



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:32 AM UTC

PDB ID : 3VI7 / pdb_00003vi7
Title : Human hematopoietic prostaglandin D synthase inhibitor complex structures
Authors : Kado, Y.; Inoue, T.
Deposited on : 2011-09-21
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

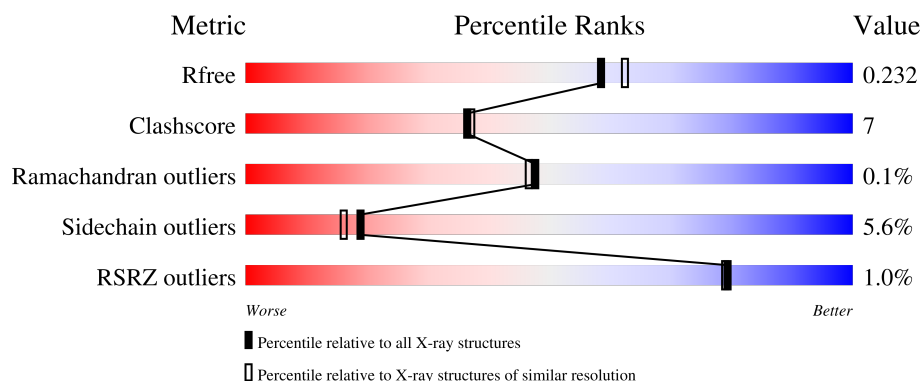
1 Overall quality at a glance

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	198	
1	B	198	
1	C	198	
1	D	198	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7479 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.

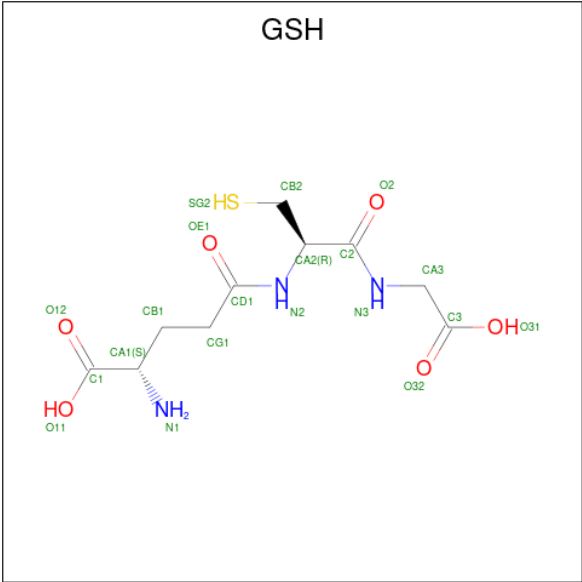
- Molecule 1 is a protein called Hematopoietic prostaglandin D synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	B	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	C	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			
1	D	198	Total	C	N	O	S	0	0	0
			1638	1058	273	298	9			

There are 4 discrepancies between the modelled and reference sequences:

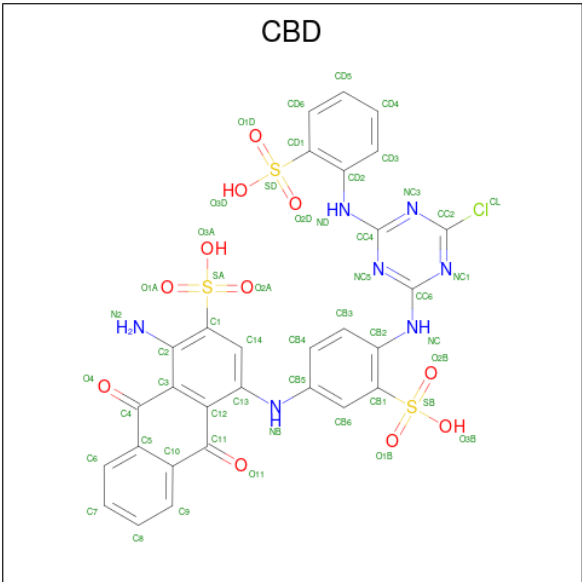
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	ASN	engineered mutation	UNP O60760
B	344	MET	ASN	engineered mutation	UNP O60760
C	544	MET	ASN	engineered mutation	UNP O60760
D	744	MET	ASN	engineered mutation	UNP O60760

- 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		
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 CIBACRON BLUE (CCD ID: CBD) (formula: $C_{29}H_{20}ClN_7O_{11}S_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		
3	B	1	Total	C	Cl	N	O	S	0	0
			51	29	1	7	11	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

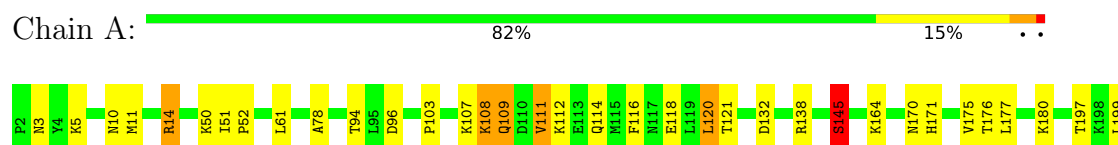
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	219	Total	O	0	0
			219	219		
5	B	216	Total	O	0	0
			216	216		
5	C	145	Total	O	0	0
			145	145		
5	D	163	Total	O	0	0
			163	163		

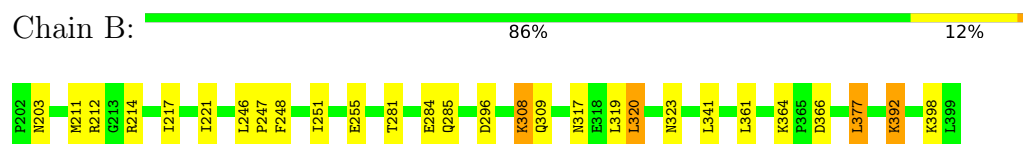
3 Residue-property plots

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.

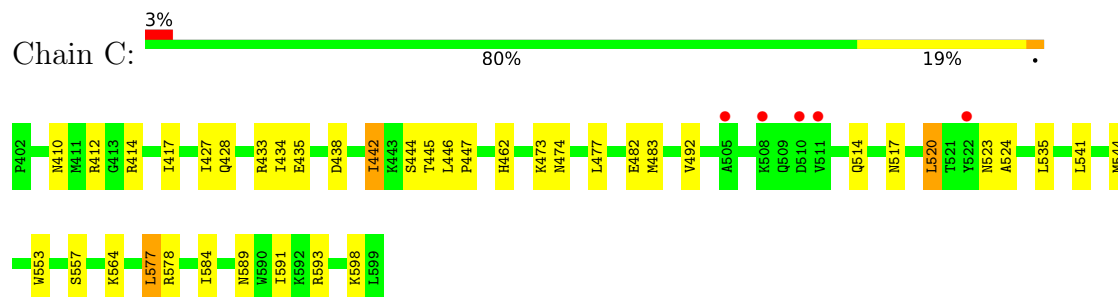
- Molecule 1: Hematopoietic prostaglandin D synthase



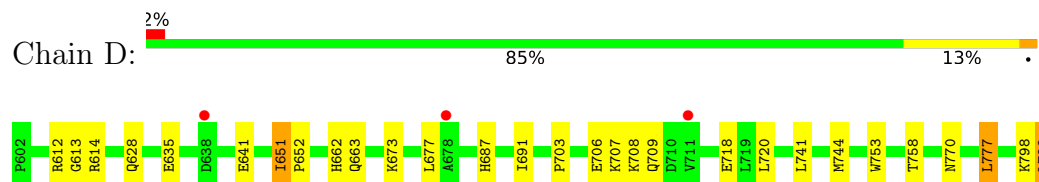
- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



- Molecule 1: Hematopoietic prostaglandin D synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.04Å 47.36Å 184.94Å 90.00° 97.41° 90.00°	Depositor
Resolution (Å)	45.85 – 2.00 45.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.85-2.00) 97.6 (45.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.233 0.174 , 0.232	Depositor DCC
R_{free} test set	2840 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7479	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 31.35 % 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 1.1231e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CBD, GSH, CA

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	1.40	5/1681 (0.3%)	1.19	2/2283 (0.1%)
1	B	1.39	6/1681 (0.4%)	1.17	3/2283 (0.1%)
1	C	1.25	2/1681 (0.1%)	1.20	5/2283 (0.2%)
1	D	1.30	1/1681 (0.1%)	1.16	1/2283 (0.0%)
All	All	1.34	14/6724 (0.2%)	1.18	11/9132 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	317	ASN	C-O	-7.43	1.15	1.24
1	C	417	ILE	CA-CB	6.83	1.63	1.54
1	A	145	SER	CA-C	6.34	1.60	1.52
1	A	175	VAL	CA-CB	6.05	1.62	1.54
1	B	251	ILE	N-CA	6.00	1.51	1.46
1	B	217	ILE	CA-CB	5.88	1.61	1.54
1	B	251	ILE	CA-C	5.80	1.57	1.52
1	D	799	LEU	CG-CD1	-5.66	1.33	1.52
1	A	94	THR	N-CA	5.48	1.52	1.46
1	B	221	ILE	C-O	5.35	1.30	1.24
1	A	11	MET	C-O	5.30	1.30	1.23
1	A	121	THR	N-CA	5.23	1.52	1.46
1	C	492	VAL	CA-CB	5.16	1.60	1.54
1	B	211	MET	CG-SD	5.07	1.93	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ALA	N-CA-C	6.59	118.55	111.36
1	A	112	LYS	N-CA-C	-6.55	103.83	110.97
1	B	361	LEU	N-CA-C	6.23	118.87	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	584	ILE	CA-C-N	-5.89	112.95	119.19
1	C	584	ILE	C-N-CA	-5.89	112.95	119.19
1	B	212	ARG	N-CA-C	-5.49	104.94	111.03
1	C	517	ASN	N-CA-C	5.32	117.08	111.28
1	D	758	THR	N-CA-C	-5.31	105.39	111.07
1	B	309	GLN	N-CA-C	5.23	116.98	111.28
1	C	412	ARG	N-CA-C	-5.13	105.33	111.03
1	C	591	ILE	N-CA-C	5.05	115.77	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1622	28	0
1	B	1638	0	1622	13	0
1	C	1638	0	1622	15	0
1	D	1638	0	1622	25	0
2	A	20	0	15	4	0
2	B	20	0	15	3	0
2	C	20	0	15	0	0
2	D	20	0	15	1	0
3	A	51	0	20	10	0
3	B	51	0	20	10	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	219	0	0	10	0
5	B	216	0	0	5	1
5	C	145	0	0	3	1
5	D	163	0	0	4	0
All	All	7479	0	6588	96	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 7.

All (96) 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:D:612:ARG:H	1:D:799:LEU:HD21	1.03	1.11
1:A:199:LEU:HD13	3:A:201:CBD:HB4	1.43	1.00
2:B:400:GSH:HB22	3:B:401:CBD:O1B	1.61	0.98
3:A:201:CBD:CB6	3:A:201:CBD:H14	1.99	0.92
1:D:613:GLY:H	1:D:799:LEU:HD11	1.36	0.91
1:D:612:ARG:N	1:D:799:LEU:HD21	1.89	0.88
1:A:14:ARG:NH2	1:A:96:ASP:OD1	2.08	0.85
1:B:214:ARG:NH1	2:B:400:GSH:O11	2.09	0.85
1:A:132:ASP:OD1	1:A:171:HIS:HD2	1.60	0.84
1:D:770:ASN:ND2	5:D:840:HOH:O	2.11	0.82
1:D:613:GLY:H	1:D:799:LEU:CD1	1.92	0.82
3:A:201:CBD:C14	3:A:201:CBD:HB6	2.11	0.80
1:A:138:ARG:NH1	5:A:285:HOH:O	2.17	0.77
1:D:613:GLY:N	1:D:799:LEU:HD11	2.00	0.77
1:A:176:THR:HG22	1:A:180:LYS:HE2	1.67	0.76
1:D:706:GLU:OE1	1:D:708:LYS:HG3	1.87	0.75
3:A:201:CBD:H14	3:A:201:CBD:HB6	1.67	0.74
1:D:612:ARG:HB2	1:D:799:LEU:HG	1.68	0.74
3:A:201:CBD:CL	5:A:288:HOH:O	2.42	0.73
1:C:410:ASN:HD22	1:C:433:ARG:HH11	1.34	0.73
1:B:320:LEU:HG	1:B:364:LYS:HB2	1.71	0.72
3:A:201:CBD:CB6	3:A:201:CBD:C14	2.58	0.72
1:A:50:LYS:HD3	2:A:200:GSH:HG12	1.72	0.71
5:A:413:HOH:O	1:D:662:HIS:HD2	1.74	0.70
1:D:651:ILE:HB	1:D:652:PRO:HA	1.71	0.70
1:B:319:LEU:HA	1:B:323:ASN:HD22	1.56	0.70
3:B:401:CBD:HD5	5:B:679:HOH:O	1.90	0.70
1:A:120:LEU:HG	1:A:164:LYS:HB2	1.75	0.69
1:A:14:ARG:HD2	2:A:200:GSH:HB12	1.78	0.65
1:A:108:LYS:HB2	1:A:111:VAL:HG13	1.78	0.65
1:B:255:GLU:OE1	5:B:418:HOH:O	2.16	0.63
1:A:14:ARG:NH1	2:A:200:GSH:O11	2.26	0.62
1:C:541:LEU:HG	1:C:577:LEU:HD11	1.81	0.61
1:A:14:ARG:HH22	1:A:96:ASP:CG	2.07	0.61
1:B:284:GLU:OE2	5:B:774:HOH:O	2.16	0.61
1:A:177:LEU:HA	1:A:180:LYS:HE3	1.81	0.61
5:B:691:HOH:O	1:C:462:HIS:HE1	1.85	0.60
3:B:401:CBD:CB6	3:B:401:CBD:H14	2.32	0.59
3:B:401:CBD:H9	5:B:37:HOH:O	2.02	0.59
1:C:589:ASN:HB3	5:C:616:HOH:O	2.02	0.58
3:A:201:CBD:H9	5:A:653:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:NE2	1:A:118:GLU:OE1	2.27	0.57
1:A:14:ARG:CD	2:A:200:GSH:HB12	2.35	0.57
1:D:612:ARG:NH2	1:D:799:LEU:HB2	2.20	0.56
1:C:410:ASN:ND2	1:C:433:ARG:HH11	2.02	0.56
3:A:201:CBD:O11	3:A:201:CBD:NB	2.36	0.55
1:D:753:TRP:CD1	1:D:777:LEU:HD13	2.43	0.54
1:C:482:GLU:HG2	5:C:788:HOH:O	2.09	0.53
3:B:401:CBD:O11	3:B:401:CBD:NB	2.29	0.52
1:D:741:LEU:HG	1:D:777:LEU:HD11	1.92	0.52
1:D:799:LEU:N	1:D:799:LEU:CD2	2.73	0.51
1:C:410:ASN:HD22	1:C:433:ARG:HD3	1.76	0.51
1:C:553:TRP:CD1	1:C:577:LEU:HD13	2.46	0.51
2:B:400:GSH:CB2	3:B:401:CBD:O1B	2.47	0.50
1:B:281:THR:O	1:B:285:GLN:HG3	2.12	0.50
1:A:199:LEU:CD1	3:A:201:CBD:HB4	2.28	0.50
1:A:5:LYS:HE3	5:A:651:HOH:O	2.10	0.50
1:C:473:LYS:O	1:C:474:ASN:HB2	2.12	0.50
1:B:214:ARG:NH2	1:B:296:ASP:OD1	2.44	0.50
1:D:628:GLN:NE2	5:D:348:HOH:O	2.44	0.50
1:D:691:ILE:HG12	5:D:827:HOH:O	2.12	0.50
1:C:557:SER:OG	1:C:578:ARG:HD2	2.13	0.49
1:A:103:PRO:HD2	1:A:116:PHE:CE1	2.49	0.48
1:D:612:ARG:H	1:D:799:LEU:CD2	1.97	0.48
1:D:703:PRO:HB2	1:D:706:GLU:HB2	1.95	0.48
1:D:614:ARG:HE	2:D:800:GSH:C1	2.27	0.48
1:D:799:LEU:N	1:D:799:LEU:HD22	2.28	0.48
1:A:50:LYS:HE2	5:D:573:HOH:O	2.13	0.47
1:B:247:PRO:HB2	1:B:248:PHE:CD1	2.49	0.47
1:A:170:ASN:ND2	5:A:840:HOH:O	2.39	0.47
1:D:662:HIS:O	1:D:663:GLN:HB2	2.14	0.46
3:B:401:CBD:CB6	3:B:401:CBD:C14	2.89	0.46
1:A:10:ASN:O	1:A:197:THR:HG21	2.16	0.46
5:A:413:HOH:O	1:D:662:HIS:CD2	2.59	0.46
1:B:341:LEU:HG	1:B:377:LEU:HD11	1.99	0.45
3:B:401:CBD:C14	3:B:401:CBD:HB6	2.47	0.45
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.32	0.44
1:C:435:GLU:HB3	5:C:626:HOH:O	2.17	0.44
1:A:132:ASP:OD1	1:A:171:HIS:CD2	2.53	0.44
1:A:199:LEU:HD13	3:A:201:CBD:CB4	2.31	0.44
3:B:401:CBD:H14	3:B:401:CBD:HB6	1.99	0.44
1:B:398:LYS:HD3	3:B:401:CBD:HD6	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	5:A:460:HOH:O	2.17	0.43
1:B:366:ASP:C	1:B:366:ASP:OD1	2.62	0.43
1:A:3:ASN:ND2	5:A:287:HOH:O	2.53	0.42
1:B:308:LYS:HB2	1:B:308:LYS:HE2	1.63	0.42
1:D:798:LYS:O	1:D:799:LEU:HB2	2.19	0.41
1:B:392:LYS:HB3	1:B:392:LYS:HE3	1.82	0.41
1:C:438:ASP:O	1:C:442:ILE:HG13	2.21	0.41
1:C:483:MET:HE3	1:C:483:MET:HB3	1.87	0.41
1:A:171:HIS:HE1	5:A:202:HOH:O	2.03	0.40
1:C:523:ASN:O	1:C:524:ALA:C	2.63	0.40
1:A:51:ILE:HB	1:A:52:PRO:HA	2.04	0.40
1:A:61:LEU:HD23	1:D:687:HIS:CE1	2.57	0.40
1:D:651:ILE:CB	1:D:652:PRO:HA	2.47	0.40
1:C:520:LEU:HG	1:C:564:LYS:HB2	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)
5:B:846:HOH:O	5:C:801:HOH:O[1_565]	2.11	0.09

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	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
1	B	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
1	C	196/198 (99%)	191 (97%)	4 (2%)	1 (0%)	24	21
1	D	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
All	All	784/792 (99%)	765 (98%)	18 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	444	SER

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	178/178 (100%)	171 (96%)	7 (4%)	28	28
1	B	178/178 (100%)	172 (97%)	6 (3%)	32	33
1	C	178/178 (100%)	162 (91%)	16 (9%)	9	6
1	D	178/178 (100%)	167 (94%)	11 (6%)	16	13
All	All	712/712 (100%)	672 (94%)	40 (6%)	19	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	107	LYS
1	A	108	LYS
1	A	109	GLN
1	A	111	VAL
1	A	120	LEU
1	A	145	SER
1	B	203	ASN
1	B	246	LEU
1	B	308	LYS
1	B	320	LEU
1	B	377	LEU
1	B	392	LYS
1	C	414	ARG
1	C	427	ILE
1	C	428	GLN
1	C	434	ILE
1	C	442	ILE
1	C	445	THR

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Mol	Chain	Res	Type
1	C	446	LEU
1	C	447	PRO
1	C	477	LEU
1	C	514	GLN
1	C	520	LEU
1	C	535	LEU
1	C	544	MET
1	C	577	LEU
1	C	593	ARG
1	C	598	LYS
1	D	635	GLU
1	D	641	GLU
1	D	651	ILE
1	D	673	LYS
1	D	677	LEU
1	D	707	LYS
1	D	709	GLN
1	D	718	GLU
1	D	720	LEU
1	D	744	MET
1	D	777	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	62	HIS
1	A	109	GLN
1	A	170	ASN
1	A	171	HIS
1	B	314	GLN
1	B	323	ASN
1	C	403	ASN
1	C	410	ASN
1	C	462	HIS
1	C	480	ASN
1	C	514	GLN
1	C	517	ASN
1	C	570	ASN
1	C	589	ASN
1	C	596	GLN
1	D	603	ASN

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Mol	Chain	Res	Type
1	D	628	GLN
1	D	662	HIS
1	D	709	GLN
1	D	729	GLN
1	D	770	ASN
1	D	796	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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
3	CBD	B	401	-	56,56,56	2.09	12 (21%)	81,87,87	2.21	24 (29%)
2	GSH	A	200	-	18,19,19	3.12	3 (16%)	21,24,24	1.70	3 (14%)
2	GSH	B	400	-	18,19,19	3.09	3 (16%)	21,24,24	1.91	5 (23%)
2	GSH	D	800	-	18,19,19	3.12	2 (11%)	21,24,24	1.81	4 (19%)
2	GSH	C	600	-	18,19,19	3.04	2 (11%)	21,24,24	1.17	3 (14%)
3	CBD	A	201	-	56,56,56	2.20	10 (17%)	81,87,87	2.12	21 (25%)

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	CBD	B	401	-	-	14/30/46/46	0/6/6/6
2	GSH	A	200	-	-	0/24/24/24	-
2	GSH	B	400	-	-	2/24/24/24	-
2	GSH	D	800	-	-	0/24/24/24	-
2	GSH	C	600	-	-	0/24/24/24	-
3	CBD	A	201	-	-	10/30/46/46	0/6/6/6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	200	GSH	OE1-CD1	9.93	1.42	1.23
2	D	800	GSH	OE1-CD1	9.36	1.41	1.23
2	C	600	GSH	OE1-CD1	9.09	1.41	1.23
2	B	400	GSH	OE1-CD1	9.00	1.41	1.23
2	B	400	GSH	O2-C2	8.61	1.39	1.23
2	D	800	GSH	O2-C2	8.60	1.39	1.23
2	C	600	GSH	O2-C2	8.52	1.39	1.23
2	A	200	GSH	O2-C2	7.99	1.38	1.23
3	B	401	CBD	O11-C11	7.96	1.37	1.22
3	A	201	CBD	O11-C11	7.67	1.36	1.22
3	A	201	CBD	CB1-SB	-6.23	1.61	1.77
3	B	401	CBD	CD1-SD	-5.88	1.62	1.77
3	A	201	CBD	C1-SA	-5.64	1.63	1.77
3	A	201	CBD	CD1-SD	-5.51	1.63	1.77
3	B	401	CBD	C1-SA	-5.39	1.63	1.77
3	B	401	CBD	CB1-SB	-5.29	1.63	1.77
3	A	201	CBD	C10-C11	-4.08	1.40	1.48
3	A	201	CBD	C5-C4	-3.99	1.40	1.48
3	A	201	CBD	CB5-NB	-3.23	1.33	1.40
3	A	201	CBD	C12-C11	-3.12	1.40	1.47
2	B	400	GSH	O11-C1	-3.12	1.20	1.30
3	B	401	CBD	C5-C4	-3.12	1.42	1.48
3	B	401	CBD	CB5-NB	-3.08	1.34	1.40
3	A	201	CBD	C3-C4	-2.90	1.40	1.47
3	B	401	CBD	C12-C11	-2.72	1.41	1.47
3	B	401	CBD	O4-C4	2.41	1.27	1.22
3	B	401	CBD	CC2-NC1	2.41	1.36	1.32
2	A	200	GSH	O11-C1	-2.33	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	CBD	C3-C4	-2.28	1.42	1.47
3	A	201	CBD	CC2-NC3	2.27	1.36	1.32
3	B	401	CBD	C10-C11	-2.17	1.44	1.48
3	B	401	CBD	CC2-NC3	2.01	1.36	1.32

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CBD	CC4-NC3-CC2	7.64	120.46	112.41
3	B	401	CBD	CC4-NC3-CC2	7.09	119.88	112.41
3	B	401	CBD	CC6-NC1-CC2	6.40	119.15	112.41
3	A	201	CBD	CC6-NC1-CC2	6.18	118.92	112.41
3	B	401	CBD	C1-C2-N2	-5.62	116.96	122.64
2	D	800	GSH	CA2-CB2-SG2	-5.27	108.22	114.16
2	A	200	GSH	CA2-CB2-SG2	-5.20	108.30	114.16
2	B	400	GSH	O11-C1-O12	-4.96	112.82	124.08
3	A	201	CBD	NC3-CC2-NC1	-4.95	120.47	129.52
3	B	401	CBD	NC3-CC2-NC1	-4.84	120.67	129.52
3	A	201	CBD	C1-C2-N2	-4.60	117.99	122.64
3	A	201	CBD	NC5-CC4-NC3	-4.48	118.91	126.26
3	B	401	CBD	CL-CC2-NC1	4.45	121.43	115.17
3	A	201	CBD	CL-CC2-NC3	4.01	120.82	115.17
3	B	401	CBD	O3B-SB-CB1	3.91	113.72	106.12
3	B	401	CBD	NC5-CC4-NC3	-3.82	120.00	126.26
2	A	200	GSH	O11-C1-O12	-3.81	115.44	124.08
3	A	201	CBD	O3A-SA-C1	3.73	113.36	106.12
3	B	401	CBD	NC5-CC6-NC1	-3.60	120.36	126.26
3	A	201	CBD	O3B-SB-CB1	3.54	113.00	106.12
3	B	401	CBD	CD6-CD1-CD2	-3.49	117.44	120.29
3	A	201	CBD	CB1-CB2-NC	-3.42	118.34	121.50
3	B	401	CBD	CC6-NC5-CC4	3.40	119.95	113.85
3	A	201	CBD	CC6-NC5-CC4	3.40	119.94	113.85
3	B	401	CBD	O3D-SD-CD1	3.36	112.66	106.12
2	B	400	GSH	OE1-CD1-CG1	-3.31	116.03	122.02
3	A	201	CBD	C14-C1-C2	-3.27	117.83	121.78
3	B	401	CBD	C14-C1-C2	-3.25	117.85	121.78
3	B	401	CBD	O11-C11-C12	-3.18	116.12	121.44
2	D	800	GSH	O11-C1-O12	-3.14	116.96	124.08
3	A	201	CBD	O3D-SD-CD1	3.07	112.08	106.12
3	A	201	CBD	CD6-CD1-CD2	-3.04	117.81	120.29
3	A	201	CBD	NC5-CC6-NC1	-3.03	121.29	126.26
2	B	400	GSH	CB2-CA2-C2	-2.97	103.04	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	CBD	C7-C8-C9	-2.83	116.75	120.24
3	B	401	CBD	CB6-CB1-CB2	-2.75	118.11	120.85
3	B	401	CBD	CD2-ND-CC4	-2.70	120.97	129.22
2	B	400	GSH	CG1-CD1-N2	2.68	120.59	115.86
2	C	600	GSH	CB1-CG1-CD1	-2.59	107.28	113.06
3	A	201	CBD	CL-CC2-NC1	2.51	118.71	115.17
3	B	401	CBD	O1A-SA-C1	2.45	112.18	106.52
3	A	201	CBD	CD2-ND-CC4	-2.43	121.79	129.22
3	A	201	CBD	CB5-NB-C13	-2.42	120.54	126.73
3	B	401	CBD	CD3-CD2-CD1	2.42	121.20	117.81
3	B	401	CBD	C9-C10-C11	2.39	123.00	119.26
3	B	401	CBD	O3A-SA-C1	2.36	110.71	106.12
3	A	201	CBD	CB3-CB2-CB1	2.32	121.07	117.81
2	C	600	GSH	O11-C1-O12	-2.28	118.91	124.08
3	B	401	CBD	CB3-CB2-CB1	2.25	120.97	117.81
3	A	201	CBD	CD3-CD2-CD1	2.21	120.91	117.81
2	D	800	GSH	C3-CA3-N3	-2.19	106.25	113.06
2	A	200	GSH	CG1-CB1-CA1	-2.17	108.88	113.86
3	B	401	CBD	C5-C4-C3	2.15	121.44	117.97
2	D	800	GSH	CA3-N3-C2	2.12	126.73	121.38
3	B	401	CBD	CB2-NC-CC6	-2.08	122.89	129.22
2	C	600	GSH	O31-C3-CA3	2.07	120.70	112.81
2	B	400	GSH	C2-CA2-N2	2.07	116.72	111.11
3	B	401	CBD	O1D-SD-CD1	2.07	111.30	106.52
3	B	401	CBD	C12-C13-NB	-2.04	117.84	120.56
3	A	201	CBD	CB6-CB1-CB2	-2.02	118.83	120.85

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	CBD	NC1-CC6-NC-CB2
3	A	201	CBD	NC5-CC6-NC-CB2
3	A	201	CBD	CD1-CD2-ND-CC4
3	B	401	CBD	CB6-CB1-SB-O2B
3	B	401	CBD	NC1-CC6-NC-CB2
3	B	401	CBD	NC5-CC6-NC-CB2
3	B	401	CBD	CD2-CD1-SD-O3D
3	B	401	CBD	CD6-CD1-SD-O1D
3	B	401	CBD	CD6-CD1-SD-O2D
3	B	401	CBD	CD6-CD1-SD-O3D
3	A	201	CBD	CB2-CB1-SB-O1B

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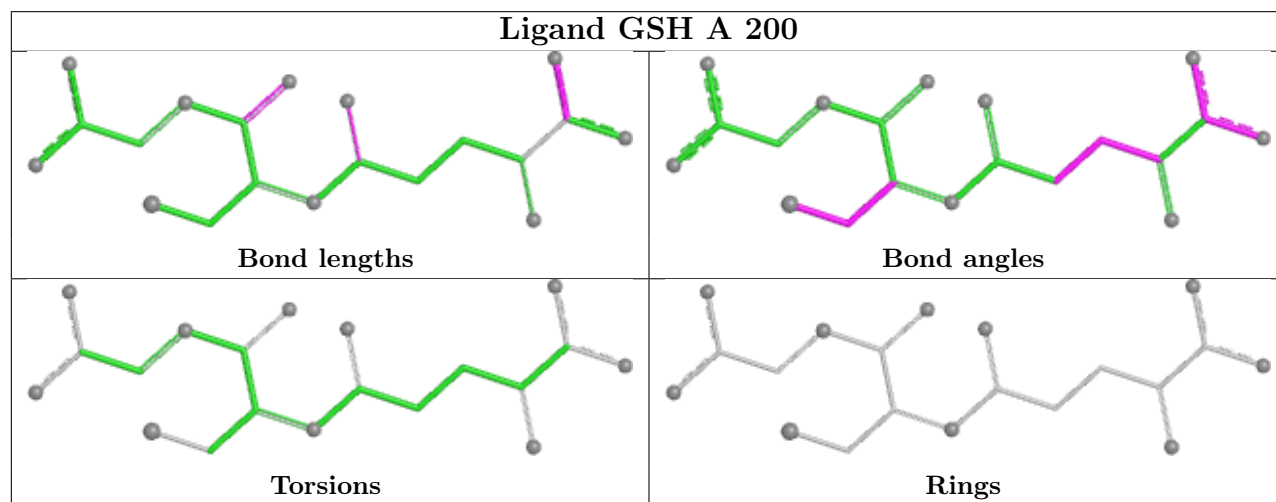
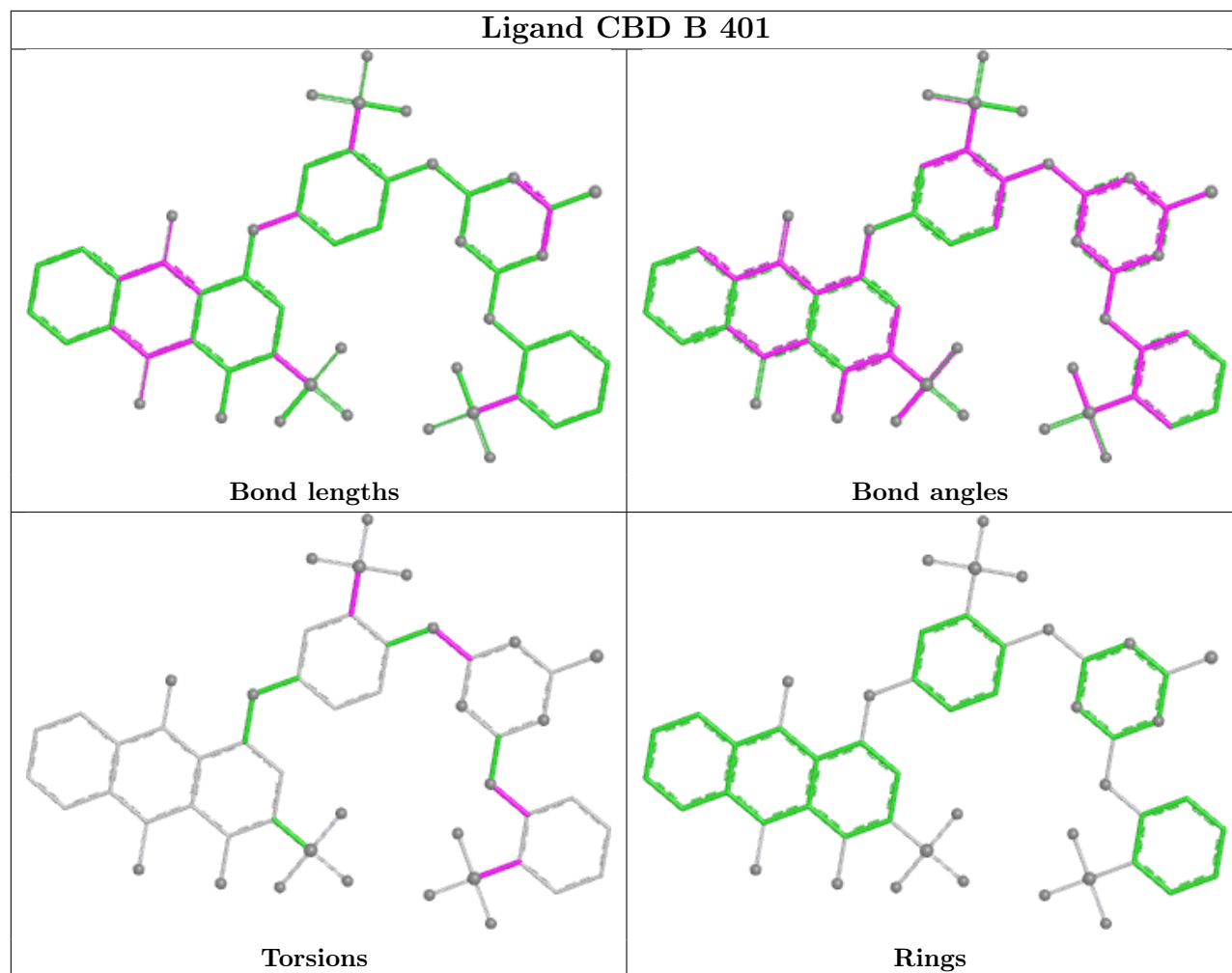
Mol	Chain	Res	Type	Atoms
3	A	201	CBD	CB2-CB1-SB-O2B
3	B	401	CBD	CD1-CD2-ND-CC4
3	A	201	CBD	CB6-CB1-SB-O1B
3	A	201	CBD	CB6-CB1-SB-O2B
3	B	401	CBD	CB6-CB1-SB-O1B
3	A	201	CBD	CB2-CB1-SB-O3B
3	A	201	CBD	CB6-CB1-SB-O3B
3	B	401	CBD	CB6-CB1-SB-O3B
3	A	201	CBD	CD3-CD2-ND-CC4
3	B	401	CBD	CD3-CD2-ND-CC4
3	B	401	CBD	CB2-CB1-SB-O2B
3	B	401	CBD	CD2-CD1-SD-O2D
2	B	400	GSH	N3-C2-CA2-N2
2	B	400	GSH	O2-C2-CA2-N2
3	B	401	CBD	CB2-CB1-SB-O3B

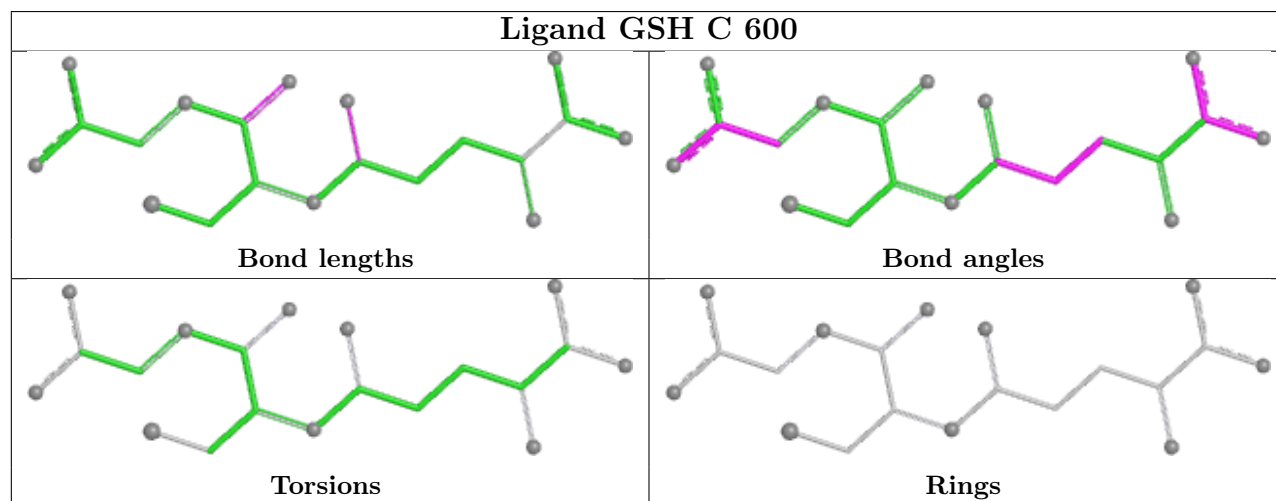
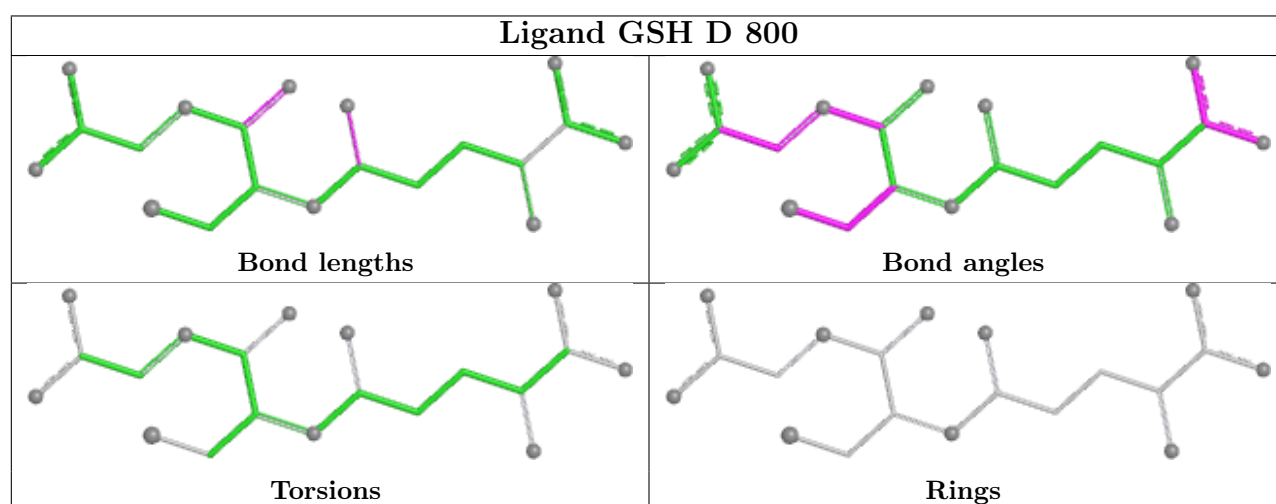
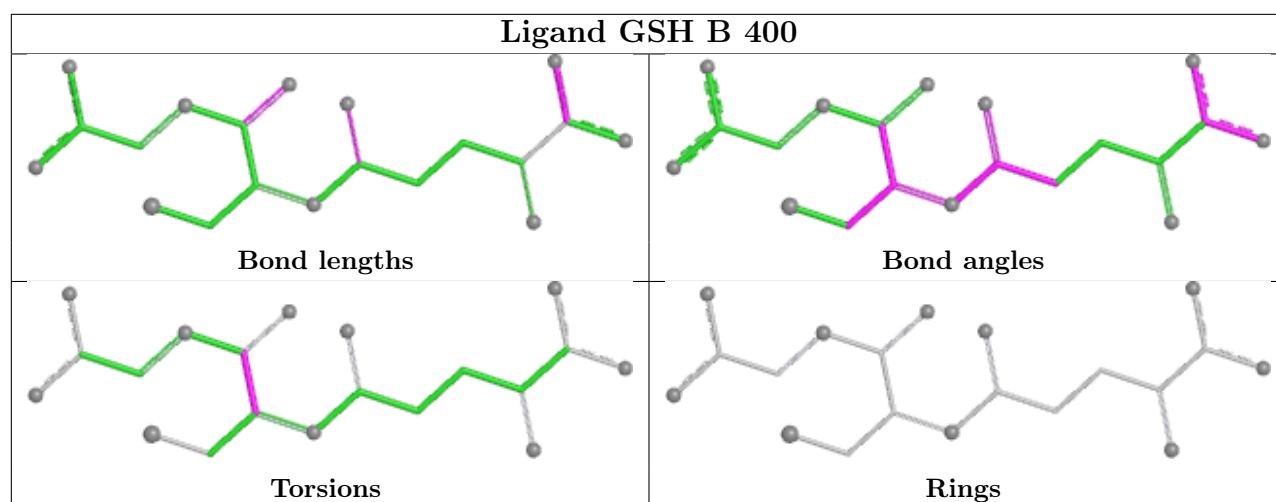
There are no ring outliers.

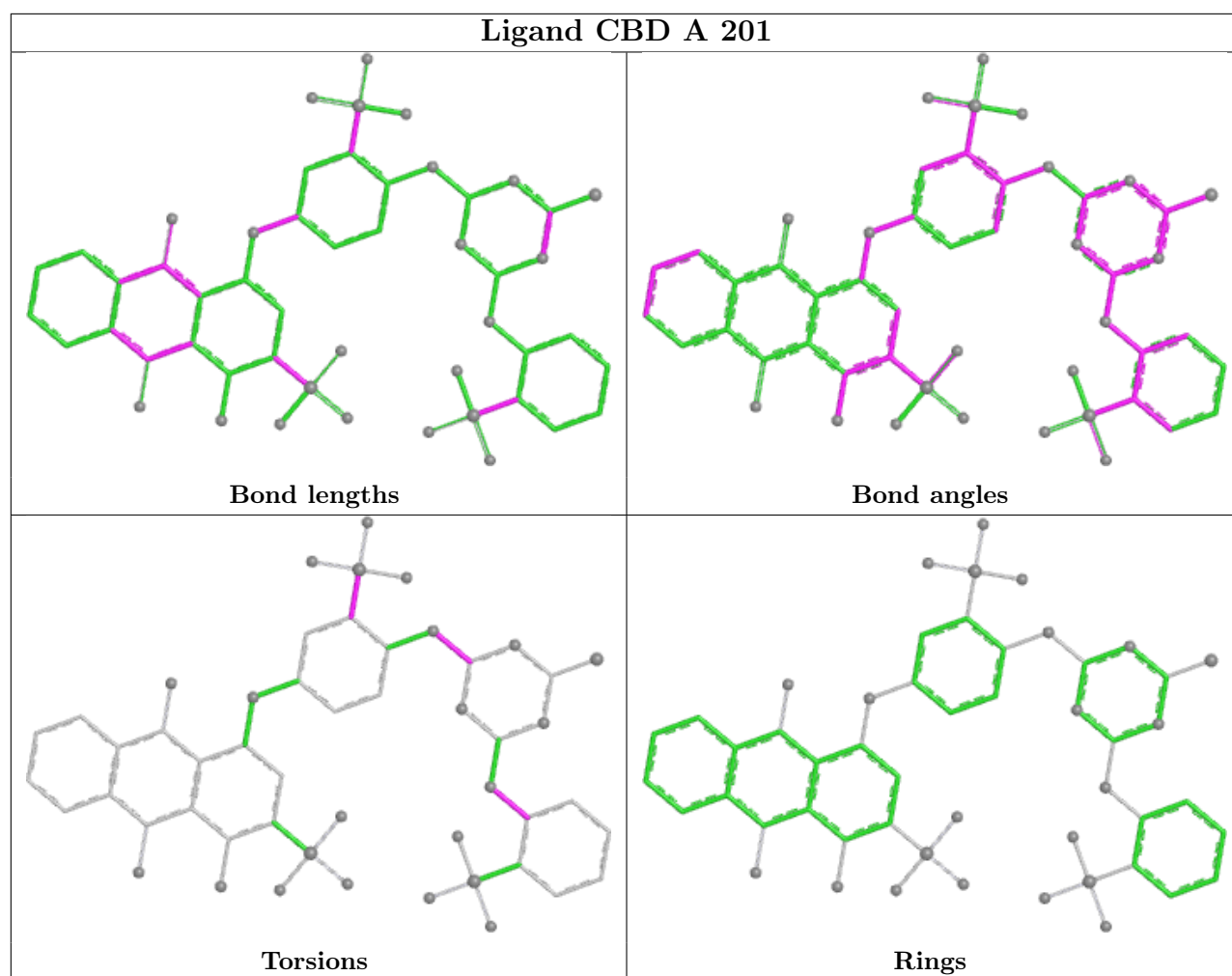
5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	CBD	10	0
2	A	200	GSH	4	0
2	B	400	GSH	3	0
2	D	800	GSH	1	0
3	A	201	CBD	10	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	198/198 (100%)	-0.48	0 100 100	9, 16, 31, 42	0
1	B	198/198 (100%)	-0.54	0 100 100	7, 15, 31, 39	0
1	C	198/198 (100%)	-0.05	5 (2%) 58 58	9, 23, 49, 61	0
1	D	198/198 (100%)	-0.16	3 (1%) 72 71	9, 22, 49, 55	0
All	All	792/792 (100%)	-0.31	8 (1%) 79 79	7, 19, 41, 61	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	522	TYR	3.9
1	D	638	ASP	2.6
1	C	505	ALA	2.6
1	C	511	VAL	2.5
1	D	678	ALA	2.4
1	D	711	VAL	2.2
1	C	508	LYS	2.2
1	C	510	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

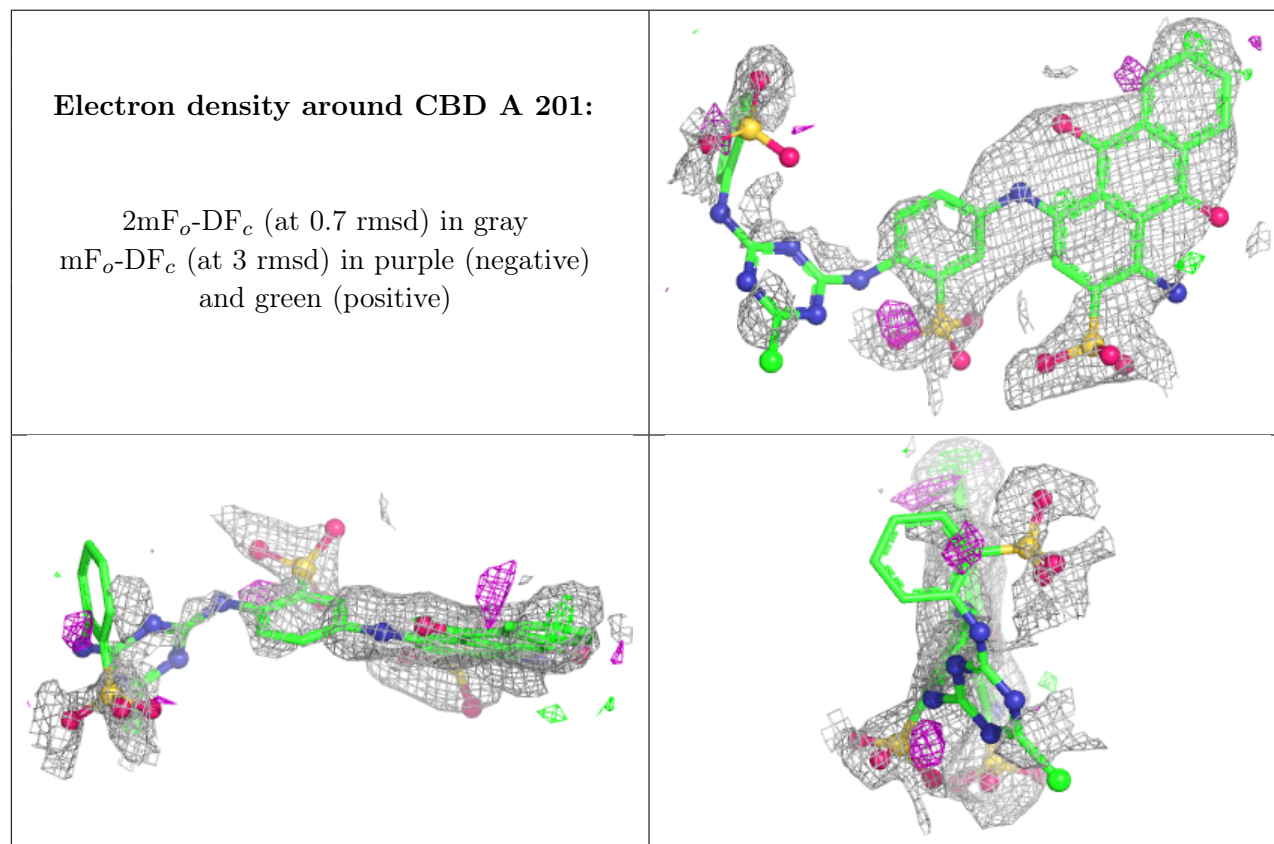
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

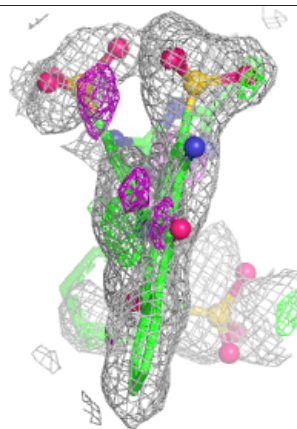
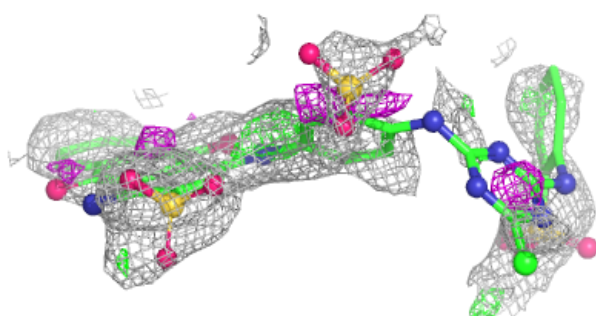
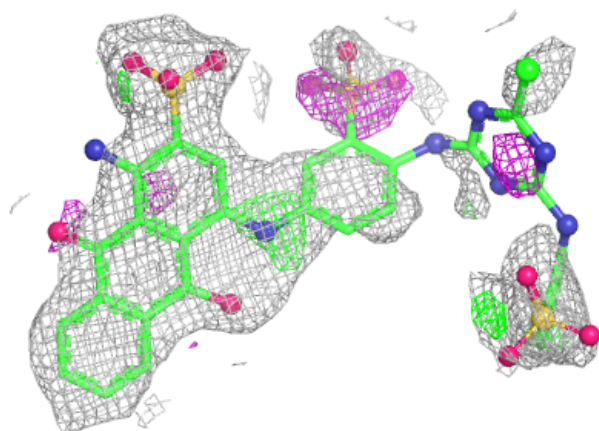
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CBD	A	201	51/51	0.72	0.20	58,86,117,118	0
3	CBD	B	401	51/51	0.79	0.18	34,76,104,104	0
2	GSH	A	200	20/20	0.92	0.11	14,39,58,60	0
2	GSH	D	800	20/20	0.92	0.10	17,36,50,51	0
2	GSH	C	600	20/20	0.94	0.07	14,28,41,41	0
2	GSH	B	400	20/20	0.94	0.09	10,33,40,41	0
4	CA	C	902	1/1	0.95	0.08	43,43,43,43	0
4	CA	D	901	1/1	0.95	0.09	37,37,37,37	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.

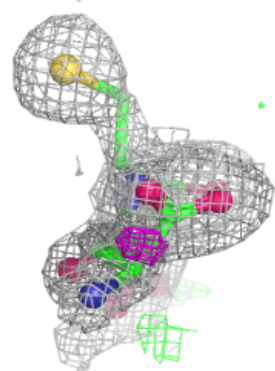
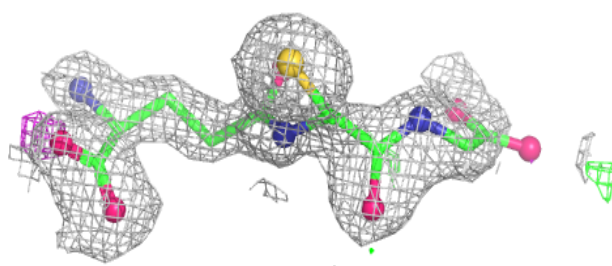
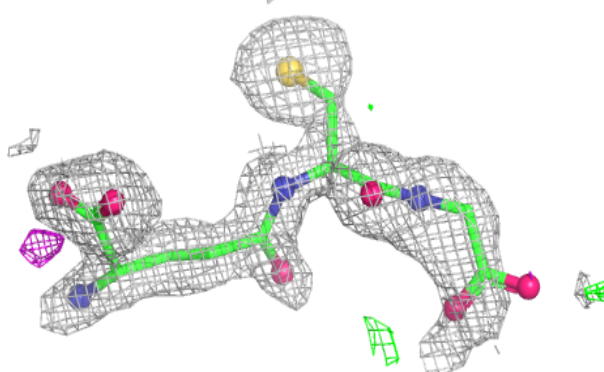


Electron density around CBD B 401:

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

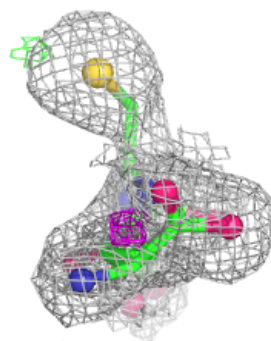
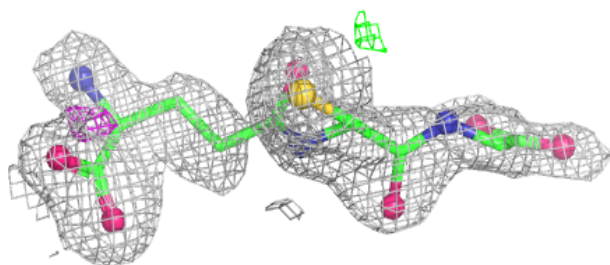
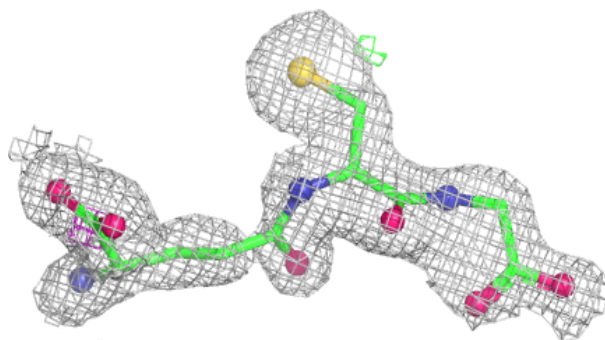
**Electron density around GSH A 200:**

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

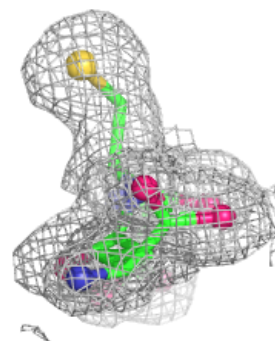
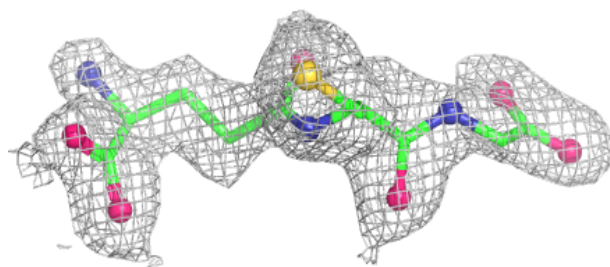
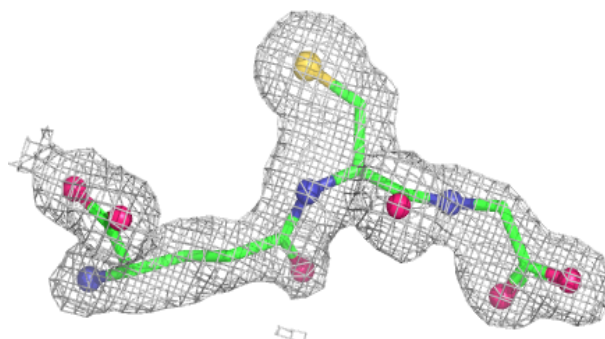


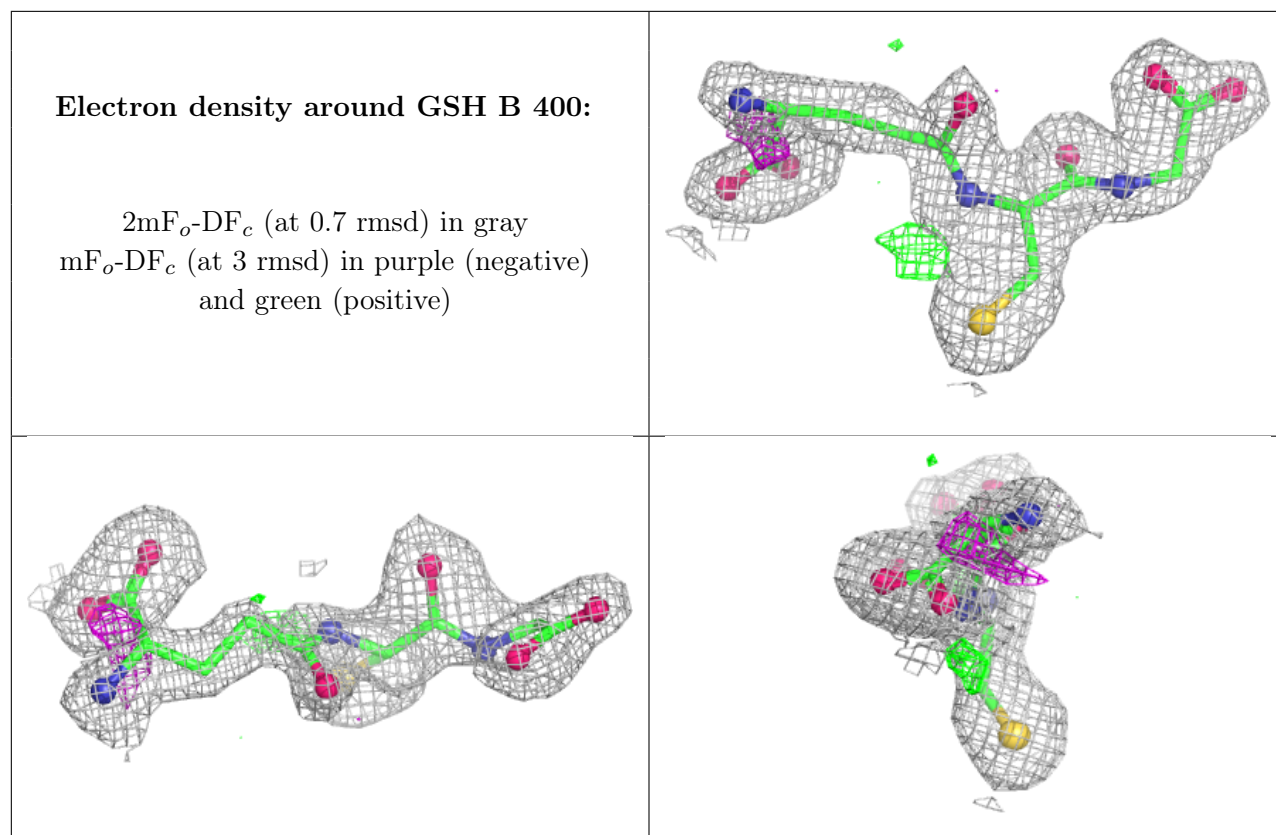
Electron density around GSH D 800:

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

**Electron density around GSH C 600:**

$2mF_o-DF_c$ (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.