13	121.38
4	C	804	GSH	C2-CA2-N2	5.93	127.14	111.11
4	C	804	GSH	CA2-N2-CD1	-5.82	107.09	121.68
4	C	804	GSH	CA3-N3-C2	-5.26	108.09	121.38
4	C	804	GSH	CB1-CG1-CD1	-4.97	101.98	113.06
4	A	800	GSH	CA2-CB2-SG2	-4.66	108.91	114.16
4	C	804	GSH	O2-C2-N3	-4.53	113.40	122.98
4	D	805	GSH	O2-C2-N3	-4.48	113.50	122.98
4	C	804	GSH	O2-C2-CA2	-4.47	111.11	120.48
4	A	799	GSH	CA3-N3-C2	-4.39	110.31	121.38
4	C	802	GSH	CB1-CA1-C1	4.32	121.89	110.45
4	A	799	GSH	CB1-CA1-N1	4.14	120.91	110.12
4	D	805	GSH	CA2-CB2-SG2	-4.01	109.64	114.16
4	D	805	GSH	CA2-C2-N3	3.87	124.85	116.54
4	C	804	GSH	CG1-CB1-CA1	3.80	122.58	113.86
4	C	804	GSH	CB1-CA1-N1	3.29	118.70	110.12
4	A	799	GSH	C3-CA3-N3	3.24	123.13	113.06
4	B	801	GSH	CB1-CA1-C1	3.22	118.97	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	799	GSH	CA2-C2-N3	3.12	123.22	116.54
4	A	800	GSH	CB1-CG1-CD1	3.06	119.89	113.06
4	B	801	GSH	CG1-CD1-N2	2.98	121.12	115.86
4	A	799	GSH	O12-C1-O11	-2.82	117.69	124.08
4	B	801	GSH	C2-CA2-N2	-2.79	103.56	111.11
4	B	801	GSH	CG1-CB1-CA1	2.76	120.20	113.86
4	A	799	GSH	CB1-CA1-C1	2.74	117.69	110.45
4	A	799	GSH	CA2-CB2-SG2	-2.73	111.08	114.16
4	D	805	GSH	CB1-CA1-C1	2.67	117.53	110.45
4	A	799	GSH	CB2-CA2-N2	-2.63	107.54	111.28
4	A	800	GSH	O12-C1-O11	-2.59	118.21	124.08
4	B	801	GSH	CA3-N3-C2	-2.49	115.08	121.38
4	C	802	GSH	O12-C1-O11	-2.42	118.59	124.08
4	C	804	GSH	O32-C3-CA3	2.31	121.59	112.81
4	B	801	GSH	CB1-CA1-N1	2.29	116.09	110.12
4	A	799	GSH	C2-CA2-N2	-2.25	105.01	111.11
4	A	799	GSH	OE1-CD1-CG1	-2.20	118.04	122.02
4	A	799	GSH	CG1-CD1-N2	2.18	119.70	115.86
4	C	802	GSH	CG1-CB1-CA1	2.12	118.74	113.86
5	D	807	GOL	O1-C1-C2	2.12	119.92	110.38
4	C	803	GSH	C2-CA2-N2	2.11	116.81	111.11
4	A	799	GSH	O2-C2-CA2	-2.07	116.14	120.48
4	B	801	GSH	CA2-CB2-SG2	2.06	116.48	114.16
5	C	810	GOL	O3-C3-C2	-2.05	101.16	110.38
4	C	803	GSH	CA2-CB2-SG2	-2.02	111.88	114.16

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	800	GSH	CA1
4	B	801	GSH	CA1
4	C	802	GSH	CA1
4	C	803	GSH	CA1
4	C	804	GSH	CA1
4	D	805	GSH	CA1

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	799	GSH	C1-CA1-CB1-CG1
4	B	801	GSH	O11-C1-CA1-N1
4	B	801	GSH	N1-CA1-CB1-CG1

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Mol	Chain	Res	Type	Atoms
4	B	801	GSH	C1-CA1-CB1-CG1
4	C	802	GSH	C1-CA1-CB1-CG1
4	C	804	GSH	O11-C1-CA1-N1
4	C	804	GSH	CG1-CD1-N2-CA2
4	C	804	GSH	OE1-CD1-N2-CA2
4	C	804	GSH	N2-CA2-CB2-SG2
4	D	805	GSH	O31-C3-CA3-N3
5	A	811	GOL	C1-C2-C3-O3
5	B	806	GOL	O1-C1-C2-C3
5	B	806	GOL	C1-C2-C3-O3
5	B	806	GOL	O2-C2-C3-O3
5	C	808	GOL	O1-C1-C2-C3
5	C	810	GOL	C1-C2-C3-O3
5	C	813	GOL	O1-C1-C2-C3
4	A	799	GSH	O2-C2-N3-CA3
4	C	804	GSH	O2-C2-N3-CA3
4	D	805	GSH	O2-C2-N3-CA3
4	C	804	GSH	CA2-C2-N3-CA3
4	D	805	GSH	CA2-C2-N3-CA3
4	A	799	GSH	CA2-C2-N3-CA3
4	D	805	GSH	CA1-CB1-CG1-CD1
4	B	801	GSH	O12-C1-CA1-N1
4	C	804	GSH	O12-C1-CA1-N1
4	D	805	GSH	O12-C1-CA1-N1
4	D	805	GSH	O32-C3-CA3-N3
5	C	813	GOL	O1-C1-C2-O2
5	A	814	GOL	C1-C2-C3-O3
5	C	813	GOL	C1-C2-C3-O3
5	A	811	GOL	O2-C2-C3-O3
4	A	799	GSH	O31-C3-CA3-N3
5	B	806	GOL	O1-C1-C2-O2
5	C	808	GOL	O1-C1-C2-O2
4	A	800	GSH	O12-C1-CA1-N1
4	A	799	GSH	O32-C3-CA3-N3
4	D	805	GSH	O11-C1-CA1-CB1
5	D	809	GOL	O1-C1-C2-O2
4	C	802	GSH	O11-C1-CA1-N1
4	D	805	GSH	O11-C1-CA1-N1
4	C	804	GSH	C1-CA1-CB1-CG1
4	D	805	GSH	O12-C1-CA1-CB1
4	C	804	GSH	CA1-CB1-CG1-CD1
5	C	810	GOL	O2-C2-C3-O3

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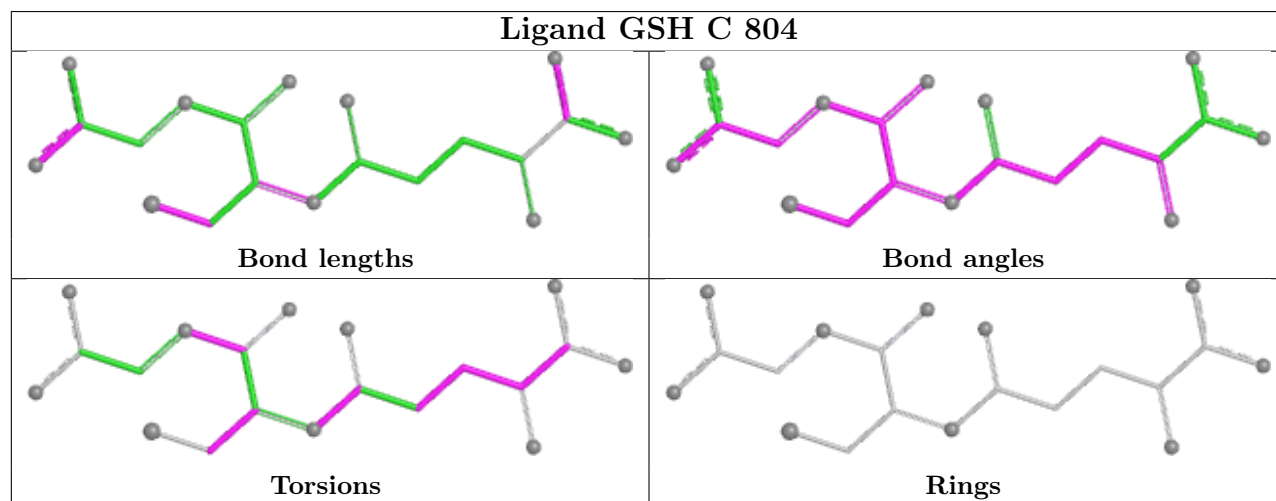
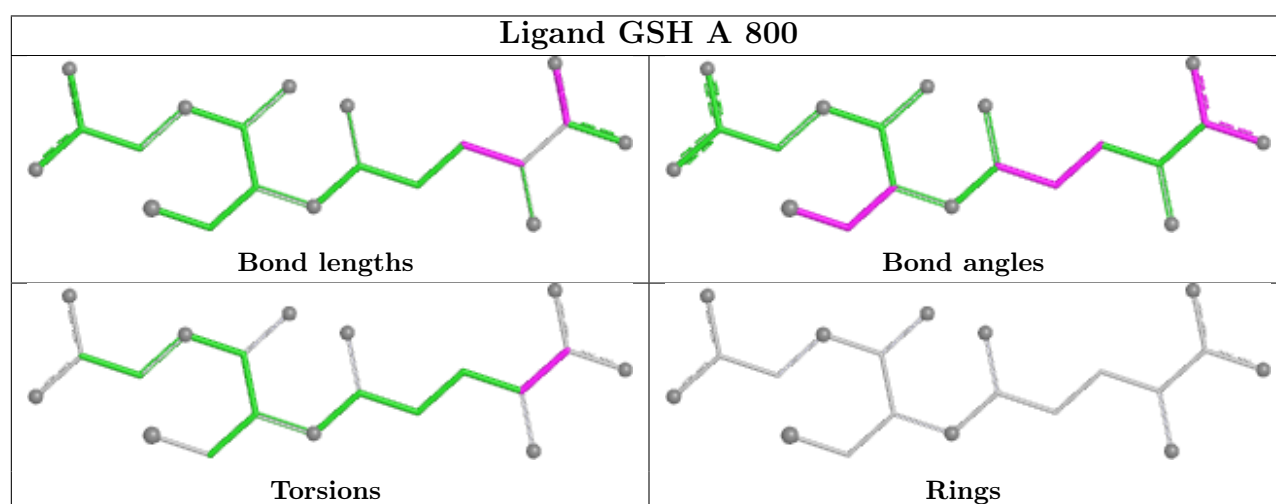
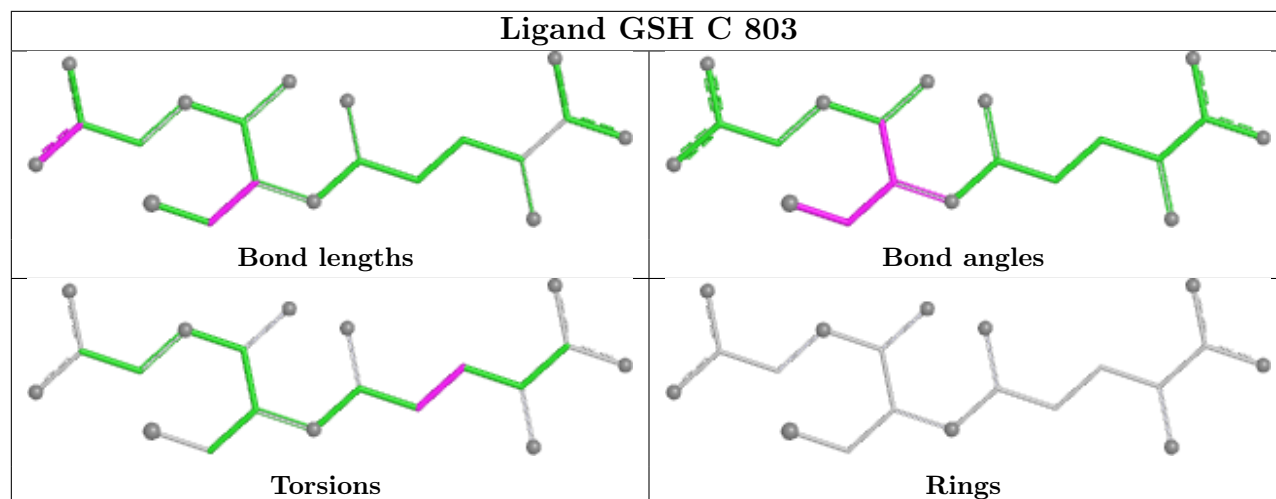
Mol	Chain	Res	Type	Atoms
5	C	813	GOL	O2-C2-C3-O3
4	C	802	GSH	O12-C1-CA1-N1
4	B	801	GSH	O31-C3-CA3-N3
5	A	814	GOL	O2-C2-C3-O3
5	C	812	GOL	C1-C2-C3-O3
4	A	799	GSH	O12-C1-CA1-N1
5	D	807	GOL	O2-C2-C3-O3
4	A	799	GSH	C3-CA3-N3-C2
4	C	804	GSH	C2-CA2-CB2-SG2
4	C	803	GSH	CA1-CB1-CG1-CD1
4	A	799	GSH	O11-C1-CA1-N1
4	A	800	GSH	O11-C1-CA1-N1

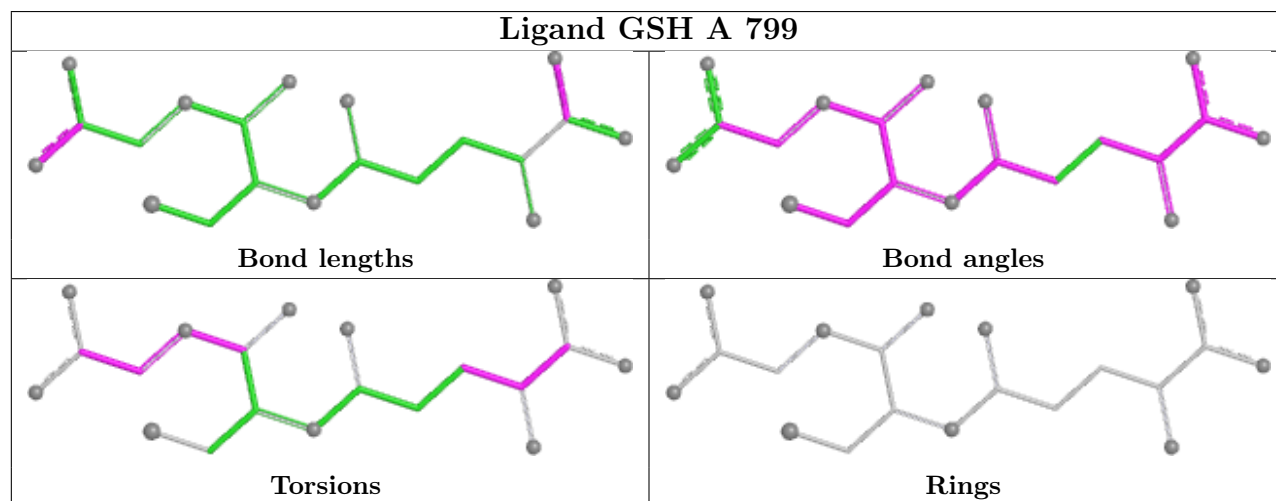
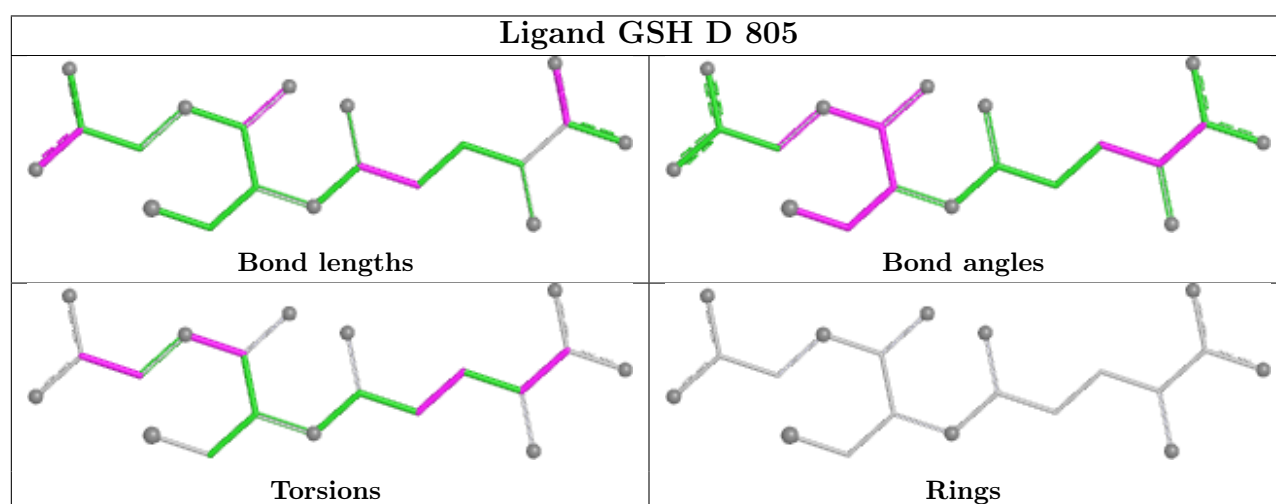
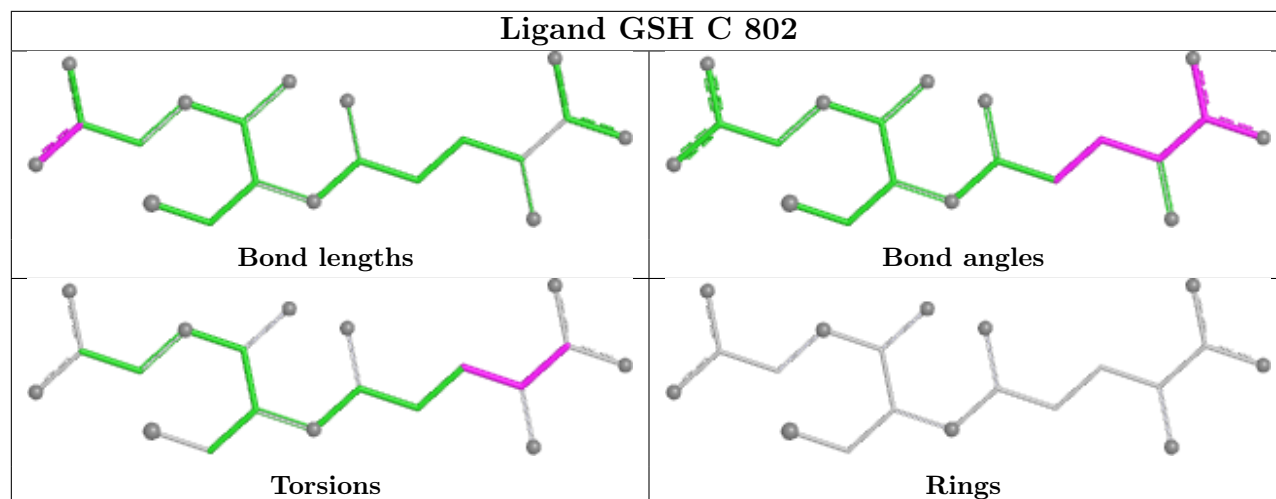
There are no ring outliers.

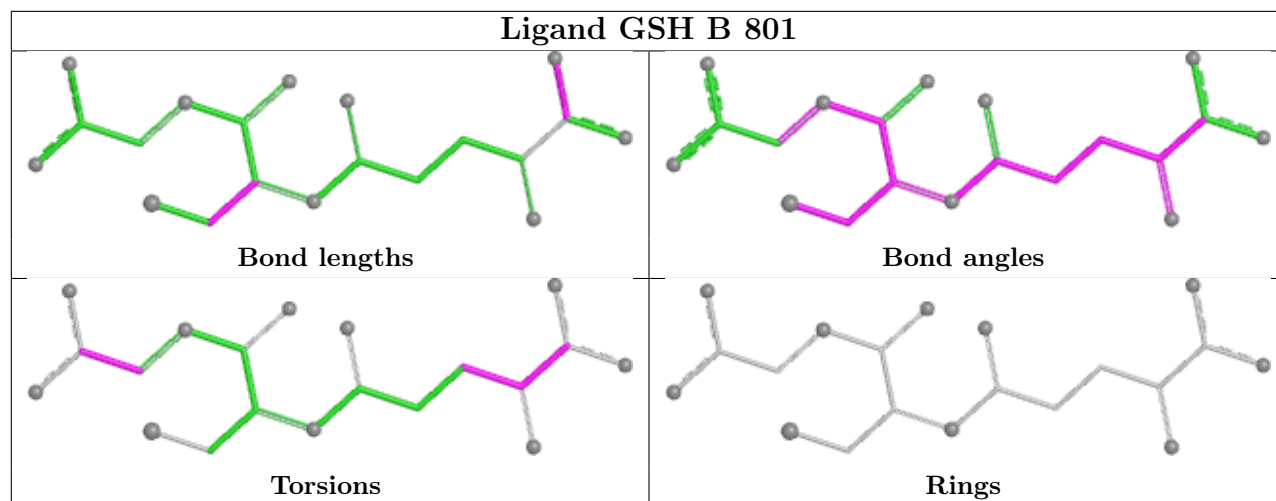
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	807	GOL	1	0
4	C	803	GSH	1	0
4	C	802	GSH	2	0
5	A	814	GOL	5	0
4	D	805	GSH	2	0
5	B	806	GOL	1	0
4	A	799	GSH	2	0
5	C	812	GOL	3	0
5	C	810	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	228/231 (98%)	0.13	16 (7%)	22	26	16, 23, 55, 84	3 (1%)
1	B	224/231 (96%)	0.59	26 (11%)	9	11	17, 27, 56, 66	5 (2%)
1	C	227/231 (98%)	0.06	16 (7%)	22	26	19, 25, 53, 76	1 (0%)
1	D	223/231 (96%)	0.76	24 (10%)	11	12	23, 32, 66, 75	3 (1%)
All	All	902/924 (97%)	0.38	82 (9%)	15	17	16, 27, 61, 84	12 (1%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	ALA	6.1
1	D	156	GLY	5.9
1	D	95	ALA	5.6
1	B	125	LEU	5.2
1	A	91	ASN	5.2
1	C	91	ASN	4.7
1	A	156	GLY	4.6
1	B	156	GLY	4.6
1	C	228	TYR	4.5
1	B	123	TRP	4.4
1	D	223	VAL	4.2
1	B	158	GLY	4.1
1	C	156	GLY	4.1
1	D	91	ASN	4.0
1	A	229	GLY	3.9
1	B	116	TYR	3.9
1	D	116	TYR	3.8
1	A	230	VAL	3.7
1	D	123	TRP	3.6
1	A	90	ALA	3.6
1	C	158	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	155	GLY	3.6
1	B	5[A]	LYS	3.5
1	D	224	LEU	3.5
1	A	2	ALA	3.5
1	B	124	ARG	3.4
1	A	158	GLY	3.4
1	B	157	GLY	3.4
1	D	222	GLY	3.4
1	B	92	SER	3.3
1	D	89	PRO	3.3
1	D	157	GLY	3.1
1	C	93	GLY	3.1
1	D	120	SER	3.0
1	A	95	ALA	3.0
1	A	157	GLY	3.0
1	D	159	GLY	2.9
1	B	115	LEU	2.9
1	C	5	LYS	2.9
1	B	218	TYR	2.9
1	C	224	LEU	2.9
1	D	132	ALA	2.8
1	A	123	TRP	2.8
1	D	226	LYS	2.8
1	B	159	GLY	2.8
1	B	122	LEU	2.7
1	B	119	GLY	2.7
1	A	5	LYS	2.6
1	D	3	GLU	2.6
1	C	159	GLY	2.6
1	A	4	GLU	2.5
1	D	134	GLY	2.5
1	B	95	ALA	2.5
1	D	131	ALA	2.5
1	B	99	TYR	2.4
1	C	95	ALA	2.4
1	B	94	ASP	2.4
1	B	90	ALA	2.4
1	C	90	ALA	2.4
1	A	224	LEU	2.4
1	B	181	ARG	2.4
1	B	131	ALA	2.4
1	B	184	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	118	CYS	2.4
1	B	3	GLU	2.3
1	D	98	ALA	2.3
1	D	160	GLY	2.3
1	A	228	TYR	2.3
1	D	113	ARG	2.3
1	B	120	SER	2.2
1	C	94	ASP	2.2
1	C	92	SER	2.2
1	A	155	GLY	2.1
1	A	222	GLY	2.1
1	B	126	LYS	2.1
1	C	96	ASP	2.1
1	C	225	LYS	2.1
1	D	122	LEU	2.1
1	B	142	ARG	2.1
1	C	40	GLY	2.0
1	C	157	GLY	2.0
1	B	127	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	A	838	1/1	0.73	0.11	93,93,93,93	0
5	GOL	A	814	6/6	0.74	0.19	69,72,74,78	0
4	GSH	C	804	20/20	0.78	0.39	46,73,81,81	20
3	CL	D	832	1/1	0.81	0.21	79,79,79,79	0

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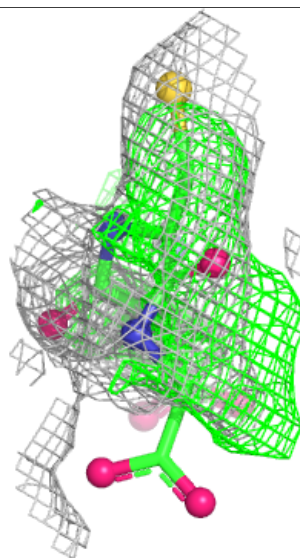
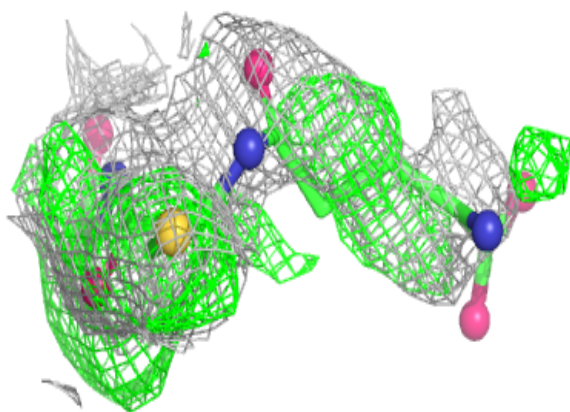
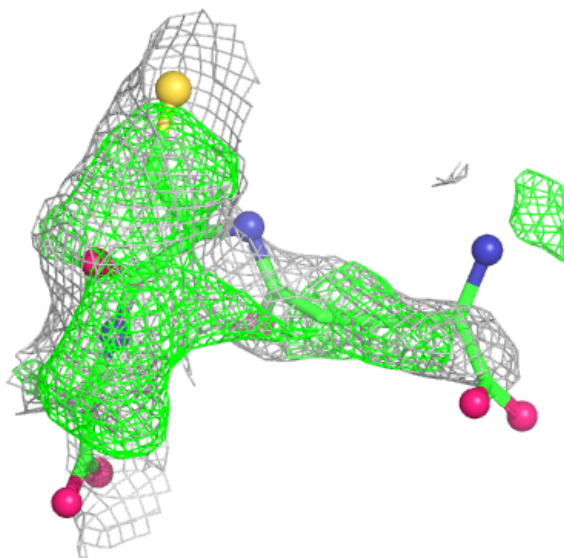
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	806	6/6	0.82	0.22	65,75,77,78	0
5	GOL	C	810	6/6	0.84	0.12	48,53,56,63	0
5	GOL	C	812	6/6	0.84	0.18	63,67,69,69	0
5	GOL	D	809	6/6	0.85	0.14	52,61,62,64	0
3	CL	C	829	1/1	0.86	0.15	74,74,74,74	0
3	CL	B	831	1/1	0.86	0.17	70,70,70,70	0
5	GOL	C	813	6/6	0.89	0.14	48,64,67,69	0
5	GOL	D	807	6/6	0.89	0.09	40,55,58,59	0
3	CL	C	828	1/1	0.89	0.33	67,67,67,67	0
4	GSH	D	805	20/20	0.90	0.11	35,43,57,58	0
5	GOL	A	811	6/6	0.90	0.15	73,80,80,81	0
3	CL	A	825	1/1	0.90	0.24	65,65,65,65	0
3	CL	A	826	1/1	0.91	0.19	73,73,73,73	0
3	CL	B	820	1/1	0.91	0.15	65,65,65,65	0
5	GOL	C	808	6/6	0.91	0.10	43,54,56,57	0
3	CL	D	834	1/1	0.91	0.16	58,58,58,58	0
4	GSH	B	801	20/20	0.92	0.09	29,39,57,58	0
3	CL	A	837	1/1	0.92	0.21	72,72,72,72	0
4	GSH	C	803	20/20	0.93	0.11	32,37,68,69	0
3	CL	B	835	1/1	0.93	0.16	68,68,68,68	0
4	GSH	A	799	20/20	0.93	0.10	29,33,54,56	0
3	CL	A	823	1/1	0.93	0.14	58,58,58,58	0
3	CL	A	836	1/1	0.94	0.27	61,61,61,61	0
3	CL	A	827	1/1	0.94	0.14	62,62,62,62	0
4	GSH	C	802	20/20	0.94	0.09	32,39,51,53	0
4	GSH	A	800	20/20	0.95	0.09	33,39,69,73	0
3	CL	D	819	1/1	0.95	0.30	55,55,55,55	0
3	CL	C	824	1/1	0.95	0.15	54,54,54,54	0
2	MG	A	817	1/1	0.97	0.10	60,60,60,60	0
3	CL	C	830	1/1	0.97	0.28	65,65,65,65	0
3	CL	C	822	1/1	0.97	0.09	52,52,52,52	0
2	MG	A	815	1/1	0.98	0.04	38,38,38,38	0
3	CL	C	833	1/1	0.98	0.07	52,52,52,52	0
2	MG	C	816	1/1	0.98	0.03	41,41,41,41	0
3	CL	D	821	1/1	0.99	0.06	51,51,51,51	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.

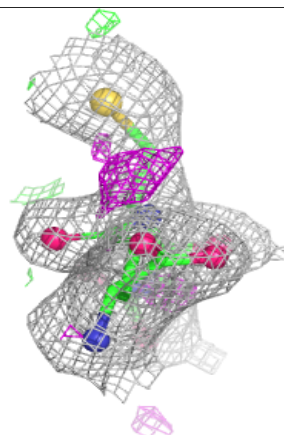
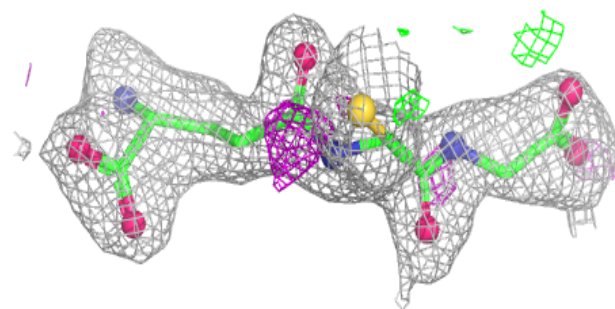
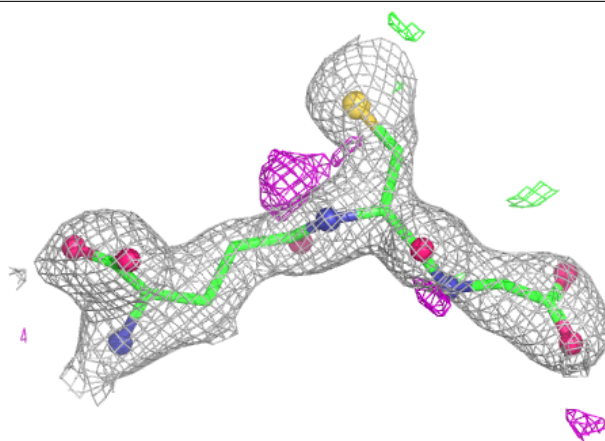
Electron density around GSH C 804:

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

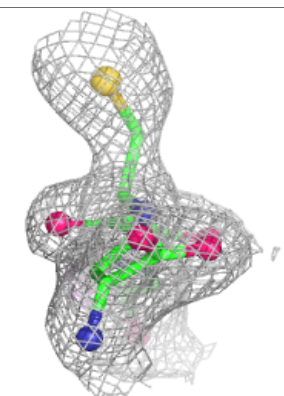
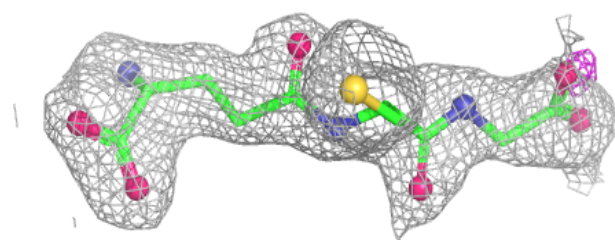
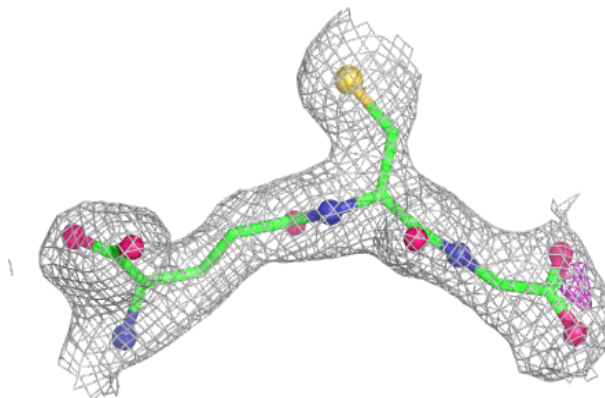


Electron density around GSH D 805:

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

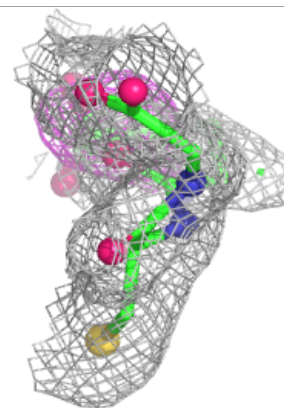
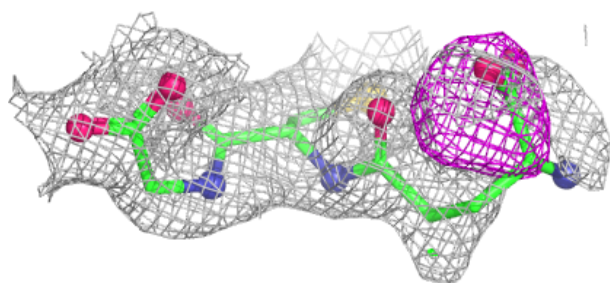
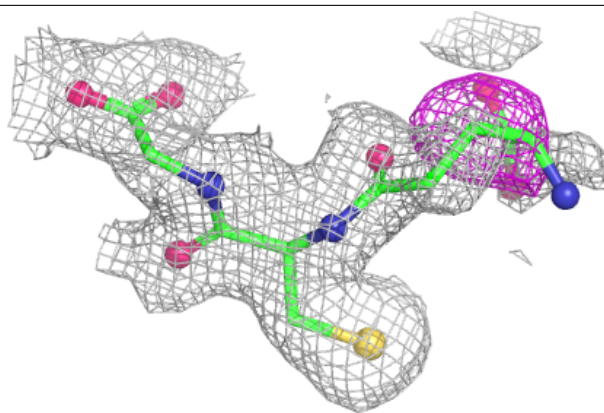
**Electron density around GSH B 801:**

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

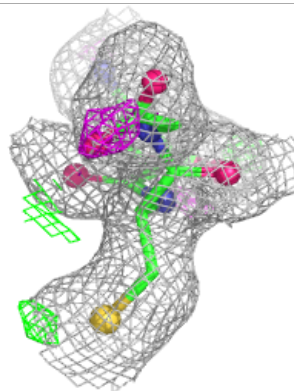
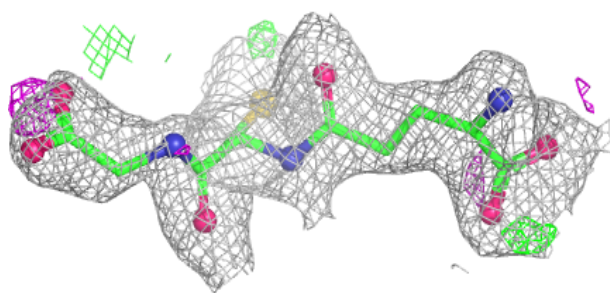
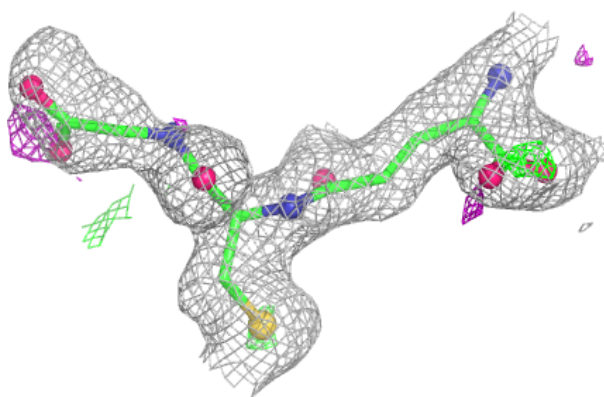


Electron density around GSH C 803:

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and green (positive)

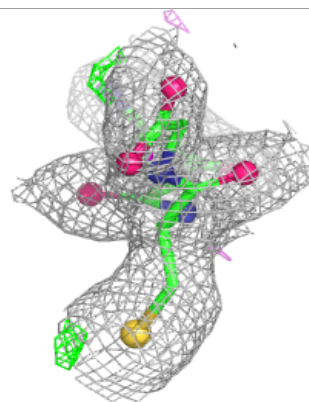
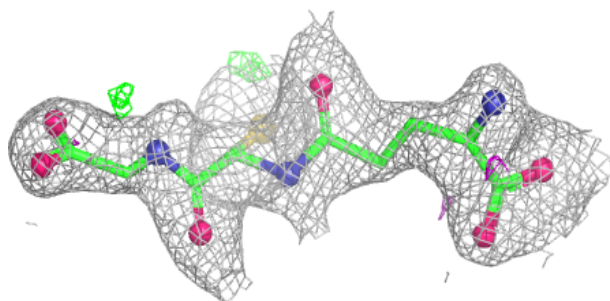
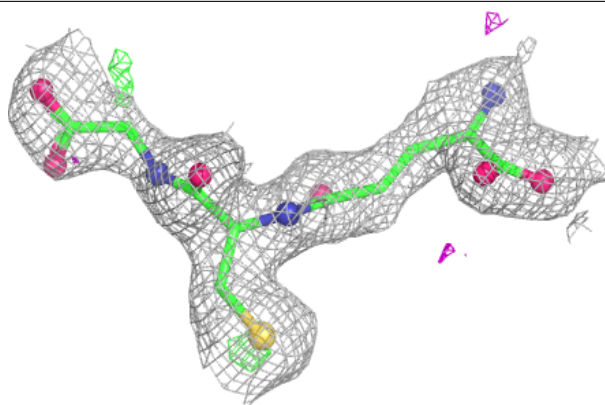
**Electron density around GSH A 799:**

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



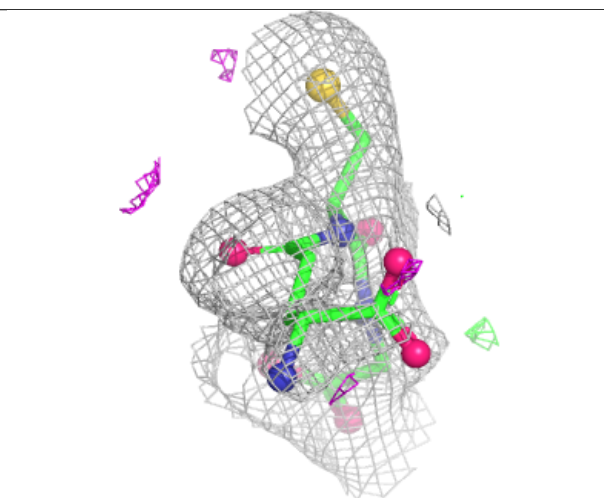
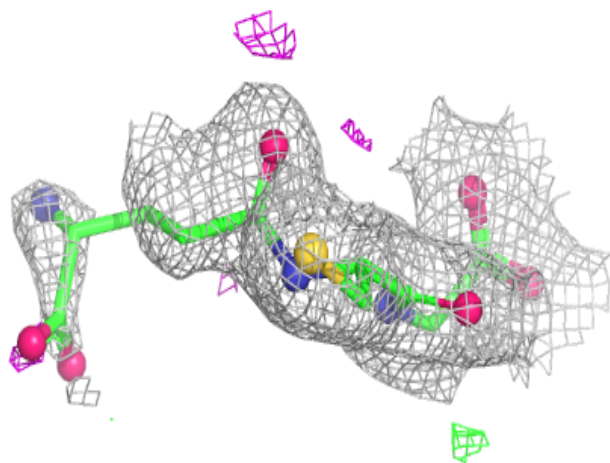
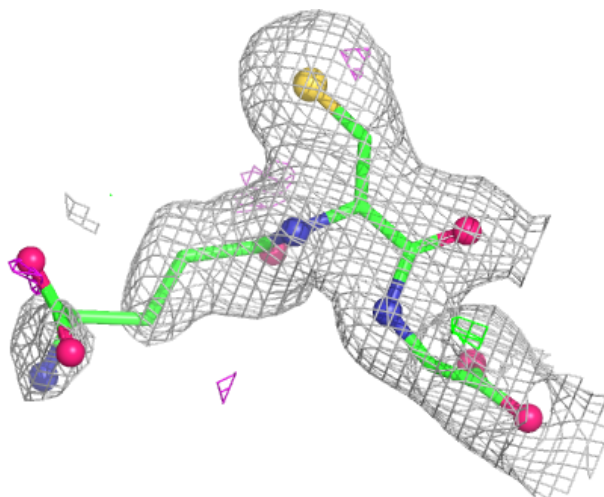
Electron density around GSH C 802:

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



Electron density around GSH A 800:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.