



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:53 pm BST

PDB ID : 1V40
Title : First Inhibitor Complex Structure of Human Hematopoietic Prostaglandin D Synthase
Authors : Inoue, T.; Okano, Y.; Kado, Y.; Aritake, K.; Irikura, D.; Uodome, N.; Kinugasa, S.; Okazaki, N.; Matsumura, H.; Kai, Y.; Urade, Y.
Deposited on : 2003-11-07
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

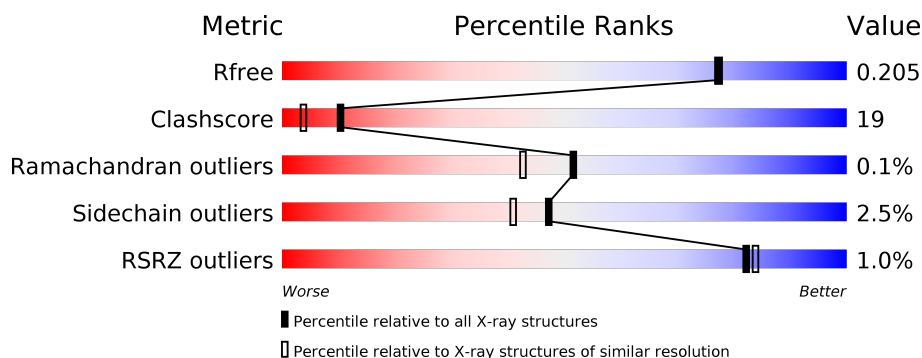
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>26%</div> </div> <div></div> </div>
1	B	198	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>23%</div> </div> <div></div> </div>
1	C	198	<div> <div></div> <div> <div></div> <div>80%</div> <div>20%</div> </div> <div></div> </div>
1	D	198	<div> <div></div> <div> <div></div> <div>82%</div> <div>16%</div> </div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	O16	A	3201	-	-	X	X
4	O16	B	3401	-	-	X	X
4	O16	C	3601	-	-	X	-
4	O16	D	3801	-	-	X	-
5	GOL	A	3002	-	-	X	-
5	GOL	C	3003	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8268 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-requiring 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			

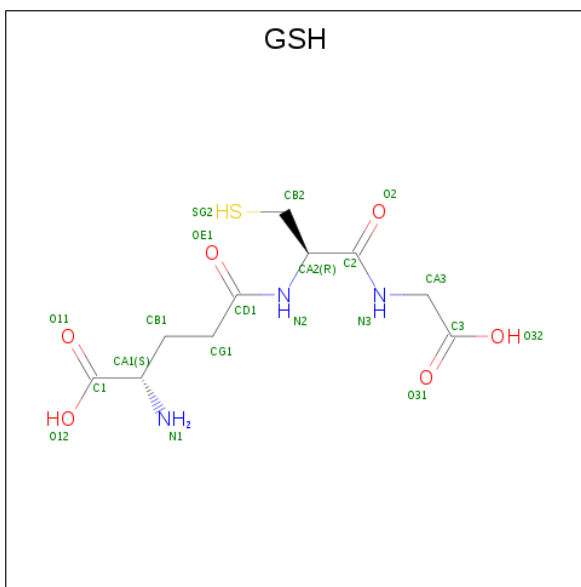
There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

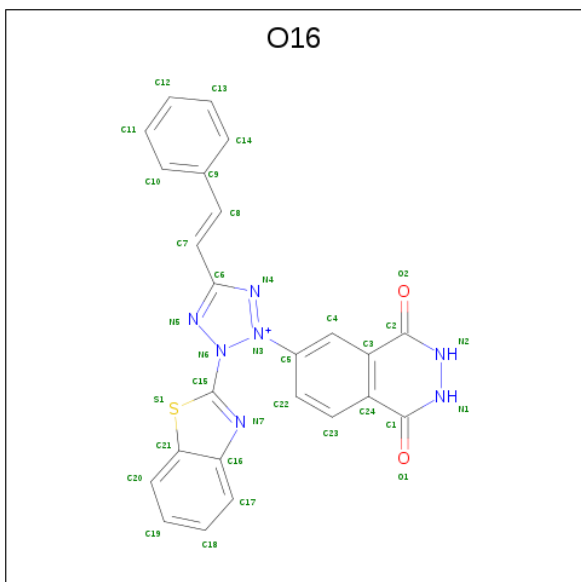
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



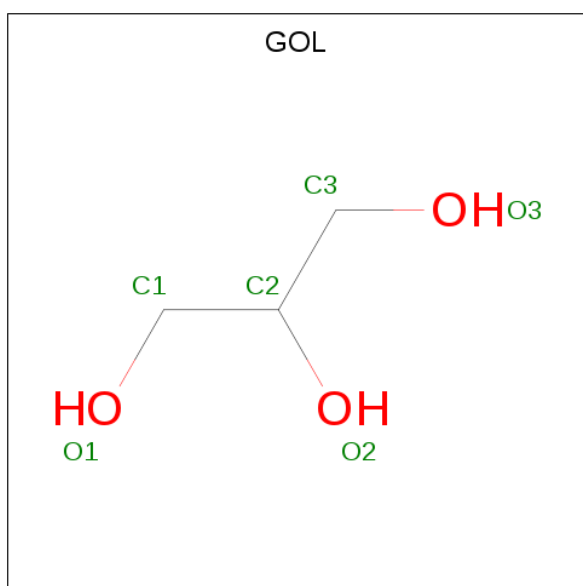
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
3	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
3	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
3	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 4 is 3-(1,3-BENZOTHAZOL-2-YL)-2-(1,4-DIOXO-1,2,3,4-TETRAHYDROPHTHALAZIN-6-YL)-5-[(E)-2-PHENYLVINYL]-3H-TETRAAZOL-2-IUM (three-letter code: O16) (formula: C₂₄H₁₆N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	24	7	2	1		
4	B	1	Total	C	N	O	S	0	0
			34	24	7	2	1		
4	C	1	Total	C	N	O	S	0	0
			34	24	7	2	1		
4	D	1	Total	C	N	O	S	0	0
			34	24	7	2	1		

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



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	D	1	Total	C	O	0	0
			6	3	3		

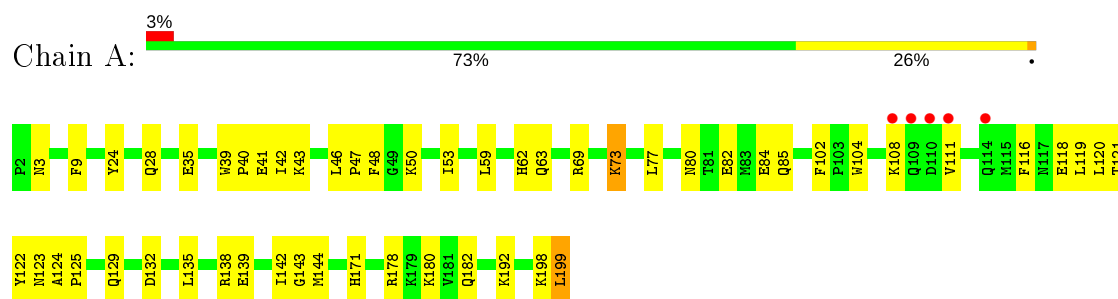
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	459	Total 459	O 459	0	0
6	B	310	Total 310	O 310	0	0
6	C	319	Total 319	O 319	0	0
6	D	374	Total 374	O 374	0	0

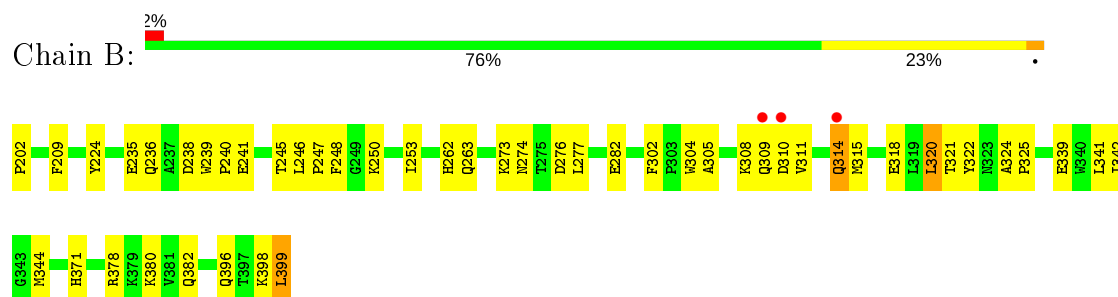
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

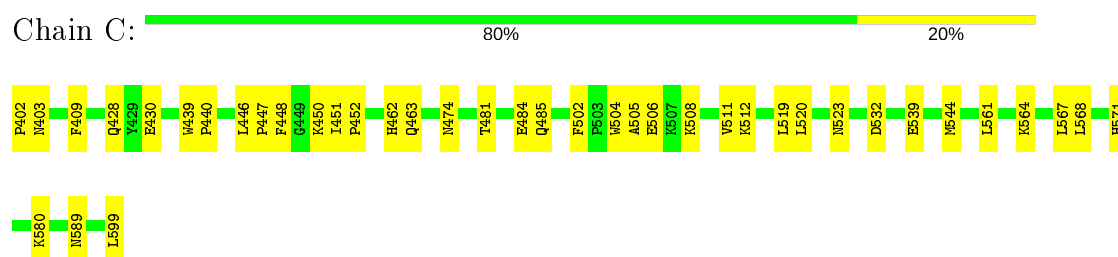
- Molecule 1: Glutathione-requiring prostaglandin D synthase



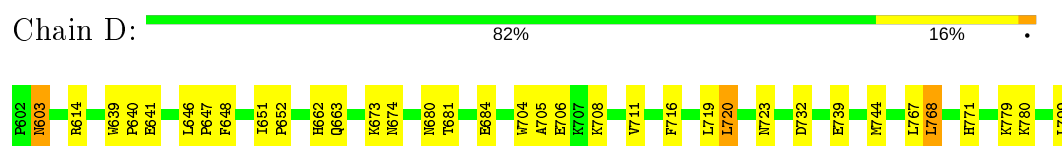
- Molecule 1: Glutathione-requiring prostaglandin D synthase



- Molecule 1: Glutathione-requiring prostaglandin D synthase



- Molecule 1: Glutathione-requiring prostaglandin D synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.29 Å 49.24 Å 94.53 Å 93.25° 89.98° 90.01°	Depositor
Resolution (Å)	35.05 – 1.90 35.05 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.2 (35.05-1.90) 93.9 (35.05-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 1.89 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.215 0.187 , 0.205	Depositor DCC
R_{free} test set	2420 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.480 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8268	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, GSH, O16

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	0.31	0/1681	0.56	0/2283
1	B	0.36	0/1681	0.56	0/2283
1	C	0.34	0/1681	0.55	0/2283
1	D	0.34	0/1681	0.56	0/2283
All	All	0.34	0/6724	0.56	0/9132

There are no bond length outliers.

There are no bond angle outliers.

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	71	0
1	B	1638	0	1622	63	0
1	C	1638	0	1622	61	0
1	D	1638	0	1622	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	15	0	0
3	B	20	0	15	1	0
3	C	20	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	20	0	15	0	0
4	A	34	0	16	9	0
4	B	34	0	16	13	0
4	C	34	0	16	26	0
4	D	34	0	16	23	0
5	A	12	0	15	6	0
5	B	6	0	8	0	0
5	C	12	0	15	3	1
5	D	6	0	8	0	0
6	A	459	0	0	17	0
6	B	310	0	0	13	0
6	C	319	0	0	6	1
6	D	374	0	0	11	2
All	All	8268	0	6658	249	2

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 19.

All (249) 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:C:504:TRP:CB	4:C:3601:O16:H22	0.99	1.45
1:C:504:TRP:HB3	4:C:3601:O16:C22	1.43	1.41
1:C:599:LEU:HD12	4:C:3601:O16:C17	1.53	1.39
1:B:304:TRP:HB2	4:B:3401:O16:C22	1.64	1.28
1:D:799:LEU:HD12	4:D:3801:O16:C17	1.62	1.27
1:C:599:LEU:HD12	4:C:3601:O16:C16	1.67	1.23
1:A:9:PHE:HE1	4:A:3201:O16:O2	0.89	1.21
1:D:799:LEU:HD12	4:D:3801:O16:C16	1.69	1.21
1:C:504:TRP:HB2	4:C:3601:O16:C22	1.62	1.20
5:C:3003:GOL:C3	5:C:3003:GOL:O3	1.90	1.20
1:D:705:ALA:HB2	4:D:3801:O16:O1	1.41	1.16
1:B:304:TRP:HB2	4:B:3401:O16:H22	1.24	1.16
1:C:505:ALA:HB2	4:C:3601:O16:O1	1.01	1.15
1:A:104:TRP:HB2	4:A:3201:O16:H22	1.27	1.14
1:C:599:LEU:HD12	4:C:3601:O16:H17	1.20	1.13
1:D:799:LEU:HD12	4:D:3801:O16:H17	1.32	1.10
1:B:304:TRP:CB	4:B:3401:O16:H22	1.86	1.04
1:C:599:LEU:CD1	4:C:3601:O16:H17	1.86	1.04
1:C:599:LEU:CD1	4:C:3601:O16:C17	2.38	1.02
1:C:599:LEU:CD1	4:C:3601:O16:N7	2.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:LEU:HD12	4:D:3801:O16:N7	1.73	1.01
1:D:705:ALA:HB2	4:D:3801:O16:C1	1.91	1.00
1:C:599:LEU:HD12	4:C:3601:O16:N7	1.76	1.00
4:D:3801:O16:S1	4:D:3801:O16:C4	2.49	1.00
1:B:304:TRP:CB	4:B:3401:O16:C22	2.39	0.99
1:A:104:TRP:CB	4:A:3201:O16:H22	1.93	0.98
1:A:108:LYS:HE2	1:A:111:VAL:HG11	1.42	0.98
1:A:108:LYS:HB2	1:A:111:VAL:HG12	1.44	0.97
1:D:704:TRP:HB2	4:D:3801:O16:C22	1.94	0.97
1:B:308:LYS:HE2	1:B:311:VAL:HG11	1.47	0.97
1:D:799:LEU:CD1	4:D:3801:O16:N7	2.29	0.96
1:C:504:TRP:CG	4:C:3601:O16:H22	2.02	0.95
4:D:3801:O16:S1	4:D:3801:O16:H4	2.07	0.95
1:C:504:TRP:HB2	4:C:3601:O16:H22	1.13	0.94
1:C:504:TRP:HB2	4:C:3601:O16:C23	1.98	0.94
1:D:799:LEU:CD1	4:D:3801:O16:H17	1.99	0.93
1:D:705:ALA:CB	4:D:3801:O16:O1	2.18	0.92
1:D:799:LEU:CD1	4:D:3801:O16:C17	2.47	0.92
1:C:599:LEU:CD1	4:C:3601:O16:C16	2.49	0.90
1:A:119:LEU:HA	1:A:123:ASN:HD22	1.37	0.90
1:B:305:ALA:HB2	4:B:3401:O16:O1	1.72	0.89
1:A:129:GLN:HB2	6:A:4350:HOH:O	1.73	0.87
1:A:9:PHE:HE1	4:A:3201:O16:C2	1.87	0.87
1:B:308:LYS:HB2	1:B:311:VAL:HG12	1.57	0.87
1:C:505:ALA:N	4:C:3601:O16:H23	1.90	0.86
1:B:247:PRO:HG3	6:B:4008:HOH:O	1.75	0.85
1:B:304:TRP:CG	4:B:3401:O16:H22	2.11	0.85
1:C:589:ASN:HB2	6:C:3898:HOH:O	1.77	0.83
1:D:704:TRP:HB2	4:D:3801:O16:H22	1.61	0.82
1:D:799:LEU:CD1	4:D:3801:O16:C16	2.55	0.80
1:C:599:LEU:HD13	4:C:3601:O16:N7	1.95	0.79
1:D:704:TRP:CB	4:D:3801:O16:C22	2.61	0.79
1:B:305:ALA:HB2	4:B:3401:O16:C1	2.14	0.78
1:A:108:LYS:HE2	1:A:111:VAL:CG1	2.14	0.78
1:D:647:PRO:HG3	6:D:4053:HOH:O	1.82	0.77
1:C:447:PRO:HG3	6:C:3659:HOH:O	1.84	0.75
1:A:108:LYS:HB2	1:A:111:VAL:CG1	2.16	0.75
1:C:504:TRP:CB	4:C:3601:O16:C23	2.59	0.74
3:B:3400:GSH:O32	4:B:3401:O16:N2	2.20	0.74
1:B:396:GLN:HG2	6:B:4147:HOH:O	1.87	0.74
1:A:102:PHE:HE2	1:A:120:LEU:HD11	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:739:GLU:HG2	1:D:780:LYS:HE2	1.69	0.73
1:B:304:TRP:CD1	4:B:3401:O16:H22	2.23	0.72
1:B:273:LYS:NZ	1:C:485:GLN:OE1	2.19	0.71
1:A:119:LEU:HD23	1:A:123:ASN:ND2	2.05	0.71
1:B:304:TRP:HB2	4:B:3401:O16:C23	2.20	0.71
1:D:646:LEU:HB3	1:D:647:PRO:HD2	1.72	0.71
1:D:779:LYS:HE2	6:D:3914:HOH:O	1.89	0.70
1:D:647:PRO:HG2	1:D:648:PHE:H	1.56	0.70
1:A:119:LEU:HD23	1:A:123:ASN:HD22	1.57	0.69
1:D:767:LEU:HG	1:D:768:LEU:HD13	1.74	0.69
1:A:138:ARG:NH1	6:A:4040:HOH:O	2.24	0.69
1:A:116:PHE:O	1:A:120:LEU:HD13	1.92	0.68
1:A:104:TRP:HB2	4:A:3201:O16:C22	2.14	0.68
1:B:247:PRO:HG2	1:B:248:PHE:H	1.57	0.68
1:B:398:LYS:HB3	1:B:399:LEU:HD12	1.76	0.68
1:C:539:GLU:HG2	1:C:580:LYS:HE2	1.75	0.68
1:B:305:ALA:CB	4:B:3401:O16:O1	2.42	0.68
1:A:180:LYS:HD2	6:A:4080:HOH:O	1.94	0.67
1:D:799:LEU:HD13	4:D:3801:O16:N7	2.08	0.67
1:A:39:TRP:HB3	1:A:40:PRO:HD3	1.77	0.66
1:C:446:LEU:HB3	1:C:447:PRO:HD2	1.76	0.66
1:B:276:ASP:HB3	6:B:4152:HOH:O	1.95	0.66
1:C:561:LEU:HD21	1:C:568:LEU:HD13	1.77	0.66
1:A:43:LYS:HE2	5:A:3001:GOL:O1	1.94	0.66
1:B:311:VAL:HB	6:B:4045:HOH:O	1.95	0.66
1:C:504:TRP:HB3	4:C:3601:O16:H22	0.66	0.66
1:A:102:PHE:HE2	1:A:120:LEU:CD1	2.10	0.65
1:A:73:LYS:HG2	6:D:3815:HOH:O	1.95	0.65
1:A:124:ALA:HB3	1:A:125:PRO:HD3	1.79	0.65
1:A:47:PRO:HG2	1:A:48:PHE:H	1.61	0.64
1:A:35:GLU:OE2	6:A:3908:HOH:O	2.14	0.64
1:A:198:LYS:HB3	1:A:199:LEU:HD12	1.78	0.64
1:A:85:GLN:OE1	1:D:673:LYS:HE2	1.98	0.64
1:A:9:PHE:CD1	4:A:3201:O16:O2	2.44	0.64
1:B:308:LYS:HB2	1:B:311:VAL:CG1	2.28	0.64
1:C:568:LEU:N	1:C:568:LEU:HD12	2.13	0.63
1:C:402:PRO:N	6:C:3652:HOH:O	2.32	0.63
1:C:519:LEU:HA	1:C:523:ASN:HD22	1.65	0.62
1:B:324:ALA:HB3	1:B:325:PRO:HD3	1.81	0.62
1:A:178:ARG:O	1:A:182:GLN:HG3	1.99	0.61
1:D:704:TRP:CB	4:D:3801:O16:H22	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:708:LYS:HB2	1:D:711:VAL:HG12	1.82	0.61
1:D:708:LYS:HB2	1:D:711:VAL:CG1	2.31	0.60
1:B:339:GLU:HG2	1:B:380:LYS:HE2	1.82	0.60
1:B:202:PRO:N	6:B:3903:HOH:O	2.34	0.60
1:D:705:ALA:CB	4:D:3801:O16:C1	2.75	0.60
1:B:378:ARG:O	1:B:382:GLN:HG3	2.02	0.59
1:C:430:GLU:HG3	6:C:3716:HOH:O	2.01	0.59
1:C:504:TRP:C	4:C:3601:O16:H23	2.22	0.59
1:A:199:LEU:HD12	1:A:199:LEU:N	2.16	0.59
1:C:447:PRO:HG2	1:C:448:PHE:H	1.67	0.59
1:D:719:LEU:HA	1:D:723:ASN:HD22	1.68	0.59
1:A:47:PRO:HG3	6:A:4024:HOH:O	2.02	0.58
1:C:508:LYS:HB2	1:C:511:VAL:HG12	1.84	0.58
1:A:119:LEU:HA	1:A:123:ASN:ND2	2.14	0.58
1:D:780:LYS:HD2	6:D:3919:HOH:O	2.03	0.58
1:B:209:PHE:HE1	4:B:3401:O16:O2	1.87	0.58
1:B:399:LEU:HD12	1:B:399:LEU:N	2.17	0.57
1:A:46:LEU:HD21	1:A:53:ILE:HD13	1.86	0.57
1:D:681:THR:OG1	1:D:684:GLU:HG3	2.05	0.57
1:C:502:PHE:HE2	1:C:520:LEU:CD2	2.18	0.56
1:B:262:HIS:HE1	6:C:3602:HOH:O	1.88	0.56
1:B:238:ASP:CG	6:B:3933:HOH:O	2.43	0.56
1:B:302:PHE:HE2	1:B:320:LEU:HD22	1.70	0.56
1:A:108:LYS:CE	1:A:111:VAL:HG11	2.27	0.56
1:B:246:LEU:HD21	1:B:253:ILE:HD13	1.86	0.56
1:C:532:ASP:OD1	1:C:571:HIS:HD2	1.90	0.55
1:B:398:LYS:HD3	1:B:399:LEU:HD11	1.89	0.55
1:A:171:HIS:HE1	6:A:4001:HOH:O	1.91	0.54
1:C:508:LYS:HB2	1:C:511:VAL:CG1	2.38	0.54
1:A:50:LYS:HE2	6:A:4117:HOH:O	2.07	0.54
1:C:539:GLU:HG2	1:C:580:LYS:CE	2.37	0.53
1:A:69:ARG:O	1:A:73:LYS:HD2	2.09	0.53
1:A:138:ARG:HH11	1:A:138:ARG:HG3	1.73	0.53
1:A:139:GLU:HG2	1:A:180:LYS:HE2	1.90	0.53
1:C:481:THR:OG1	1:C:484:GLU:HG3	2.09	0.53
1:C:439:TRP:HB3	1:C:440:PRO:HD3	1.91	0.52
1:D:732:ASP:OD1	1:D:771:HIS:HD2	1.92	0.52
1:B:246:LEU:CD2	1:B:253:ILE:HD13	2.39	0.52
1:A:3:ASN:N	1:A:3:ASN:HD22	2.08	0.52
1:B:245:THR:HG21	6:B:4139:HOH:O	2.08	0.52
1:B:282:GLU:OE1	1:C:474:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:CD2	1:A:53:ILE:HD13	2.40	0.52
1:C:505:ALA:CA	4:C:3601:O16:O1	2.54	0.52
1:C:502:PHE:HE2	1:C:520:LEU:HD22	1.75	0.52
1:B:308:LYS:HE2	1:B:311:VAL:CG1	2.31	0.51
1:B:246:LEU:HB3	1:B:247:PRO:HD2	1.92	0.51
1:A:143:GLY:H	5:A:3002:GOL:H12	1.74	0.51
1:B:247:PRO:HG2	1:B:248:PHE:N	2.26	0.51
1:D:780:LYS:HG3	6:D:3918:HOH:O	2.09	0.50
1:B:314:GLN:HA	1:B:314:GLN:NE2	2.26	0.50
1:D:708:LYS:HE2	1:D:711:VAL:HG11	1.92	0.50
1:B:262:HIS:HD2	6:B:3940:HOH:O	1.94	0.50
1:D:647:PRO:HG2	1:D:648:PHE:N	2.27	0.49
1:C:504:TRP:HB2	4:C:3601:O16:H23	1.87	0.49
1:A:104:TRP:CB	4:A:3201:O16:C22	2.78	0.49
1:A:135:LEU:O	1:A:138:ARG:NH1	2.46	0.49
1:B:236:GLN:O	1:B:240:PRO:HD3	2.12	0.49
1:B:322:TYR:O	1:B:325:PRO:HD2	2.13	0.49
1:C:448:PHE:O	1:C:450:LYS:HG2	2.13	0.49
1:D:662:HIS:O	1:D:663:GLN:HB2	2.12	0.49
1:A:139:GLU:CG	1:A:180:LYS:HE2	2.43	0.49
1:B:380:LYS:HD3	6:B:4063:HOH:O	2.11	0.49
1:A:199:LEU:HD13	4:A:3201:O16:H17	1.94	0.49
1:B:310:ASP:OD2	1:B:311:VAL:N	2.41	0.49
1:C:567:LEU:HB3	1:C:568:LEU:HD12	1.93	0.48
1:C:462:HIS:O	1:C:463:GLN:HB2	2.13	0.48
1:A:102:PHE:CE2	1:A:120:LEU:HD11	2.42	0.48
1:C:567:LEU:HD23	1:C:568:LEU:HD11	1.94	0.48
1:D:716:PHE:O	1:D:720:LEU:HD22	2.13	0.48
1:B:273:LYS:NZ	6:B:4203:HOH:O	2.45	0.48
1:D:767:LEU:HG	1:D:768:LEU:CD1	2.44	0.48
1:D:680:ASN:ND2	6:D:4110:HOH:O	2.45	0.48
1:A:143:GLY:N	5:A:3002:GOL:H12	2.30	0.47
1:D:639:TRP:HB3	1:D:640:PRO:HD3	1.95	0.47
1:C:504:TRP:C	4:C:3601:O16:C23	2.83	0.47
1:A:80:ASN:ND2	6:A:3973:HOH:O	2.47	0.47
1:B:371:HIS:HE1	6:B:4051:HOH:O	1.97	0.47
1:B:302:PHE:HE2	1:B:320:LEU:CD2	2.27	0.47
1:A:24:TYR:CD2	1:A:77:LEU:HD11	2.50	0.47
1:A:82:GLU:OE1	1:D:674:ASN:ND2	2.46	0.46
1:B:262:HIS:O	1:B:263:GLN:HB2	2.15	0.46
1:D:651:ILE:HB	1:D:652:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:HIS:HE1	6:D:3814:HOH:O	1.97	0.46
1:A:46:LEU:HD22	1:A:53:ILE:HG21	1.97	0.46
1:B:396:GLN:NE2	6:B:4195:HOH:O	2.49	0.46
1:D:704:TRP:HB2	4:D:3801:O16:C23	2.44	0.46
1:A:192:LYS:NZ	6:A:4250:HOH:O	2.49	0.45
1:C:508:LYS:HE2	1:C:511:VAL:HG11	1.96	0.45
1:A:142:ILE:HA	5:A:3002:GOL:H32	1.98	0.45
1:B:314:GLN:HE21	1:B:314:GLN:CA	2.28	0.45
1:C:403:ASN:HB3	6:C:3916:HOH:O	2.16	0.45
1:B:341:LEU:C	1:B:342:ILE:HD12	2.37	0.45
1:D:799:LEU:CG	4:D:3801:O16:H17	2.45	0.45
1:D:739:GLU:HG2	1:D:780:LYS:CE	2.41	0.45
1:B:339:GLU:CG	1:B:380:LYS:HE2	2.47	0.44
1:C:409:PHE:CE1	1:C:451:ILE:HD11	2.53	0.44
1:A:62:HIS:O	1:A:63:GLN:HB2	2.17	0.44
1:C:451:ILE:HB	1:C:452:PRO:HA	1.98	0.44
1:A:102:PHE:CE2	1:A:120:LEU:CD1	2.97	0.44
1:A:47:PRO:HA	6:A:4114:HOH:O	2.17	0.44
1:B:342:ILE:HD12	1:B:342:ILE:N	2.33	0.44
1:A:47:PRO:CG	6:A:4024:HOH:O	2.64	0.44
1:A:62:HIS:HD2	6:A:3952:HOH:O	2.00	0.44
1:A:42:ILE:HD13	6:A:3940:HOH:O	2.18	0.43
1:A:132:ASP:OD1	1:A:171:HIS:HD2	2.01	0.43
1:B:341:LEU:HB3	1:B:342:ILE:HD12	2.00	0.43
1:C:599:LEU:CG	4:C:3601:O16:H17	2.47	0.43
1:D:603:ASN:ND2	6:D:3856:HOH:O	2.51	0.43
1:A:28:GLN:HG3	6:A:4164:HOH:O	2.18	0.43
1:A:84:GLU:HG2	5:A:3002:GOL:H11	1.99	0.43
1:A:59:LEU:HD12	6:A:3954:HOH:O	2.18	0.43
1:B:239:TRP:HB3	1:B:240:PRO:HD3	2.00	0.43
1:C:567:LEU:CB	1:C:568:LEU:HD12	2.49	0.43
1:D:767:LEU:CG	1:D:768:LEU:HD13	2.47	0.43
1:A:48:PHE:O	1:A:50:LYS:HG2	2.19	0.43
1:C:511:VAL:HG13	1:C:512:LYS:N	2.34	0.43
1:B:236:GLN:HA	1:B:236:GLN:NE2	2.34	0.43
1:B:240:PRO:HB2	1:B:241:GLU:OE1	2.18	0.43
1:D:780:LYS:HD3	6:D:3920:HOH:O	2.18	0.43
1:C:568:LEU:CD1	1:C:568:LEU:N	2.80	0.43
1:B:273:LYS:O	1:B:274:ASN:HB2	2.19	0.42
1:C:506:GLU:HG2	1:C:511:VAL:HG13	2.01	0.42
5:C:3003:GOL:C2	5:C:3003:GOL:O3	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ALA:HB1	4:C:3601:O16:O1	1.99	0.42
1:D:771:HIS:HE1	6:D:4030:HOH:O	2.01	0.42
1:A:122:TYR:O	1:A:125:PRO:HD2	2.19	0.42
1:A:199:LEU:CD1	4:A:3201:O16:H17	2.49	0.42
1:A:142:ILE:HG23	5:A:3002:GOL:H32	2.00	0.42
1:B:224:TYR:CD2	1:B:277:LEU:HD11	2.54	0.42
1:D:706:GLU:HG2	1:D:711:VAL:HG13	2.02	0.42
1:A:121:THR:HG23	6:A:4237:HOH:O	2.20	0.42
1:A:138:ARG:HD2	6:A:4127:HOH:O	2.20	0.42
1:B:236:GLN:HA	1:B:236:GLN:HE21	1.84	0.41
1:C:428:GLN:NE2	5:C:3003:GOL:O1	2.45	0.41
1:D:704:TRP:HB3	4:D:3801:O16:C22	2.47	0.41
3:C:3600:GSH:HB22	4:C:3601:O16:O2	2.21	0.41
1:B:239:TRP:HA	1:B:239:TRP:CE3	2.56	0.41
4:D:3801:O16:H14	4:D:3801:O16:H7	1.88	0.41
1:D:614:ARG:NH2	6:D:3872:HOH:O	2.54	0.41
1:C:520:LEU:HG	1:C:564:LYS:HB2	2.03	0.41
1:A:39:TRP:CE3	1:A:39:TRP:HA	2.56	0.41
1:B:202:PRO:CA	6:B:3903:HOH:O	2.69	0.41
4:B:3401:O16:C4	4:B:3401:O16:S1	3.09	0.41
1:C:447:PRO:HG2	1:C:448:PHE:N	2.35	0.41
1:C:539:GLU:HG2	1:C:580:LYS:NZ	2.36	0.40
1:B:248:PHE:O	1:B:250:LYS:HG2	2.21	0.40
1:B:321:THR:HG22	1:B:322:TYR:CE2	2.57	0.40

All (2) 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:C:3003:GOL:O3	6:D:3992:HOH:O[1_455]	1.99	0.21
6:C:3682:HOH:O	6:D:3992:HOH:O[1_455]	2.17	0.03

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%)	189 (96%)	7 (4%)	0	100	100
1	B	196/198 (99%)	189 (96%)	6 (3%)	1 (0%)	29	18
1	C	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
1	D	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
All	All	784/792 (99%)	761 (97%)	22 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	GLN

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%)	173 (97%)	5 (3%)	43	36
1	B	178/178 (100%)	171 (96%)	7 (4%)	32	23
1	C	178/178 (100%)	177 (99%)	1 (1%)	86	87
1	D	178/178 (100%)	173 (97%)	5 (3%)	43	36
All	All	712/712 (100%)	694 (98%)	18 (2%)	47	41

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	73	LYS
1	A	118	GLU
1	A	144	MET
1	A	199	LEU
1	B	235	GLU
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	315	MET
1	B	318	GLU
1	B	320	LEU
1	B	344	MET
1	B	399	LEU
1	C	544	MET
1	D	603	ASN
1	D	641	GLU
1	D	720	LEU
1	D	744	MET
1	D	768	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	28	GLN
1	A	36	GLN
1	A	62	HIS
1	A	80	ASN
1	A	114	GLN
1	A	123	ASN
1	A	170	ASN
1	A	171	HIS
1	B	203	ASN
1	B	228	GLN
1	B	236	GLN
1	B	262	HIS
1	B	314	GLN
1	B	370	ASN
1	B	371	HIS
1	B	396	GLN
1	C	403	ASN
1	C	428	GLN
1	C	436	GLN
1	C	462	HIS
1	C	514	GLN
1	C	523	ASN
1	C	570	ASN
1	C	571	HIS
1	D	603	ASN
1	D	628	GLN

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Mol	Chain	Res	Type
1	D	636	GLN
1	D	662	HIS
1	D	680	ASN
1	D	714	GLN
1	D	723	ASN
1	D	770	ASN
1	D	771	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	C	3004	-	5,5,5	0.90	0	5,5,5	0.36	0
3	GSH	B	3400	-	12,19,19	1.19	1 (8%)	15,24,24	0.97	0
3	GSH	C	3600	-	12,19,19	1.30	2 (16%)	15,24,24	0.96	0
5	GOL	C	3003	-	5,5,5	6.48	5 (100%)	5,5,5	0.90	0
3	GSH	D	3800	-	12,19,19	1.30	2 (16%)	15,24,24	0.95	0
4	O16	D	3801	-	32,39,39	2.99	4 (12%)	34,56,56	3.03	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	O16	C	3601	1	32,39,39	3.03	4 (12%)	34,56,56	3.02	9 (26%)
5	GOL	A	3002	-	5,5,5	1.10	1 (20%)	5,5,5	0.34	0
5	GOL	A	3001	-	5,5,5	1.90	2 (40%)	5,5,5	0.26	0
4	O16	B	3401	-	32,39,39	3.07	4 (12%)	34,56,56	3.07	10 (29%)
4	O16	A	3201	1	32,39,39	3.04	4 (12%)	34,56,56	3.01	9 (26%)
5	GOL	D	3005	-	5,5,5	0.89	0	5,5,5	0.43	0
5	GOL	B	3006	-	5,5,5	1.05	0	5,5,5	0.33	0
3	GSH	A	3200	-	12,19,19	1.18	1 (8%)	15,24,24	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	3004	-	-	0/4/4/4	-
3	GSH	B	3400	-	-	0/18/24/24	-
3	GSH	C	3600	-	-	1/18/24/24	-
5	GOL	C	3003	-	-	0/4/4/4	-
3	GSH	D	3800	-	-	1/18/24/24	-
4	O16	D	3801	-	-	0/7/13/13	0/6/6/6
4	O16	C	3601	1	-	0/7/13/13	0/6/6/6
5	GOL	A	3002	-	-	0/4/4/4	-
5	GOL	A	3001	-	-	0/4/4/4	-
4	O16	B	3401	-	-	0/7/13/13	0/6/6/6
4	O16	A	3201	1	-	1/7/13/13	0/6/6/6
5	GOL	D	3005	-	-	0/4/4/4	-
5	GOL	B	3006	-	-	0/4/4/4	-
3	GSH	A	3200	-	-	1/18/24/24	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3401	O16	N5-N6	14.78	1.40	1.31
4	C	3601	O16	N5-N6	14.67	1.40	1.31
4	D	3801	O16	N5-N6	14.58	1.40	1.31
4	A	3201	O16	N5-N6	14.56	1.40	1.31
5	C	3003	GOL	O3-C3	11.31	1.90	1.42
5	C	3003	GOL	O2-C2	-8.20	1.18	1.43
4	C	3601	O16	C5-N3	-6.59	1.37	1.45
4	A	3201	O16	C5-N3	-6.29	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3401	O16	C5-N3	-6.21	1.38	1.45
4	D	3801	O16	C5-N3	-5.71	1.38	1.45
4	A	3201	O16	N4-N3	-4.79	1.28	1.31
4	B	3401	O16	N4-N3	-4.78	1.28	1.31
4	D	3801	O16	N4-N3	-4.68	1.29	1.31
4	C	3601	O16	N4-N3	-3.93	1.29	1.31
5	A	3001	GOL	O2-C2	-2.79	1.35	1.43
5	A	3001	GOL	C3-C2	-2.72	1.40	1.51
5	C	3003	GOL	C1-C2	2.34	1.61	1.51
3	D	3800	GSH	CG1-CD1	2.23	1.55	1.51
3	C	3600	GSH	CB2-CA2	2.19	1.55	1.53
3	D	3800	GSH	CB2-CA2	2.18	1.55	1.53
5	C	3003	GOL	O1-C1	2.17	1.51	1.42
4	B	3401	O16	N2-N1	2.16	1.39	1.34
4	A	3201	O16	N2-N1	2.16	1.39	1.34
4	C	3601	O16	N2-N1	2.15	1.39	1.34
5	C	3003	GOL	C3-C2	-2.12	1.43	1.51
4	D	3801	O16	N2-N1	2.11	1.39	1.34
3	B	3400	GSH	CB2-CA2	2.05	1.55	1.53
3	A	3200	GSH	CB2-CA2	2.03	1.55	1.53
5	A	3002	GOL	O3-C3	2.02	1.51	1.42
3	C	3600	GSH	CG1-CD1	2.02	1.55	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3801	O16	N5-N6-N3	-12.24	105.17	110.36
4	B	3401	O16	N5-N6-N3	-12.06	105.24	110.36
4	A	3201	O16	N5-N6-N3	-11.69	105.40	110.36
4	C	3601	O16	N5-N6-N3	-11.63	105.43	110.36
4	B	3401	O16	C16-C21-S1	-7.32	102.14	111.85
4	D	3801	O16	C16-C21-S1	-7.32	102.14	111.85
4	A	3201	O16	C16-C21-S1	-7.29	102.18	111.85
4	C	3601	O16	C16-C21-S1	-7.27	102.21	111.85
4	C	3601	O16	N4-N3-N6	-6.84	107.46	110.36
4	A	3201	O16	N4-N3-N6	-6.64	107.54	110.36
4	D	3801	O16	N4-N3-N6	-6.05	107.79	110.36
4	B	3401	O16	N4-N3-N6	-6.04	107.80	110.36
4	B	3401	O16	C21-C16-N7	3.38	115.92	108.04
4	A	3201	O16	C21-C16-N7	3.32	115.76	108.04
4	D	3801	O16	C21-C16-N7	3.30	115.71	108.04
4	C	3601	O16	C21-C16-N7	3.24	115.58	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3401	O16	C5-N3-N4	3.23	126.42	123.50
4	A	3201	O16	C5-N3-N4	3.21	126.40	123.50
4	C	3601	O16	N5-C6-N4	-3.19	109.41	111.92
4	D	3801	O16	C2-N2-N1	3.07	122.14	119.32
4	B	3401	O16	C1-N1-N2	3.06	122.13	119.32
4	C	3601	O16	C2-N2-N1	3.05	122.13	119.32
4	A	3201	O16	C1-N1-N2	3.04	122.12	119.32
4	D	3801	O16	N5-C6-N4	-3.01	109.55	111.92
4	C	3601	O16	C5-N3-N4	2.99	126.20	123.50
4	B	3401	O16	C2-N2-N1	2.97	122.05	119.32
4	B	3401	O16	N5-C6-N4	-2.94	109.60	111.92
4	D	3801	O16	C5-N3-N4	2.91	126.12	123.50
4	A	3201	O16	N5-C6-N4	-2.90	109.64	111.92
4	D	3801	O16	C1-N1-N2	2.86	121.95	119.32
4	A	3201	O16	C2-N2-N1	2.83	121.93	119.32
4	B	3401	O16	C17-C16-C21	-2.77	115.66	120.53
4	D	3801	O16	C17-C16-C21	-2.64	115.88	120.53
4	A	3201	O16	C17-C16-C21	-2.64	115.88	120.53
4	C	3601	O16	C1-N1-N2	2.55	121.67	119.32
4	C	3601	O16	C17-C16-C21	-2.49	116.15	120.53
4	B	3401	O16	C14-C9-C10	2.38	121.16	117.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3600	GSH	N1-CA1-CB1-CG1
3	D	3800	GSH	N1-CA1-CB1-CG1
3	A	3200	GSH	N1-CA1-CB1-CG1
4	A	3201	O16	C4-C5-N3-N6

There are no ring outliers.

9 monomers are involved in 81 short contacts:

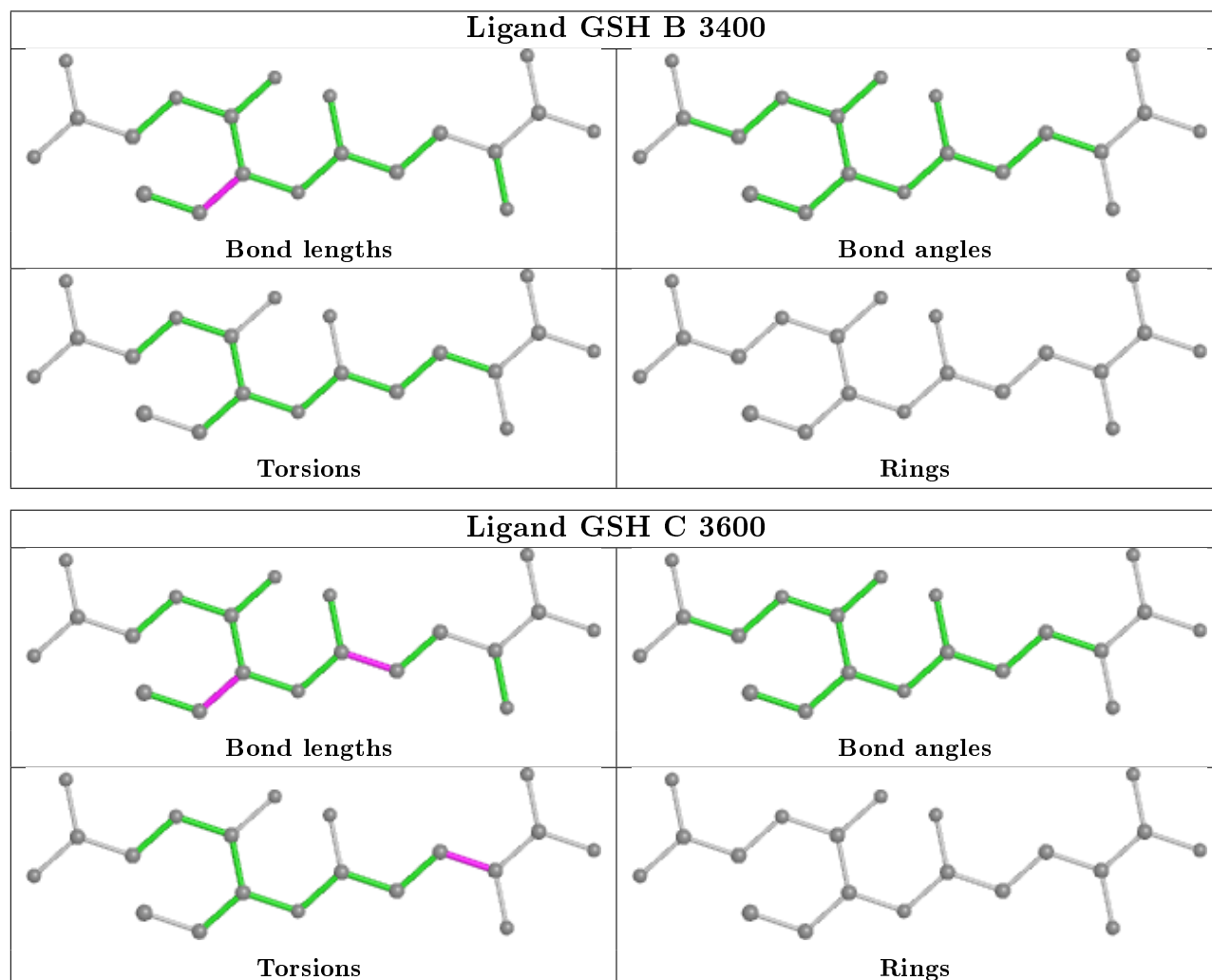
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3400	GSH	1	0
3	C	3600	GSH	1	0
5	C	3003	GOL	3	1
4	D	3801	O16	23	0
4	C	3601	O16	26	0
5	A	3002	GOL	5	0

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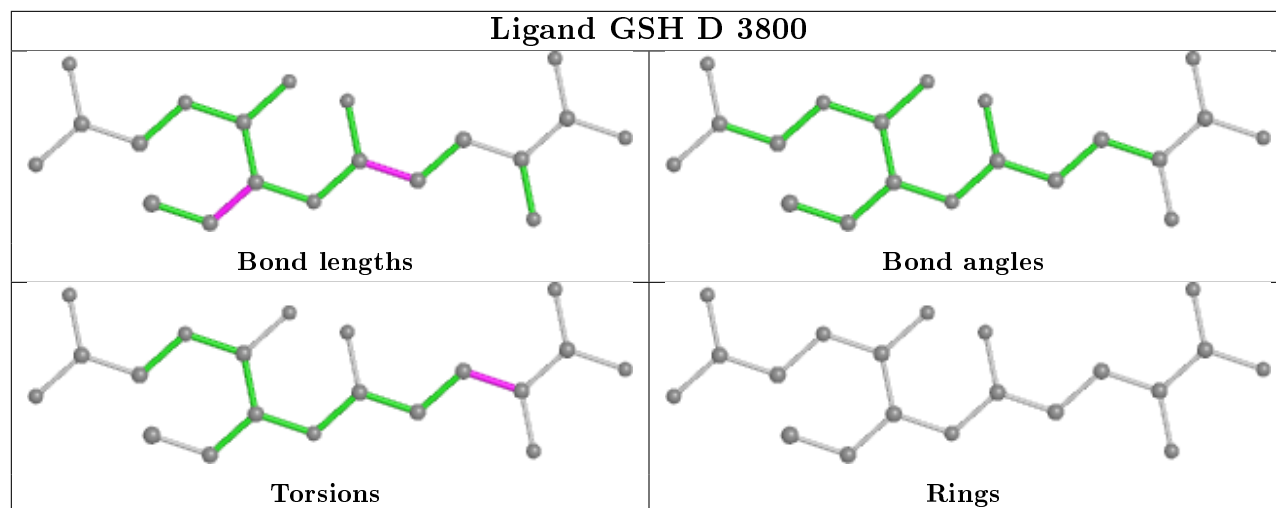
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3001	GOL	1	0
4	B	3401	O16	13	0
4	A	3201	O16	9	0

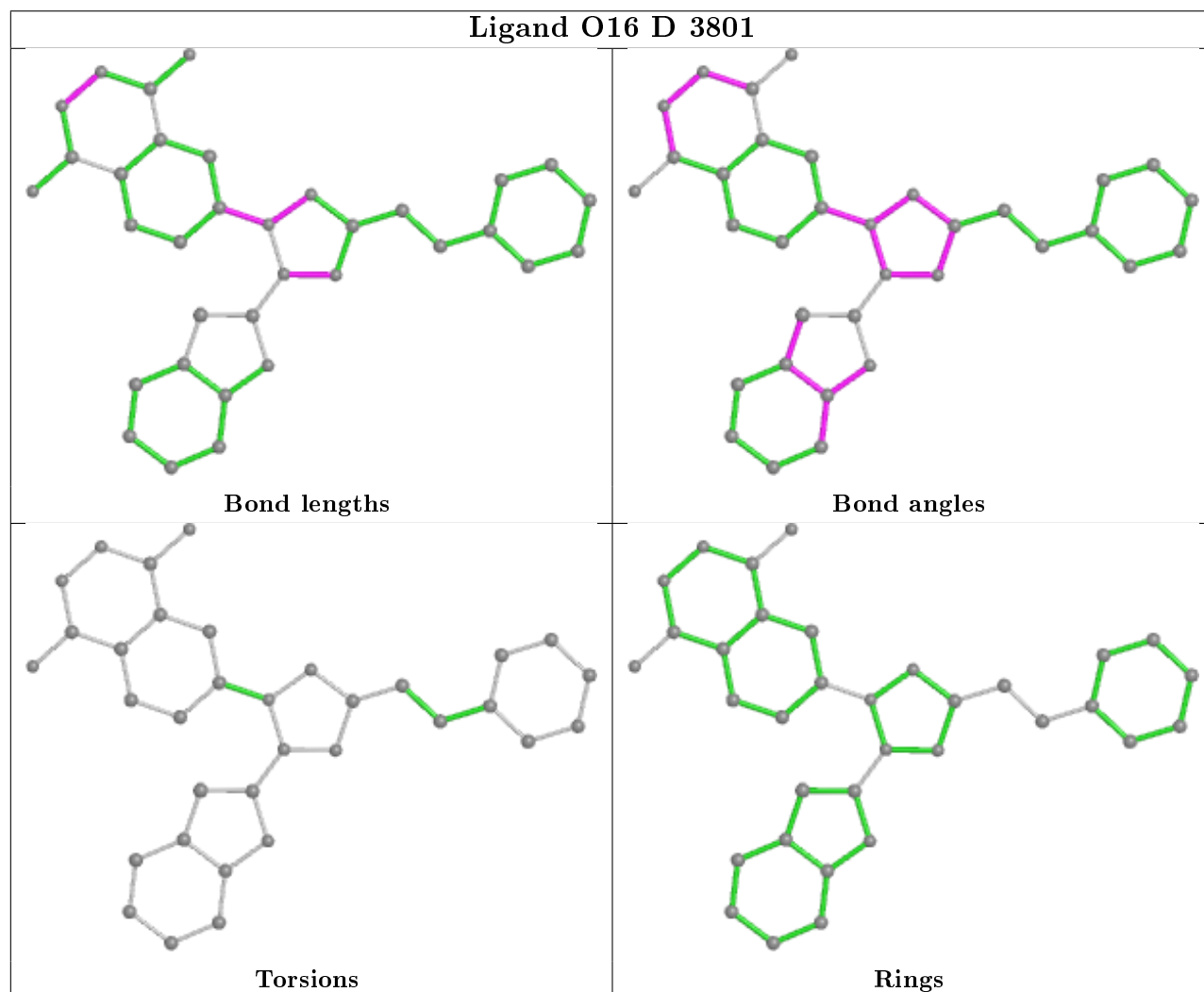
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

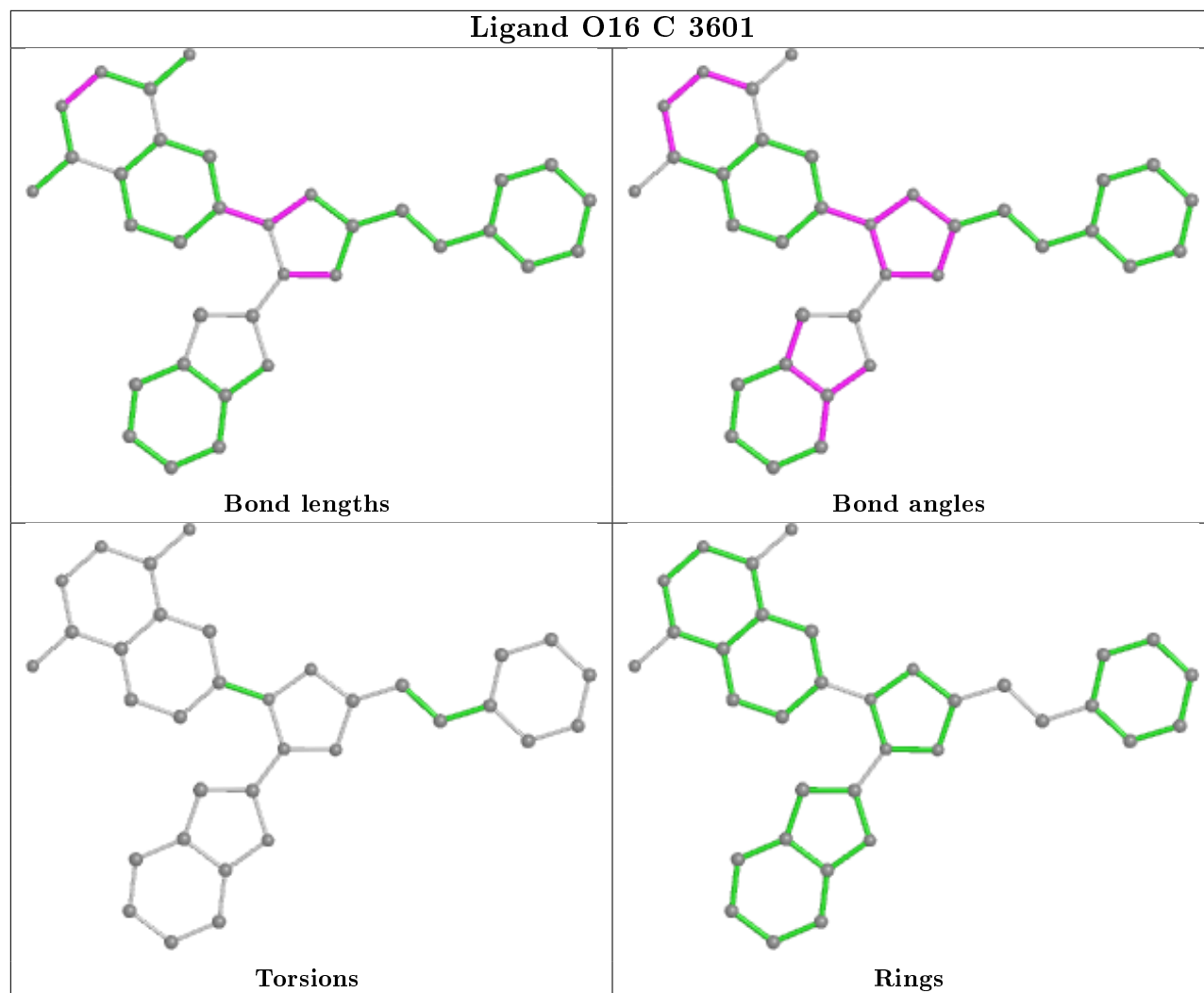


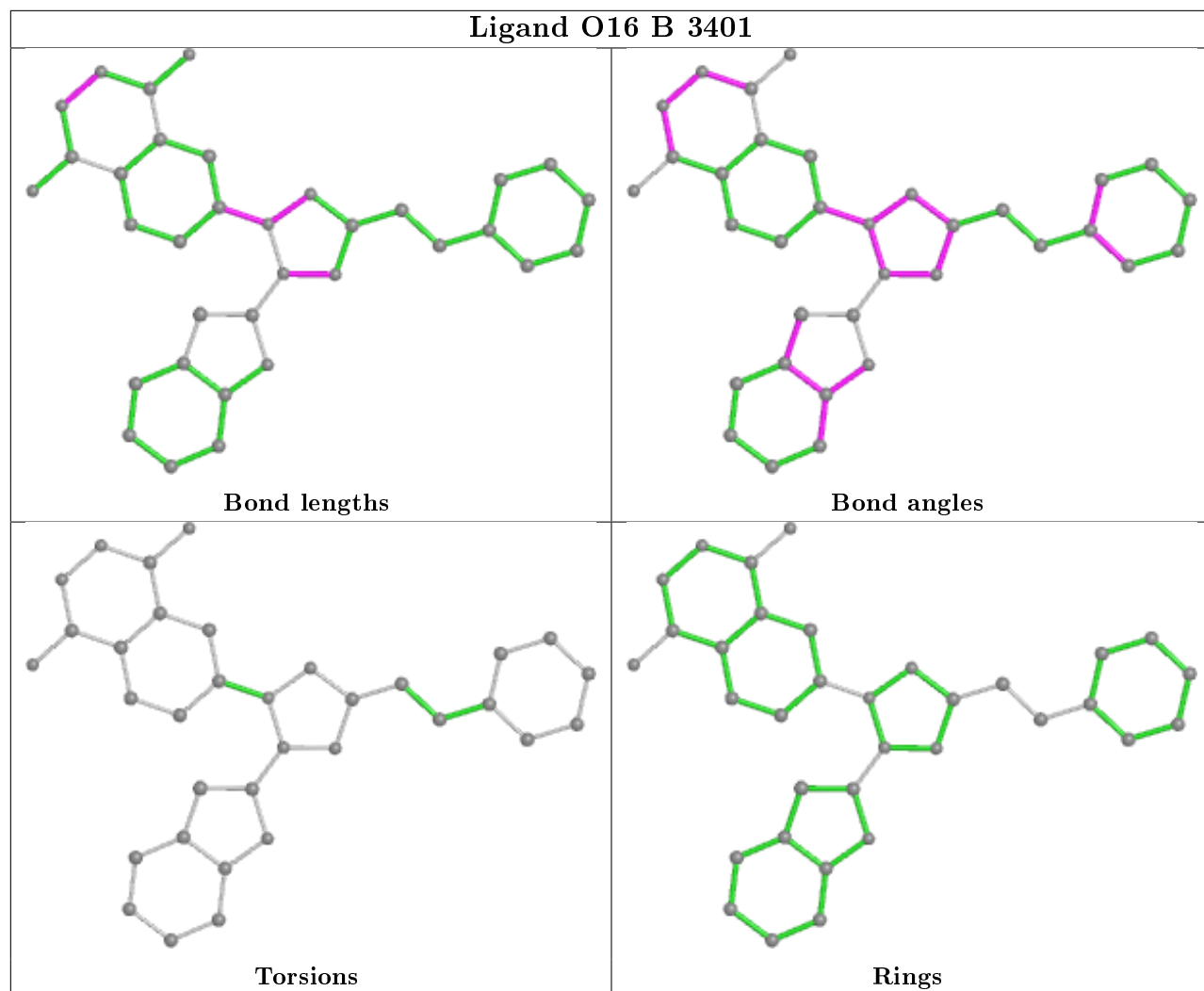
Ligand GSH D 3800

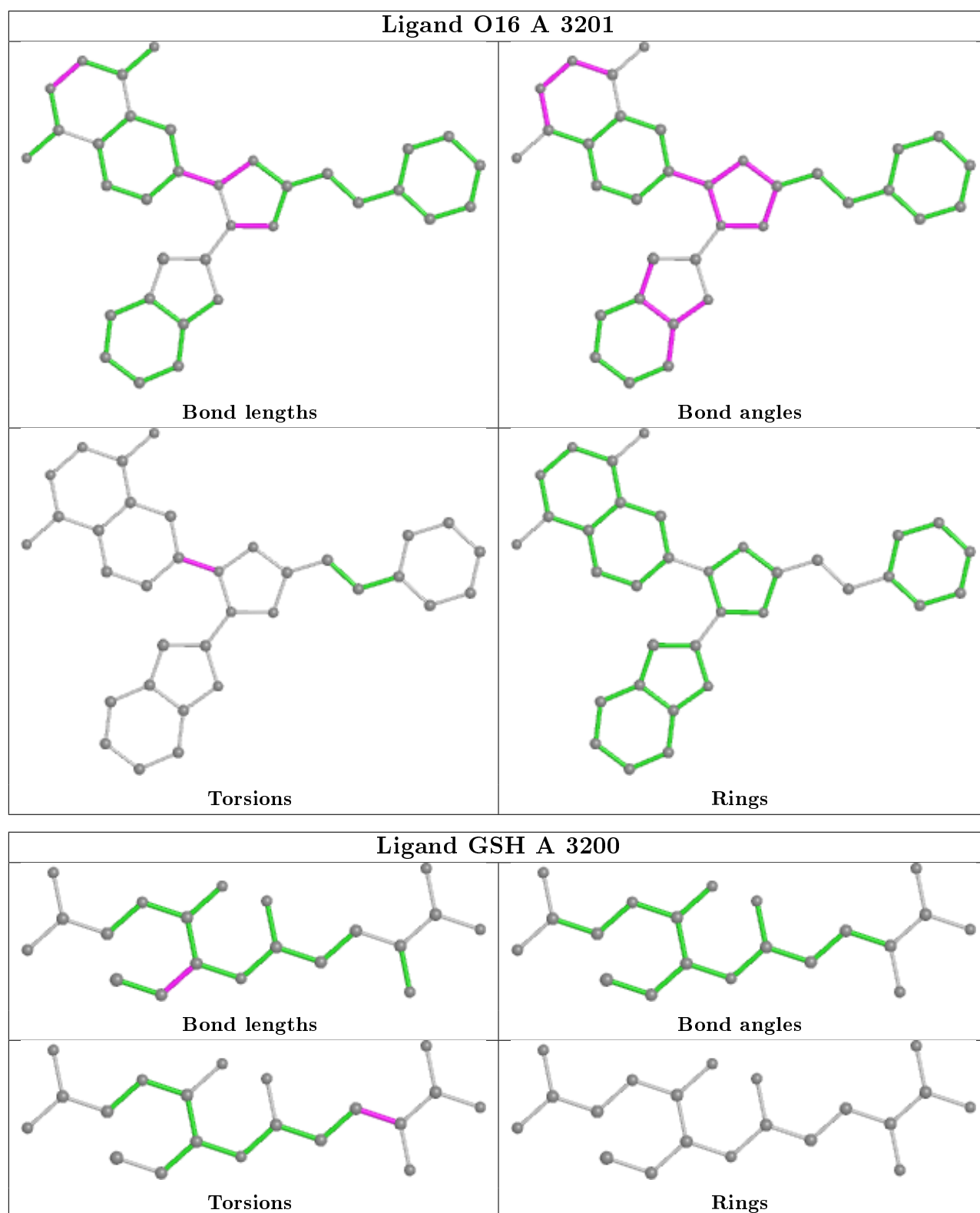


Ligand O16 D 3801









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.13	5 (2%) 57 60	8, 21, 46, 54	0
1	B	198/198 (100%)	-0.16	3 (1%) 73 76	9, 21, 46, 55	0
1	C	198/198 (100%)	-0.55	0 100 100	6, 12, 28, 36	0
1	D	198/198 (100%)	-0.53	0 100 100	6, 13, 28, 36	0
All	All	792/792 (100%)	-0.34	8 (1%) 82 84	6, 17, 41, 55	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	ASP	4.7
1	A	110	ASP	3.4
1	A	109	GLN	3.4
1	B	309	GLN	3.1
1	B	314	GLN	2.4
1	A	108	LYS	2.2
1	A	111	VAL	2.0
1	A	114	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 carbohydrates in this entry.

6.4 Ligands ⓘ

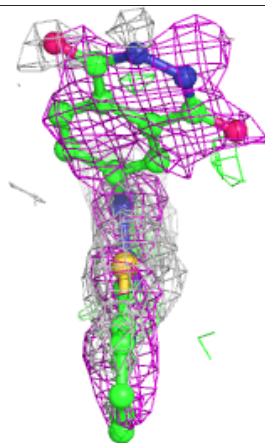
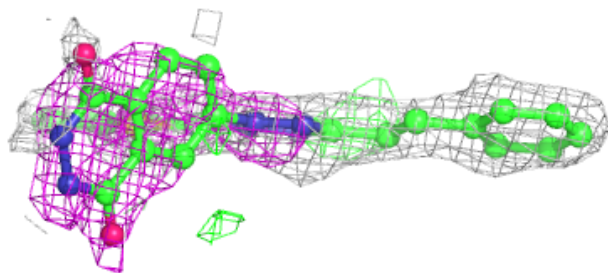
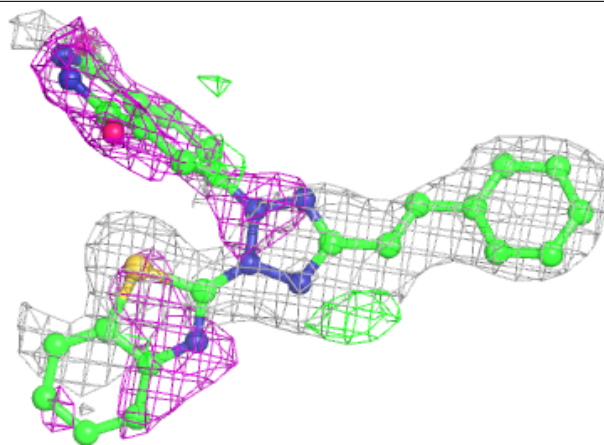
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	O16	B	3401	34/34	0.58	0.42	33,38,40,40	0
4	O16	D	3801	34/34	0.58	0.39	32,38,40,40	0
4	O16	A	3201	34/34	0.58	0.41	33,39,40,41	0
4	O16	C	3601	34/34	0.59	0.39	31,38,39,40	0
5	GOL	C	3003	6/6	0.71	0.21	31,32,32,33	0
5	GOL	A	3001	6/6	0.78	0.27	33,33,33,35	0
3	GSH	D	3800	20/20	0.83	0.14	28,34,38,38	0
5	GOL	B	3006	6/6	0.85	0.11	32,33,33,35	0
3	GSH	B	3400	20/20	0.86	0.14	25,33,38,38	0
5	GOL	D	3005	6/6	0.87	0.15	31,31,32,32	0
5	GOL	A	3002	6/6	0.87	0.13	31,32,32,34	0
3	GSH	C	3600	20/20	0.88	0.12	24,31,34,35	0
3	GSH	A	3200	20/20	0.88	0.12	30,35,40,40	0
5	GOL	C	3004	6/6	0.90	0.16	28,29,30,31	0
2	MG	A	3900	1/1	0.99	0.03	13,13,13,13	0
2	MG	B	3901	1/1	0.99	0.02	13,13,13,13	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.

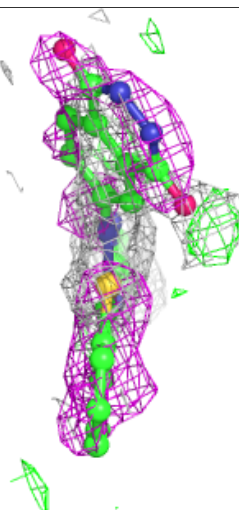
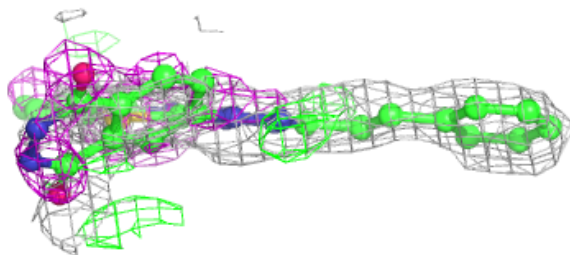
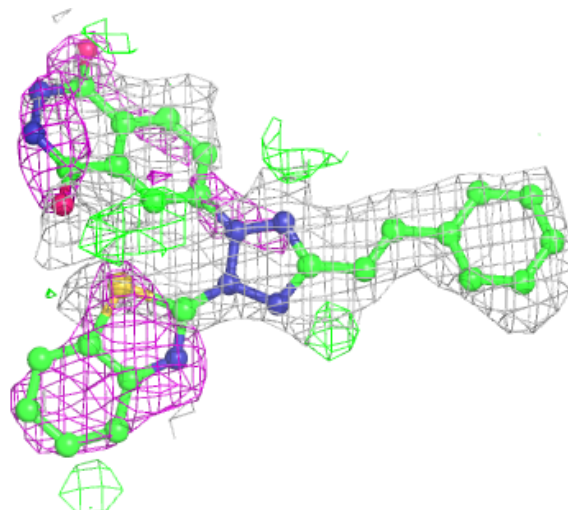
Electron density around O16 B 3401:

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



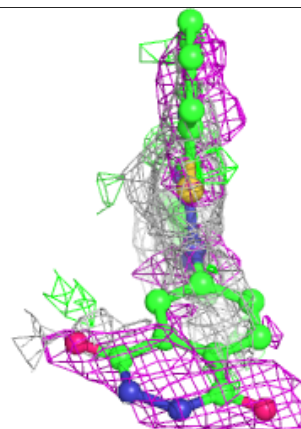
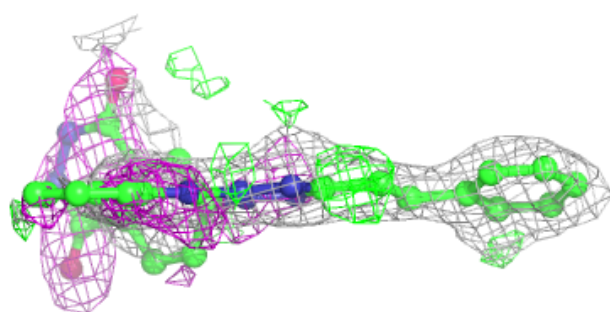
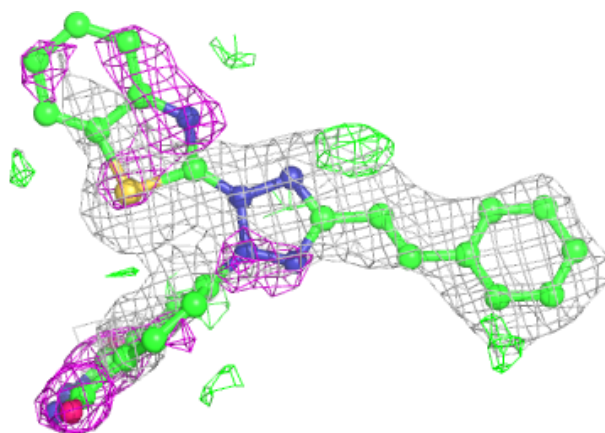
Electron density around O16 D 3801:

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



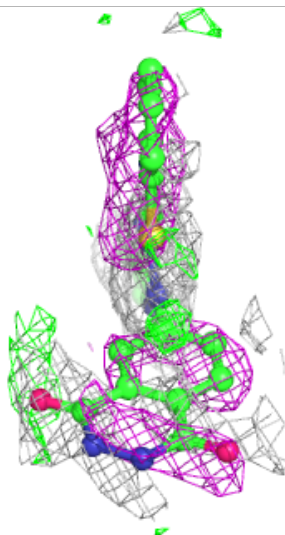
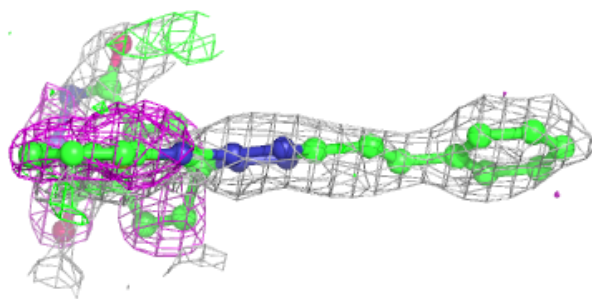
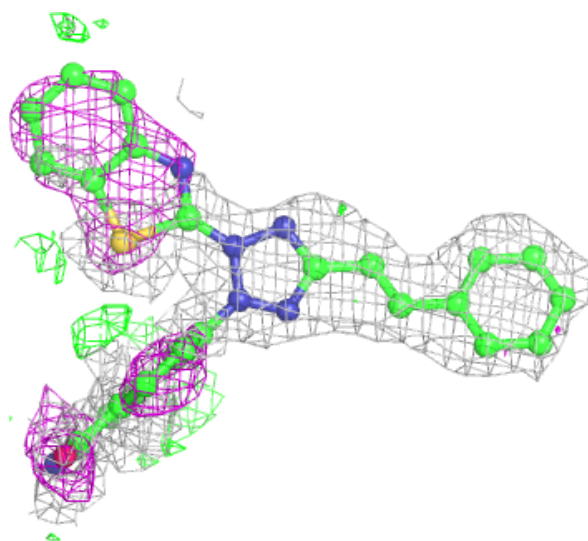
Electron density around O16 A 3201:

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



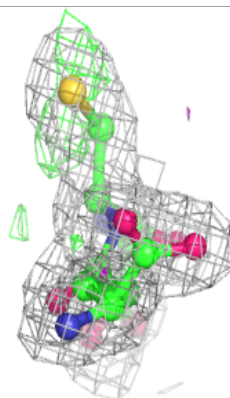
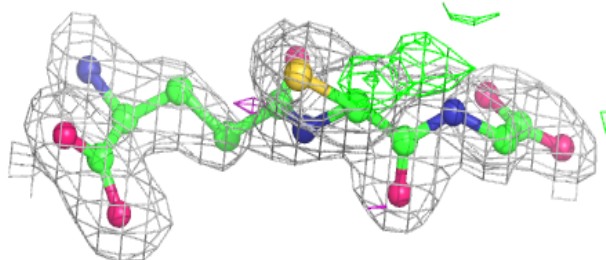
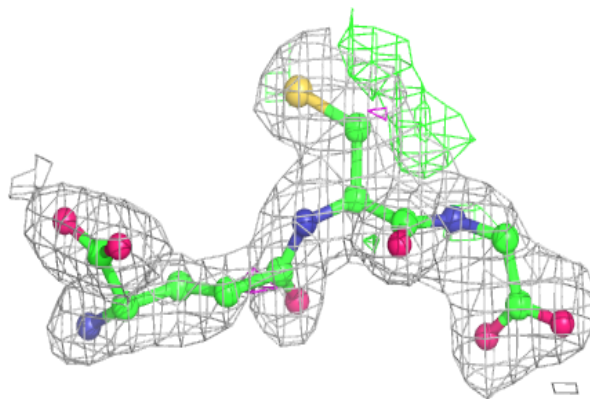
Electron density around O16 C 3601:

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

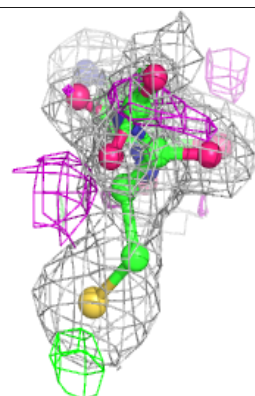
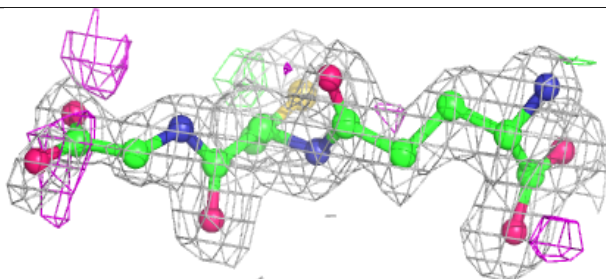
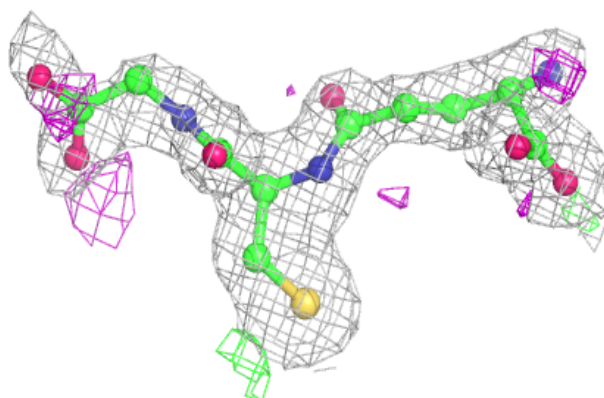


Electron density around GSH D 3800:

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

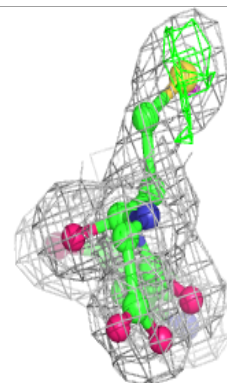
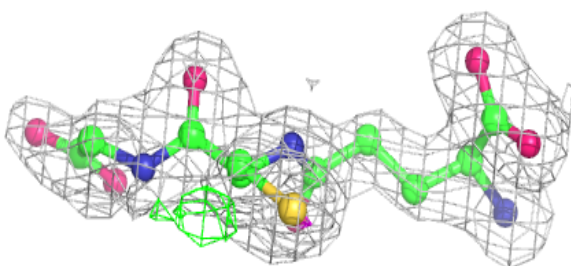
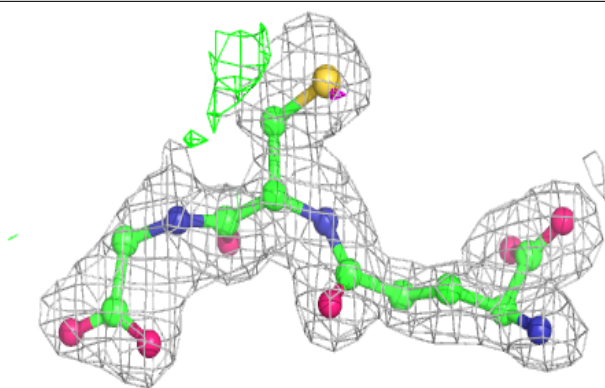
**Electron density around GSH B 3400:**

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

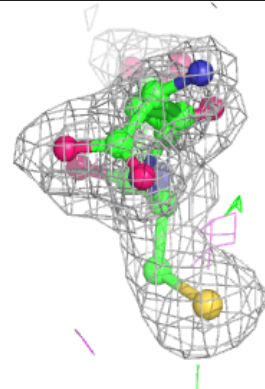
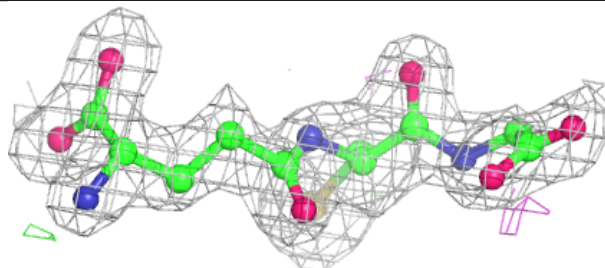
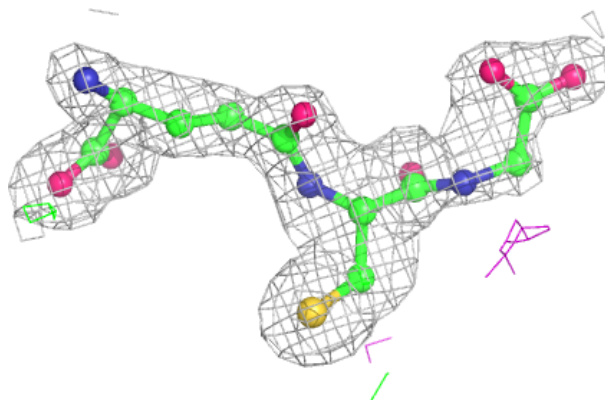


Electron density around GSH C 3600:

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

**Electron density around GSH A 3200:**

$2mF_o-DF_c$ (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.