Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 09:24 PM EST

PDB ID	:	3VI5
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 (i) 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 (i)) were used in the production of this report:

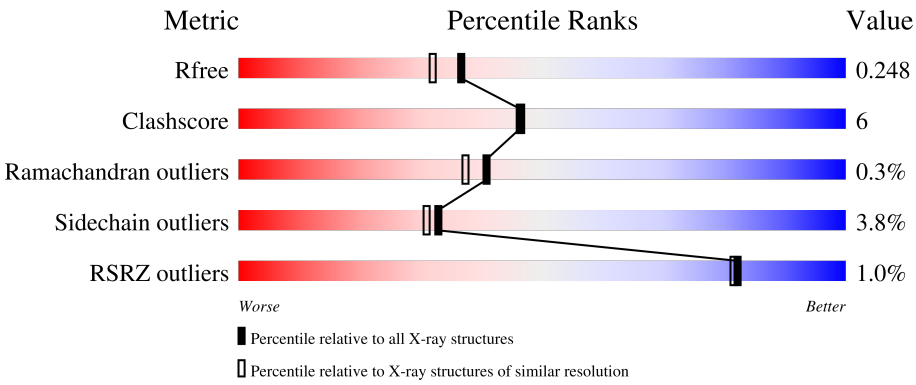
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	% 78% 21% •
1	B	198	3% 81% 16% ••
1	C	198	85% 14% ••
1	D	198	88% 11% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7363 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.

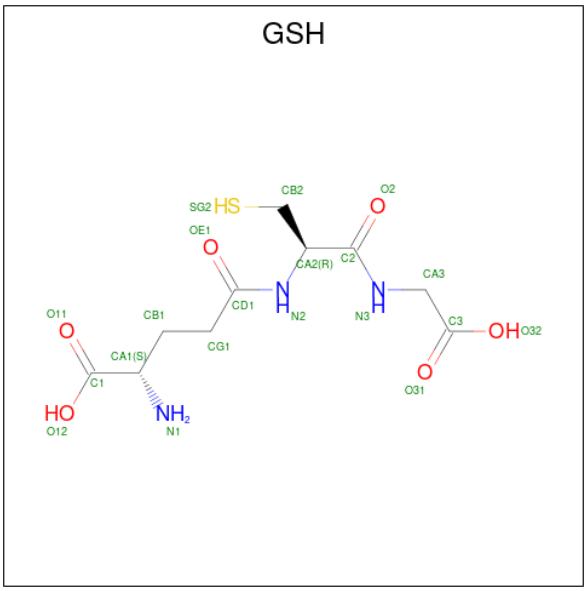
- Molecule 1 is a protein called Hematopoietic prostaglandin D synthase.

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

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 (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).

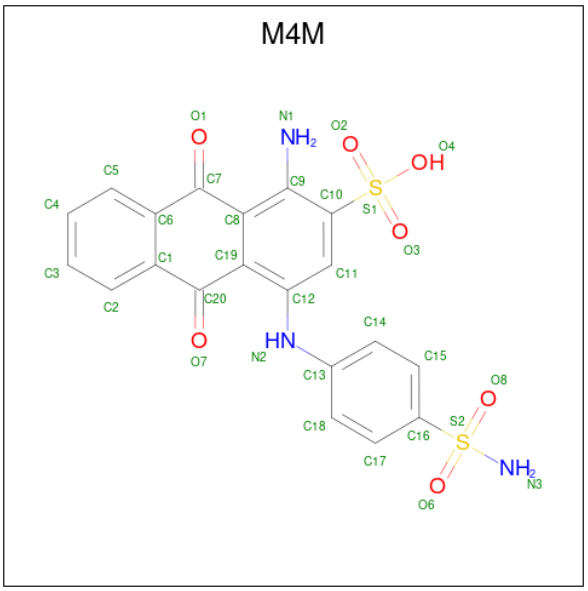


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	20	10	3	6	1	0	0
			Total	C	N	O	S		
2	B	1	20	10	3	6	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

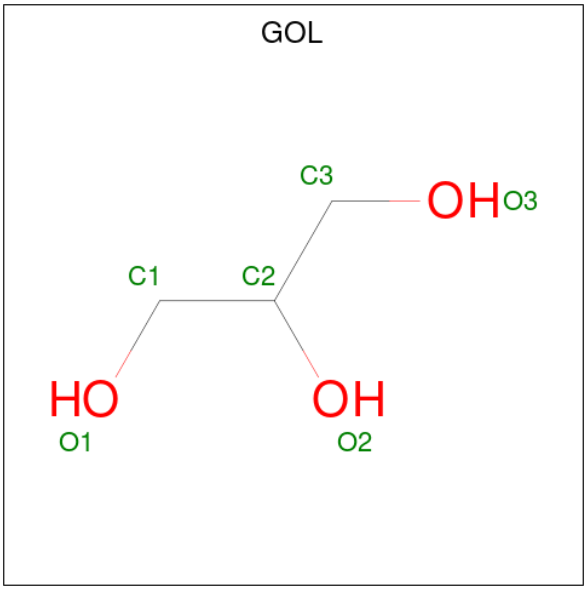
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	C	1	1	1	0	0
			Total	Ca		
3	D	1	1	1	0	0

- Molecule 4 is 1-amino-9,10-dioxo-4-[(4-sulfamoylphenyl)amino]-9,10-dihydroanthracene-2-sulfonic acid (three-letter code: M4M) (formula: $C_{20}H_{15}N_3O_7S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	32	20	3	7	2	0	0
			Total	C	N	O	S		
4	D	1	32	20	3	7	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

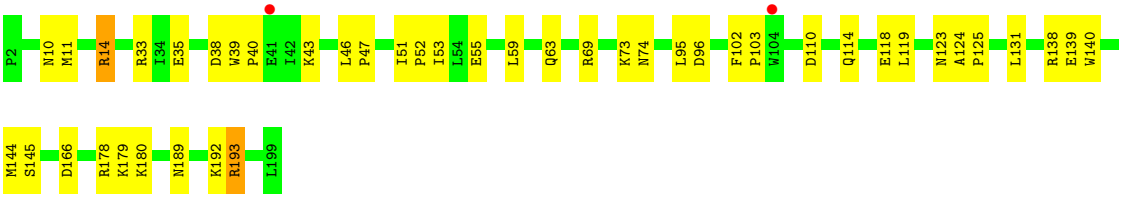
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	116	116	116	0	0
			Total	O		
6	B	112	112	112	0	0
			Total	O		
6	C	239	239	239	0	0
			Total	O		
6	D	232	232	232	0	0

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.

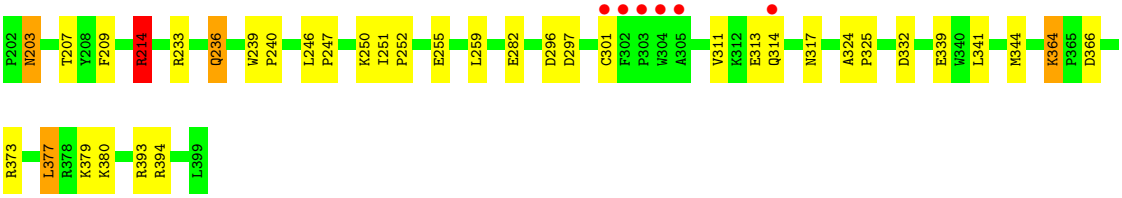
• Molecule 1: Hematopoietic prostaglandin D synthase

Chain A:



• Molecule 1: Hematopoietic prostaglandin D synthase

Chain B:



• Molecule 1: Hematopoietic prostaglandin D synthase

Chain C:

• Molecule 1: Hematopoietic prostaglandin D synthase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	47.28Å 48.99Å 91.92Å 95.80° 90.99° 90.14°	Depositor
Resolution (Å)	33.86 – 2.00 33.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (33.86-2.00) 97.2 (33.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.176 , 0.249 0.175 , 0.248	Depositor DCC
R_{free} test set	2735 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 29.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.299 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7363	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, M4M, CA, 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	0.92	0/1681	0.85	4/2283 (0.2%)
1	B	0.94	0/1681	0.88	6/2283 (0.3%)
1	C	1.23	5/1681 (0.3%)	0.93	4/2283 (0.2%)
1	D	1.27	2/1681 (0.1%)	0.96	4/2283 (0.2%)
All	All	1.10	7/6724 (0.1%)	0.91	18/9132 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	718	GLU	CB-CG	6.22	1.64	1.52
1	C	412	ARG	CG-CD	5.90	1.66	1.51
1	C	516	PHE	CD1-CE1	5.73	1.50	1.39
1	C	464	SER	CB-OG	-5.70	1.34	1.42
1	C	553	TRP	CE3-CZ3	5.43	1.47	1.38
1	D	748	TRP	CE3-CZ3	5.34	1.47	1.38
1	C	429	TYR	CD2-CE2	5.31	1.47	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	214	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	C	414	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	214	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	69	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	D	738	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	D	720	LEU	CB-CG-CD1	6.14	121.44	111.00
1	D	614	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	178	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	69	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	297	ASP	CB-CG-OD2	5.75	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	538	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	C	446	LEU	CB-CG-CD1	5.15	119.75	111.00
1	B	233	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	394	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	393	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	611	MET	CA-CB-CG	5.06	121.91	113.30
1	C	411	MET	CA-CB-CG	5.04	121.88	113.30
1	A	138	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1622	30	0
1	B	1638	0	1622	18	0
1	C	1638	0	1622	13	0
1	D	1638	0	1622	16	0
2	A	20	0	15	2	0
2	B	20	0	15	2	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	32	0	15	5	0
4	D	32	0	15	3	0
5	D	6	0	8	1	0
6	A	116	0	0	2	0
6	B	112	0	0	1	0
6	C	239	0	0	0	0
6	D	232	0	0	2	0
All	All	7363	0	6556	83	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 6.

All (83) 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)
4:C:803:M4M:H11	4:C:803:M4M:C14	1.67	1.16
4:C:803:M4M:H11	4:C:803:M4M:H14	1.28	1.08
4:D:804:M4M:H11	4:D:804:M4M:H18	1.58	0.84
1:D:708:LYS:HB2	1:D:711:VAL:HG12	1.60	0.84
1:A:43:LYS:HA	1:A:46:LEU:HD12	1.63	0.80
1:C:443:LYS:HA	1:C:446:LEU:HD22	1.65	0.78
1:A:43:LYS:HA	1:A:46:LEU:CD1	2.15	0.76
4:C:803:M4M:C14	4:C:803:M4M:C11	2.46	0.75
1:D:732:ASP:OD1	1:D:771:HIS:HD2	1.68	0.75
1:D:708:LYS:HB2	1:D:711:VAL:CG1	2.16	0.75
1:B:364:LYS:HD3	1:B:366:ASP:OD2	1.87	0.75
1:C:539:GLU:HG2	1:C:580:LYS:HE2	1.69	0.74
4:C:803:M4M:H14	4:C:803:M4M:C11	2.10	0.73
1:C:402:PRO:HG2	1:C:404:TYR:CZ	2.26	0.71
1:A:10:ASN:HD22	1:A:33:ARG:HH11	1.39	0.67
1:D:771:HIS:HE1	6:D:245:HOH:O	1.80	0.64
1:D:767:LEU:HD23	1:D:768:LEU:CD1	2.29	0.62
1:A:189:ASN:HA	1:A:192:LYS:HE2	1.81	0.61
1:A:193:ARG:HH11	1:A:193:ARG:HG3	1.67	0.60
1:B:313:GLU:OE2	1:B:313:GLU:HA	2.02	0.60
1:B:246:LEU:HB3	1:B:247:PRO:HD2	1.85	0.58
1:A:55:GLU:HA	1:A:59:LEU:O	2.04	0.58
1:A:51:ILE:HB	1:A:52:PRO:HA	1.86	0.57
1:B:341:LEU:HG	1:B:377:LEU:HD11	1.86	0.57
1:C:575:VAL:HG12	1:C:579:LYS:HE2	1.86	0.56
1:A:10:ASN:HD22	1:A:33:ARG:HD3	1.73	0.55
1:D:720:LEU:HG	1:D:764:LYS:HB2	1.90	0.54
1:A:14:ARG:NH2	1:A:96:ASP:OD1	2.37	0.53
1:A:166:ASP:OD1	1:A:166:ASP:N	2.36	0.53
1:B:214:ARG:NH2	1:B:296:ASP:OD1	2.34	0.53
1:D:732:ASP:OD1	1:D:771:HIS:CD2	2.56	0.53
1:A:43:LYS:CA	1:A:46:LEU:HD12	2.36	0.53
1:B:324:ALA:HB3	1:B:325:PRO:HD3	1.92	0.52
1:D:739:GLU:HG2	1:D:780:LYS:NZ	2.25	0.51
1:A:180:LYS:HD2	6:A:517:HOH:O	2.11	0.51
1:B:255:GLU:HA	1:B:259:LEU:O	2.12	0.50
1:C:488:VAL:HA	1:C:542:ILE:HD13	1.94	0.49
1:C:480:ASN:HD21	1:C:544:MET:HE3	1.78	0.49
1:B:313:GLU:O	1:B:317:ASN:HB2	2.13	0.49
1:A:10:ASN:ND2	1:A:33:ARG:HH11	2.10	0.49
6:A:290:HOH:O	1:D:683:MET:CE	2.61	0.48
1:C:521:THR:OG1	1:C:564:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:OE1	1:A:180:LYS:NZ	2.46	0.48
1:A:140:TRP:CD1	1:A:145:SER:HA	2.47	0.48
1:A:39:TRP:HB3	1:A:40:PRO:CD	2.44	0.47
1:B:214:ARG:HD3	2:B:400:GSH:O11	2.14	0.47
1:A:39:TRP:O	1:A:40:PRO:C	2.52	0.47
1:A:73:LYS:O	1:A:74:ASN:HB2	2.15	0.47
1:B:332:ASP:OD2	1:B:373:ARG:NH2	2.46	0.47
1:D:708:LYS:HE2	1:D:711:VAL:HG11	1.96	0.47
1:A:35:GLU:HB2	1:A:38:ASP:OD1	2.15	0.47
1:D:719:LEU:HA	1:D:723:ASN:HD22	1.81	0.46
1:B:282:GLU:OE1	1:C:474:ASN:ND2	2.48	0.45
1:D:706:GLU:HB3	1:D:712:LYS:HG3	1.98	0.45
1:B:203:ASN:ND2	6:B:429:HOH:O	2.46	0.45
1:B:236:GLN:H	1:B:236:GLN:HG2	1.37	0.45
1:A:14:ARG:HD3	2:A:200:GSH:O11	2.16	0.45
1:A:124:ALA:HB3	1:A:125:PRO:HD3	1.99	0.44
1:A:193:ARG:HG3	1:A:193:ARG:NH1	2.31	0.44
1:B:209:PHE:CE1	1:B:251:ILE:HD11	2.53	0.44
4:D:804:M4M:H11	4:D:804:M4M:C18	2.35	0.44
1:C:539:GLU:HG2	1:C:580:LYS:CE	2.42	0.44
1:B:207:THR:O	1:B:252:PRO:HA	2.19	0.43
1:D:739:GLU:HG2	1:D:780:LYS:HE2	2.01	0.43
1:A:39:TRP:HB3	1:A:40:PRO:HD3	2.00	0.43
1:A:46:LEU:HB3	1:A:47:PRO:HD2	2.01	0.43
1:A:102:PHE:HA	1:A:103:PRO:HD3	1.86	0.42
1:D:603:ASN:ND2	6:D:806:HOH:O	2.52	0.42
1:C:519:LEU:HA	1:C:523:ASN:HD22	1.84	0.42
1:A:10:ASN:ND2	1:A:33:ARG:HD3	2.33	0.42
1:B:239:TRP:O	1:B:240:PRO:C	2.58	0.42
1:D:767:LEU:HD23	1:D:768:LEU:HD11	2.00	0.42
1:A:14:ARG:HG3	2:A:200:GSH:SG2	2.60	0.41
1:A:46:LEU:HD23	1:A:53:ILE:HG21	2.01	0.41
4:D:804:M4M:O1	4:D:804:M4M:N1	2.51	0.41
1:C:480:ASN:ND2	1:C:544:MET:HE3	2.34	0.41
1:C:480:ASN:ND2	1:C:544:MET:CE	2.84	0.41
1:C:413:GLY:HA2	4:C:803:M4M:O1	2.20	0.41
1:D:796:GLN:HB3	5:D:1001:GOL:H2	2.03	0.41
1:A:95:LEU:HD21	1:A:131:LEU:HD11	2.03	0.40
1:B:250:LYS:HD2	2:B:400:GSH:OE1	2.21	0.40
1:B:339:GLU:HG3	1:B:380:LYS:HE3	2.03	0.40
1:A:119:LEU:HA	1:A:123:ASN:OD1	2.22	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	196/198 (99%)	181 (92%)	13 (7%)	2 (1%)	15	9
1	B	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
1	C	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
1	D	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
All	All	784/792 (99%)	754 (96%)	28 (4%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	63	GLN

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	178/178 (100%)	171 (96%)	7 (4%)	32	30
1	B	178/178 (100%)	168 (94%)	10 (6%)	21	17
1	C	178/178 (100%)	173 (97%)	5 (3%)	43	44
1	D	178/178 (100%)	173 (97%)	5 (3%)	43	44
All	All	712/712 (100%)	685 (96%)	27 (4%)	33	31

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	14	ARG
1	A	114	GLN
1	A	118	GLU
1	A	144	MET
1	A	179	LYS
1	A	193	ARG
1	B	203	ASN
1	B	214	ARG
1	B	236	GLN
1	B	301	CYS
1	B	311	VAL
1	B	314	GLN
1	B	344	MET
1	B	364	LYS
1	B	377	LEU
1	B	379	LYS
1	C	441	GLU
1	C	446	LEU
1	C	450	LYS
1	C	483	MET
1	C	544	MET
1	D	603	ASN
1	D	683	MET
1	D	714	GLN
1	D	720	LEU
1	D	744	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	62	HIS
1	A	80	ASN
1	A	114	GLN
1	A	126	HIS
1	A	170	ASN
1	B	203	ASN
1	B	317	ASN
1	B	396	GLN
1	C	480	ASN

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Mol	Chain	Res	Type
1	C	523	ASN
1	D	603	ASN
1	D	662	HIS
1	D	714	GLN
1	D	723	ASN
1	D	770	ASN
1	D	771	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	M4M	D	804	-	34,35,35	2.66	10 (29%)	52,55,55	2.48	19 (36%)
5	GOL	D	1001	-	5,5,5	0.73	0	5,5,5	0.48	0
2	GSH	A	200	-	18,19,19	3.06	3 (16%)	23,24,24	1.75	8 (34%)
4	M4M	C	803	-	34,35,35	2.73	10 (29%)	52,55,55	2.12	12 (23%)
2	GSH	B	400	-	18,19,19	3.03	2 (11%)	23,24,24	1.40	5 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	M4M	D	804	-	-	0/16/32/32	0/4/4/4
5	GOL	D	1001	-	-	2/4/4/4	-
2	GSH	A	200	-	-	3/24/24/24	-
4	M4M	C	803	-	-	5/16/32/32	0/4/4/4
2	GSH	B	400	-	-	0/24/24/24	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	804	M4M	C16-S2	-9.36	1.62	1.77
4	C	803	M4M	C16-S2	-9.23	1.62	1.77
2	A	200	GSH	OE1-CD1	9.04	1.41	1.23
2	B	400	GSH	O2-C2	8.83	1.40	1.23
2	B	400	GSH	OE1-CD1	8.70	1.40	1.23
2	A	200	GSH	O2-C2	8.30	1.39	1.23
4	C	803	M4M	C8-C9	6.01	1.50	1.42
4	D	804	M4M	C8-C9	5.80	1.50	1.42
4	C	803	M4M	S2-N3	-5.53	1.49	1.60
4	D	804	M4M	S2-N3	-5.17	1.50	1.60
4	C	803	M4M	C19-C12	3.90	1.49	1.41
4	D	804	M4M	C19-C12	3.87	1.49	1.41
4	C	803	M4M	O6-S2	3.61	1.50	1.43
4	D	804	M4M	O6-S2	3.51	1.50	1.43
4	C	803	M4M	O8-S2	3.41	1.50	1.43
4	C	803	M4M	C9-C10	-3.39	1.38	1.42
4	D	804	M4M	O8-S2	3.23	1.49	1.43
4	C	803	M4M	C19-C8	3.12	1.48	1.41
4	D	804	M4M	C13-N2	-2.60	1.35	1.40
4	D	804	M4M	C19-C8	2.58	1.47	1.41
4	D	804	M4M	O7-C20	2.51	1.27	1.22
4	C	803	M4M	C13-N2	-2.50	1.35	1.40
4	D	804	M4M	C17-C16	2.49	1.42	1.38
2	A	200	GSH	CB2-CA2	2.43	1.55	1.53
4	C	803	M4M	C6-C7	2.07	1.52	1.48

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	804	M4M	C8-C19-C12	-7.51	114.74	119.74
4	D	804	M4M	O8-S2-O6	-6.64	107.84	118.76
4	C	803	M4M	O8-S2-O6	-5.83	109.18	118.76
4	C	803	M4M	C8-C19-C12	-5.49	116.08	119.74
4	C	803	M4M	C13-N2-C12	-5.32	112.76	126.66
4	D	804	M4M	C19-C12-N2	-5.19	114.86	120.52
4	C	803	M4M	O3-S1-C10	5.02	114.99	106.51
4	D	804	M4M	O3-S1-C10	4.98	114.94	106.51
4	D	804	M4M	C11-C10-C9	-4.40	116.46	121.78
4	C	803	M4M	C12-C11-C10	4.39	126.41	119.47
4	D	804	M4M	C8-C9-N1	-3.92	117.11	122.65
4	D	804	M4M	O2-S1-C10	3.92	113.14	106.51
4	C	803	M4M	C11-C10-C9	-3.60	117.42	121.78
4	C	803	M4M	C10-C9-N1	-3.59	119.01	122.64
4	D	804	M4M	C12-C11-C10	3.39	124.82	119.47
4	D	804	M4M	C12-C19-C20	3.21	125.54	121.08
2	A	200	GSH	OE1-CD1-CG1	-3.20	116.16	122.02
2	A	200	GSH	CB1-CG1-CD1	-3.12	106.08	113.04
4	D	804	M4M	O1-C7-C8	-3.10	116.40	121.43
2	A	200	GSH	CA2-CB2-SG2	2.97	117.54	114.19
4	D	804	M4M	O7-C20-C1	-2.89	116.67	120.91
2	B	400	GSH	CB1-CG1-CD1	-2.60	107.22	113.04
4	D	804	M4M	C6-C7-C8	2.58	122.07	118.00
4	D	804	M4M	C17-C18-C13	-2.43	117.49	120.30
2	B	400	GSH	CG1-CD1-N2	2.38	119.95	115.83
2	A	200	GSH	O32-C3-CA3	2.35	120.92	112.74
4	D	804	M4M	C10-C9-N1	-2.33	120.28	122.64
2	A	200	GSH	O12-C1-CA1	2.33	121.31	113.38
4	C	803	M4M	C12-C19-C20	2.32	124.30	121.08
4	C	803	M4M	O1-C7-C8	-2.31	117.68	121.43
4	C	803	M4M	C8-C9-N1	-2.31	119.38	122.65
2	B	400	GSH	O12-C1-CA1	2.29	121.20	113.38
2	A	200	GSH	O32-C3-O31	-2.19	117.83	123.30
2	B	400	GSH	O12-C1-O11	-2.19	119.12	124.09
4	D	804	M4M	O3-S1-O2	-2.19	101.50	112.86
2	B	400	GSH	C3-CA3-N3	-2.18	106.33	113.06
4	D	804	M4M	C14-C13-N2	-2.14	113.47	120.64
2	A	200	GSH	CG1-CB1-CA1	-2.13	108.86	113.84
4	D	804	M4M	O8-S2-C16	2.13	109.73	107.35
4	C	803	M4M	O6-S2-N3	2.10	110.48	107.36
4	C	803	M4M	C19-C12-N2	2.03	122.73	120.52
4	D	804	M4M	O6-S2-C16	2.03	109.61	107.35
2	A	200	GSH	CB2-CA2-C2	2.01	113.91	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	804	M4M	C18-C13-C14	2.01	121.78	119.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	GSH	CA2-C2-N3-CA3
5	D	1001	GOL	C1-C2-C3-O3
2	A	200	GSH	O2-C2-N3-CA3
4	C	803	M4M	C17-C16-S2-N3
5	D	1001	GOL	O2-C2-C3-O3
4	C	803	M4M	C15-C16-S2-N3
4	C	803	M4M	C15-C16-S2-O6
4	C	803	M4M	C17-C16-S2-O6
4	C	803	M4M	C18-C13-N2-C12
2	A	200	GSH	C3-CA3-N3-C2

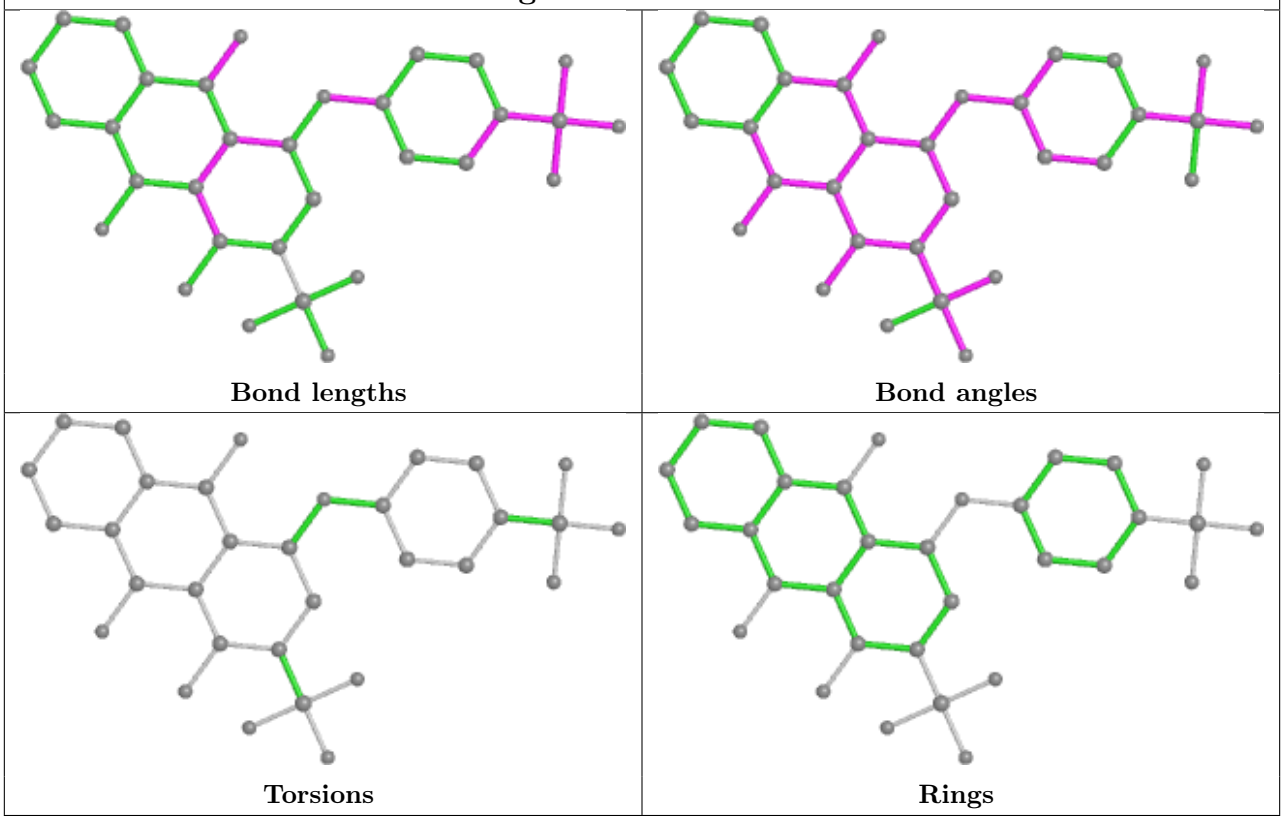
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	804	M4M	3	0
5	D	1001	GOL	1	0
2	A	200	GSH	2	0
4	C	803	M4M	5	0
2	B	400	GSH	2	0

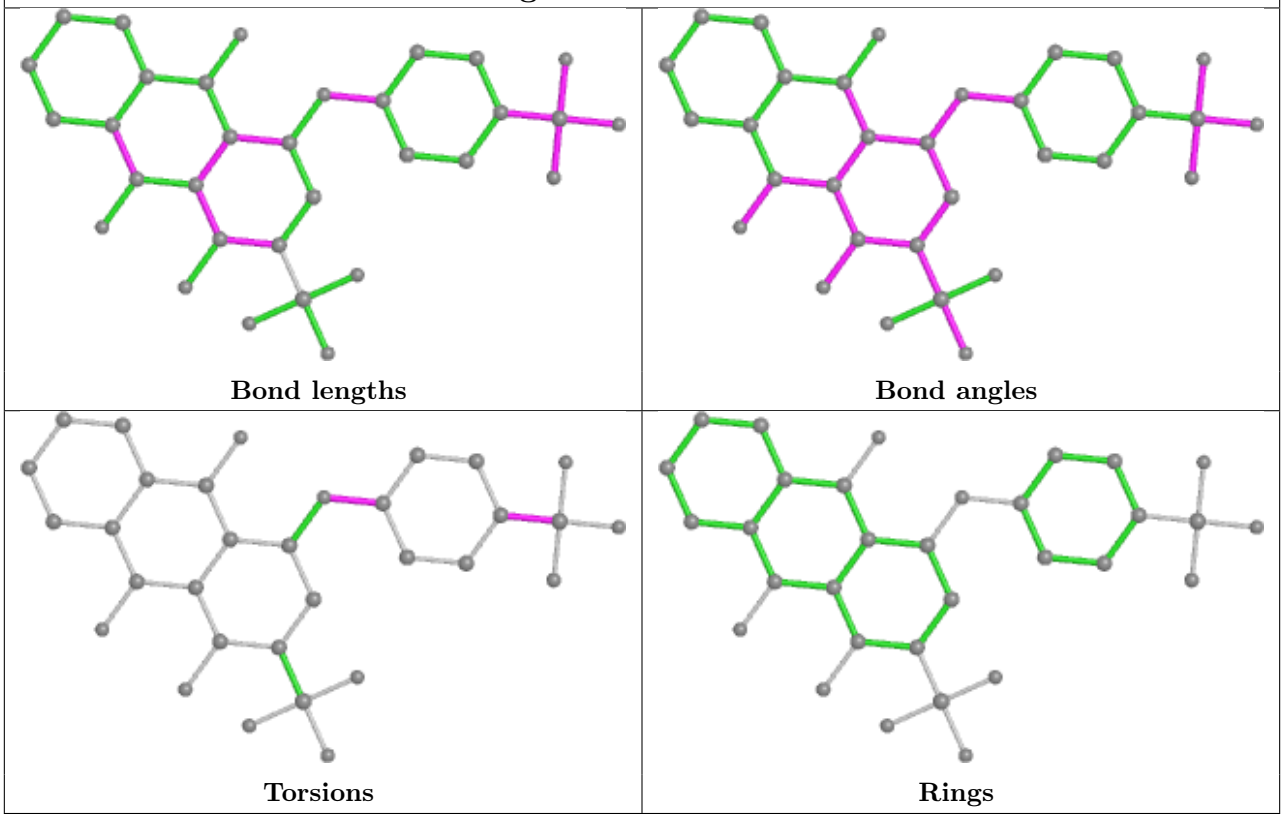
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 M4M D 804



Ligand GSH A 200

Ligand M4M C 803



Ligand GSH B 400

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%)	-0.50	2 (1%)	82	81	14, 31, 66, 81	0
1	B	198/198 (100%)	-0.44	6 (3%)	50	49	13, 30, 78, 87	0
1	C	198/198 (100%)	-0.98	0	100	100	9, 17, 36, 46	0
1	D	198/198 (100%)	-0.94	0	100	100	7, 18, 36, 50	0
All	All	792/792 (100%)	-0.71	8 (1%)	82	81	7, 24, 58, 87	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	TRP	3.4
1	B	303	PRO	3.3
1	B	301	CYS	3.2
1	B	302	PHE	3.1
1	A	104	TRP	2.7
1	B	305	ALA	2.5
1	A	41	GLU	2.3
1	B	314	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

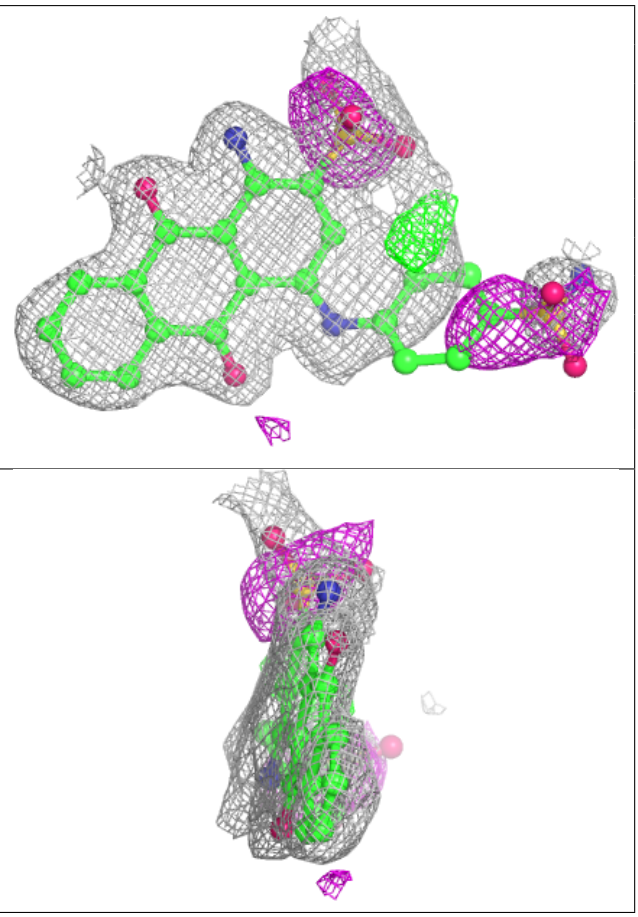
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	M4M	C	803	32/32	0.71	0.22	25,46,82,82	0
4	M4M	D	804	32/32	0.74	0.21	23,44,86,87	0
2	GSH	A	200	20/20	0.89	0.16	29,44,58,60	0
2	GSH	B	400	20/20	0.92	0.12	25,36,54,56	0
5	GOL	D	1001	6/6	0.98	0.08	26,27,29,31	0
3	CA	D	900	1/1	0.99	0.03	57,57,57,57	0
3	CA	C	901	1/1	0.99	0.04	56,56,56,56	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.

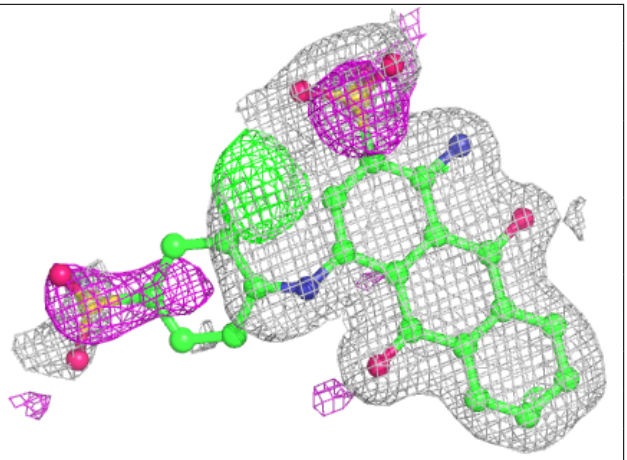
Electron density around M4M C 803:

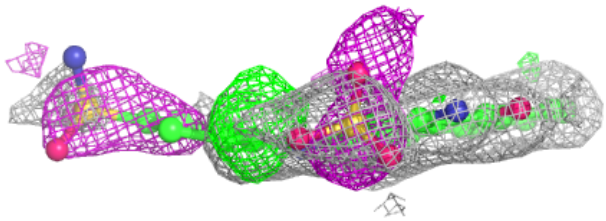
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

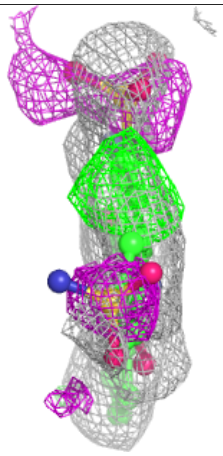


Electron density around M4M D 804:

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

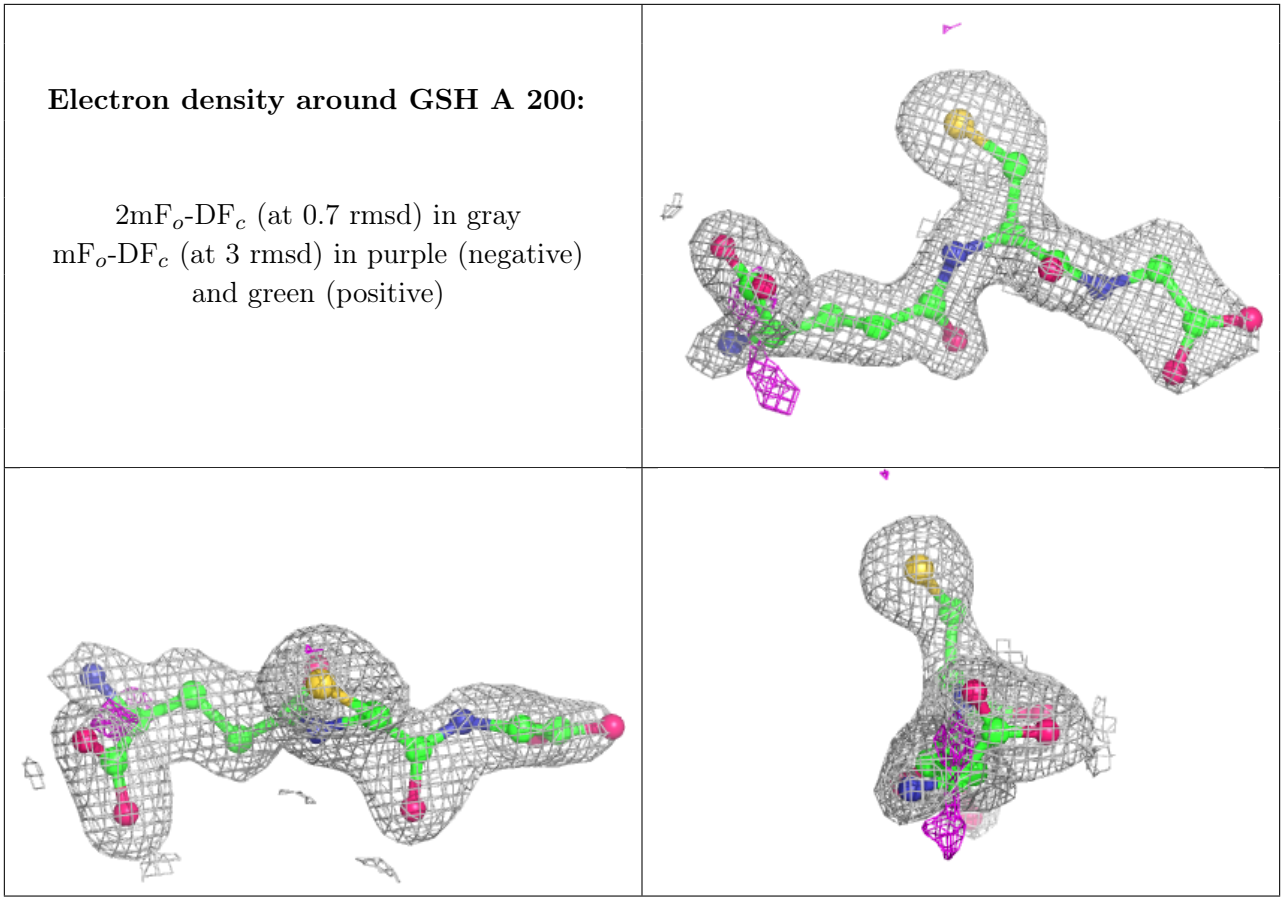






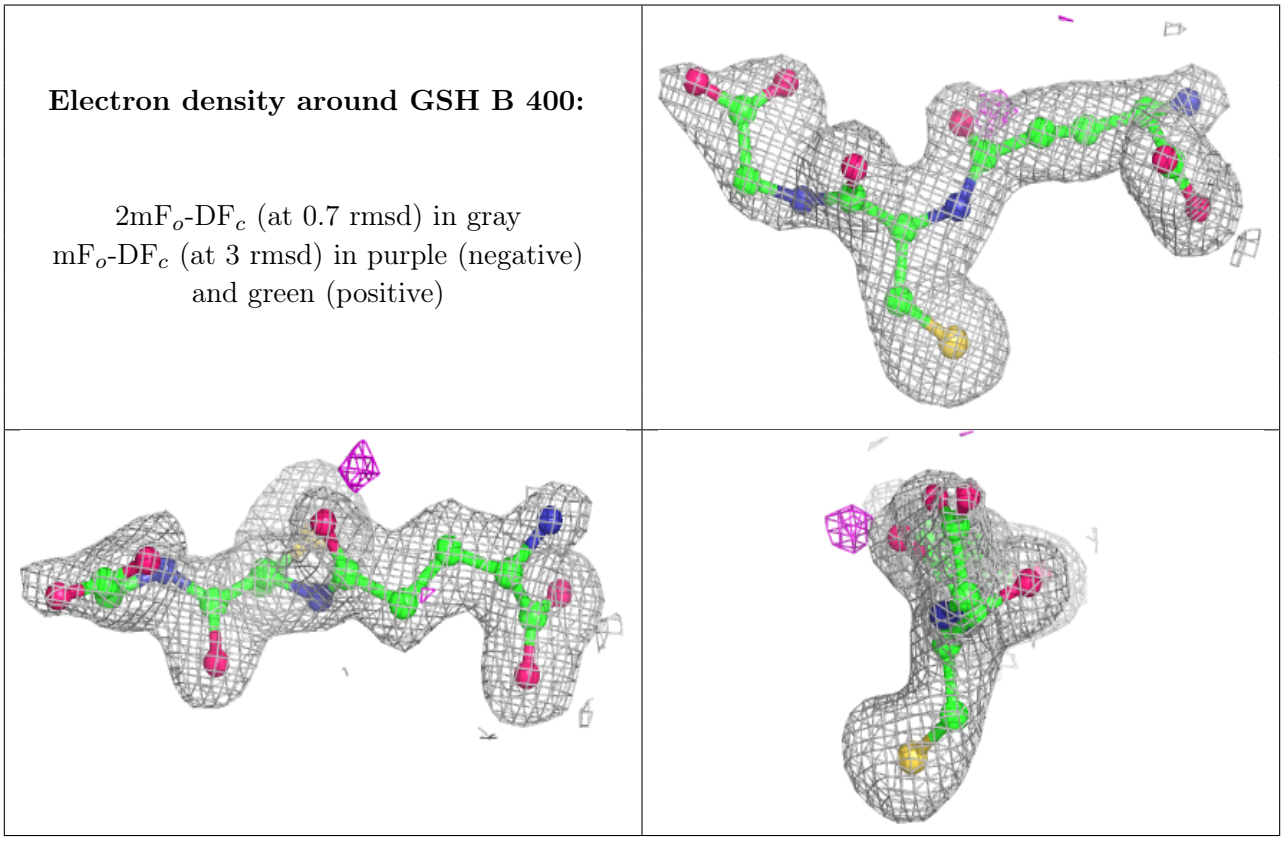
Electron density around GSH A 200:

$2mF_o$-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 B 400:

$2mF_o$-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.