



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 1, 2025 – 11:03 pm BST

PDB ID : 2X99 / pdb\_00002x99  
Title : Thioredoxin glutathione reductase from *Schistosoma mansoni* in complex with NADPH  
Authors : Angelucci, F.; Dimastrogiovanni, D.; Boumis, G.; Brunori, M.; Miele, A.E.; Saccoccia, F.; Bellelli, A.  
Deposited on : 2010-03-15  
Resolution : 2.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

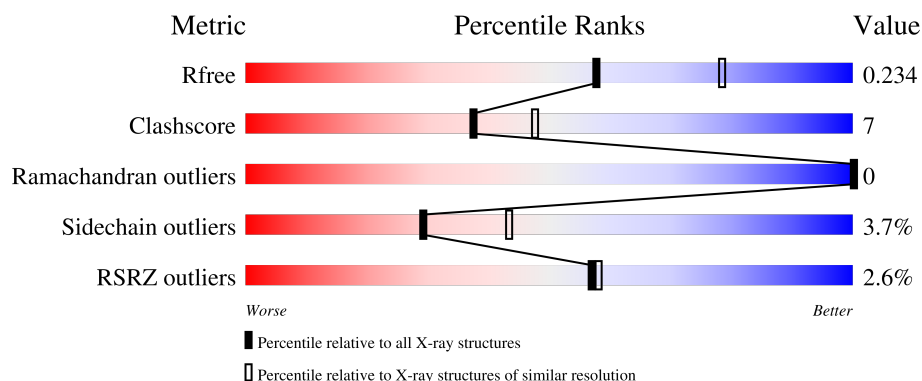
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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  $\geq 3$ , 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	598	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GSH	A	604	X	-	-	-

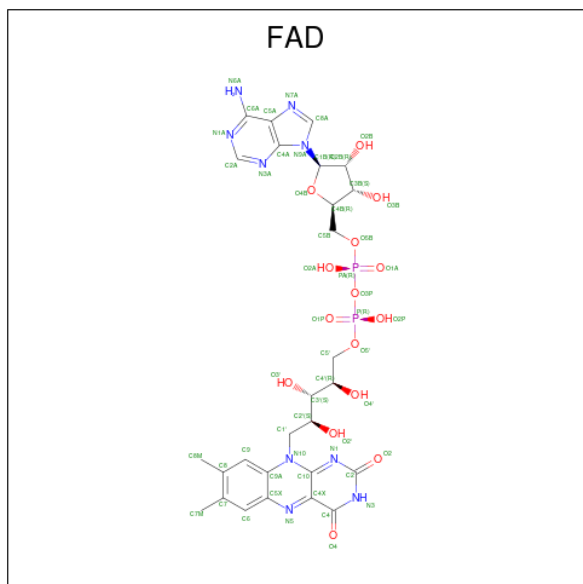


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THIOREDOXIN GLUTATHIONE REDUCTASE.

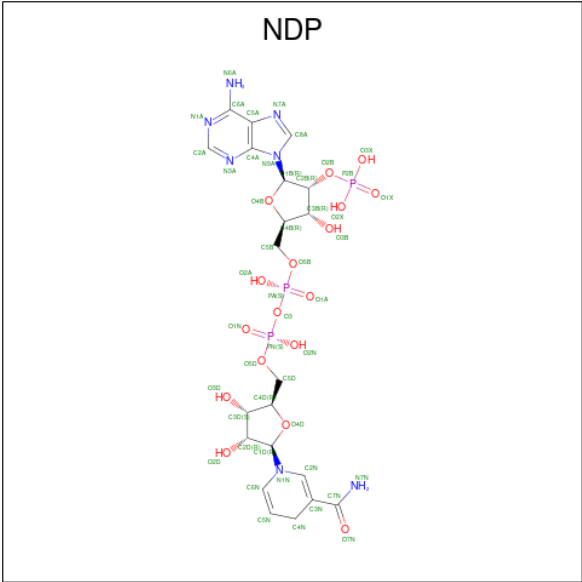
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	2	0
			4502	2858	758	862	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



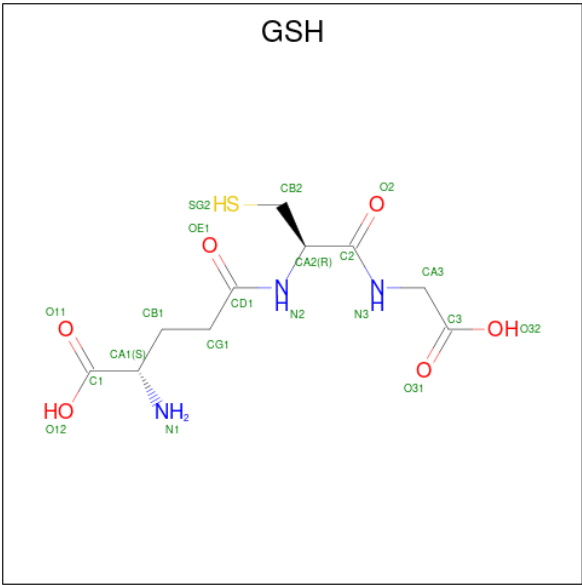
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).

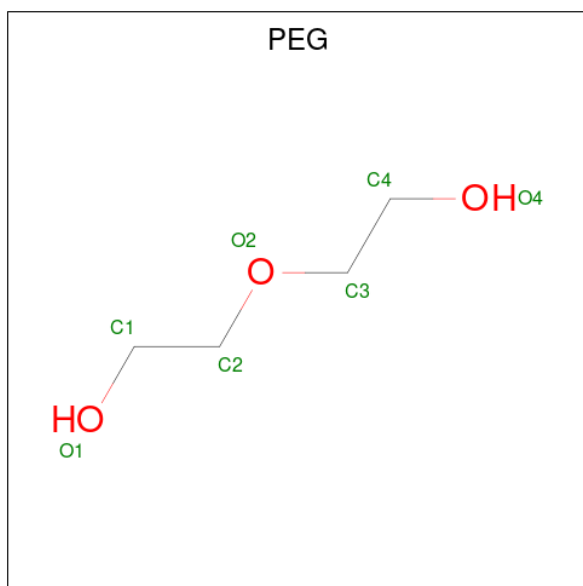


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

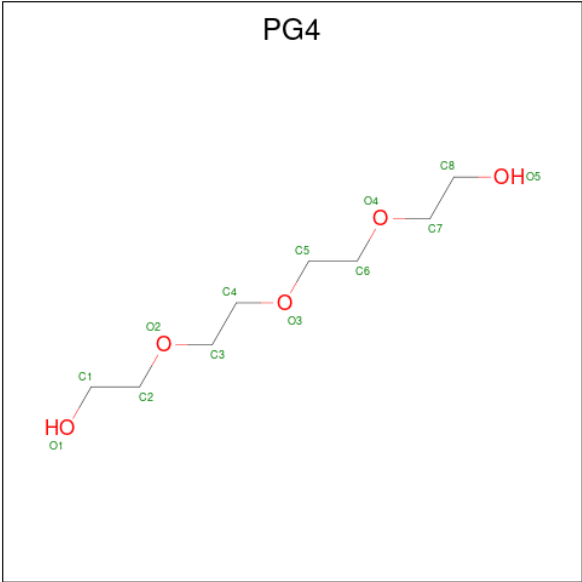
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		

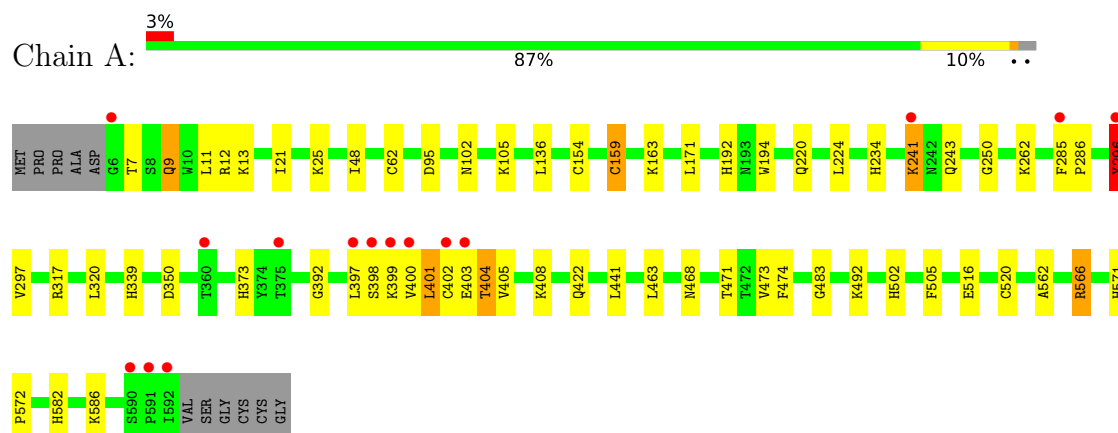
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	185	Total	O	0	0
			185	185		

### 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: THIOREDOXIN GLUTATHIONE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.50Å 102.61Å 59.94Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.30) 99.8 (40.00-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.190 , 0.231 0.192 , 0.234	Depositor DCC
$R_{free}$ test set	1743 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4936	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, CA, GSH, PG4, FAD, NDP

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	0.55	0/4595	0.64	3/6224 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	397	LEU	CB-CA-C	-10.81	89.67	110.20
1	A	582	HIS	CB-CA-C	6.07	122.53	110.40
1	A	296	TYR	CA-CB-CG	5.31	123.50	113.40

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	4502	0	4520	63	0
2	A	53	0	31	1	0
3	A	48	0	26	10	0
4	A	40	0	29	3	0
5	A	1	0	0	0	0
6	A	42	0	60	1	0
7	A	65	0	90	5	0
8	A	185	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4936	0	4756	66	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 7.

All (66) 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:A:441:LEU:HD11	1:A:471:THR:HG22	1.57	0.84
1:A:400:VAL:HG23	1:A:401:LEU:HD13	1.61	0.82
1:A:401:LEU:O	1:A:404:THR:HG23	1.77	0.82
1:A:296:TYR:CE1	3:A:602:NDP:H2D	2.15	0.81
1:A:399:LYS:O	1:A:403:GLU:HG2	1.81	0.80
1:A:401:LEU:O	1:A:404:THR:CG2	2.30	0.80
3:A:602:NDP:H62A	7:A:614:PG4:H21	1.47	0.79
1:A:339:HIS:HE1	1:A:516:GLU:OE2	1.66	0.79
1:A:402:CYS:HA	4:A:604:GSH:HB23	1.67	0.76
1:A:400:VAL:HG23	1:A:401:LEU:CD1	2.15	0.76
1:A:398:SER:O	1:A:402:CYS:HB2	1.92	0.69
1:A:194:TRP:HB2	1:A:285:PHE:HD1	1.58	0.69
1:A:13:LYS:HB3	6:A:609:PEG:H42	1.76	0.68
1:A:154[B]:CYS:HB2	1:A:159[B]:CYS:HG	1.61	0.66
1:A:339:HIS:CE1	1:A:516:GLU:OE2	2.49	0.66
1:A:296:TYR:HD2	1:A:473:VAL:HG22	1.62	0.65
1:A:154[B]:CYS:CB	1:A:159[B]:CYS:HG	2.10	0.65
1:A:296:TYR:HE1	3:A:602:NDP:H2D	1.64	0.63
1:A:194:TRP:HB2	1:A:285:PHE:CD1	2.34	0.62
1:A:398:SER:HB3	1:A:401:LEU:HB2	1.81	0.61
1:A:297:VAL:HG23	3:A:602:NDP:H6N	1.82	0.61
1:A:262:LYS:HD3	7:A:614:PG4:H82	1.83	0.60
1:A:25:LYS:HE3	4:A:603:GSH:O31	2.00	0.60
1:A:468:ASN:HD22	1:A:483:GLY:HA2	1.68	0.58
1:A:296:TYR:CD2	1:A:473:VAL:HG22	2.38	0.57
1:A:401:LEU:O	1:A:404:THR:HG22	2.08	0.54
2:A:601:FAD:H61A	4:A:604:GSH:HN12	1.57	0.51
1:A:163:LYS:HE3	1:A:474:PHE:CE1	2.45	0.51
1:A:401:LEU:C	1:A:404:THR:HG22	2.32	0.50
1:A:192:HIS:HD2	8:A:854:HOH:O	1.94	0.50
1:A:405:VAL:O	1:A:405:VAL:HG12	2.12	0.50
1:A:441:LEU:HD11	1:A:471:THR:CG2	2.36	0.50
1:A:400:VAL:CG2	1:A:401:LEU:HD13	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154[B]:CYS:HG	1:A:159[B]:CYS:HB2	1.77	0.48
1:A:241:LYS:C	1:A:243:GLN:H	2.17	0.48
1:A:105:LYS:O	7:A:615:PG4:H41	2.14	0.48
1:A:422:GLN:NE2	8:A:703:HOH:O	2.47	0.47
1:A:562:ALA:O	1:A:566:ARG:HG3	2.13	0.47
1:A:401:LEU:HA	1:A:404:THR:CG2	2.45	0.46
1:A:400:VAL:O	1:A:404:THR:HG22	2.15	0.46
1:A:9:GLN:HE21	1:A:9:GLN:H	1.64	0.46
1:A:285:PHE:CD1	1:A:286:PRO:HD2	2.51	0.46
1:A:399:LYS:O	1:A:403:GLU:CG	2.59	0.45
1:A:296:TYR:CZ	3:A:602:NDP:H2D	2.51	0.45
1:A:392:GLY:HA2	3:A:602:NDP:O3	2.16	0.45
1:A:317:ARG:HD2	3:A:602:NDP:O2X	2.16	0.45
1:A:401:LEU:HA	1:A:404:THR:HG22	1.99	0.45
1:A:398:SER:CB	1:A:401:LEU:HB2	2.47	0.44
1:A:400:VAL:HA	1:A:403:GLU:HG2	1.97	0.44
1:A:297:VAL:CG2	3:A:602:NDP:H6N	2.47	0.44
1:A:350:ASP:OD2	1:A:373:HIS:HD2	2.01	0.44
1:A:505:PHE:CZ	1:A:520:CYS:HB3	2.53	0.44
3:A:602:NDP:N7A	7:A:614:PG4:H81	2.32	0.44
1:A:401:LEU:CA	1:A:404:THR:HG22	2.48	0.44
1:A:154[B]:CYS:HB2	1:A:159[B]:CYS:SG	2.59	0.42
1:A:21:ILE:HD11	1:A:48:ILE:HD12	2.01	0.42
1:A:400:VAL:HG23	1:A:401:LEU:HD12	2.00	0.42
1:A:9:GLN:H	1:A:9:GLN:NE2	2.18	0.42
1:A:297:VAL:HG23	3:A:602:NDP:C6N	2.49	0.41
1:A:136:LEU:CD2	1:A:224:LEU:HD12	2.50	0.41
1:A:154[B]:CYS:HG	1:A:159[B]:CYS:CB	2.34	0.41
1:A:492:LYS:HG3	7:A:613:PG4:H11	2.02	0.41
1:A:571:HIS:HA	1:A:572:PRO:HA	1.71	0.41
1:A:234:HIS:HD2	1:A:250:GLY:O	2.03	0.41
1:A:11:LEU:HD23	1:A:62:CYS:HB3	2.03	0.40
1:A:400:VAL:HG23	1:A:401:LEU:N	2.37	0.40

There are no symmetry-related clashes.

## 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	587/598 (98%)	572 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	490/496 (99%)	471 (96%)	19 (4%)	27	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	9	GLN
1	A	12	ARG
1	A	95	ASP
1	A	102	ASN
1	A	159[A]	CYS
1	A	159[B]	CYS
1	A	171	LEU
1	A	220	GLN
1	A	241	LYS
1	A	296	TYR
1	A	320	LEU
1	A	401	LEU

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Mol	Chain	Res	Type
1	A	404	THR
1	A	408	LYS
1	A	463	LEU
1	A	502	HIS
1	A	566	ARG
1	A	586	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	102	ASN
1	A	173	HIS
1	A	180	HIS
1	A	192	HIS
1	A	209	ASN
1	A	219	ASN
1	A	234	HIS
1	A	242	ASN
1	A	338	ASN
1	A	339	HIS
1	A	373	HIS
1	A	422	GLN
1	A	468	ASN
1	A	514	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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
6	PEG	A	606	-	6,6,6	0.49	0	5,5,5	0.24	0
6	PEG	A	616	-	6,6,6	0.44	0	5,5,5	0.28	0
7	PG4	A	612	-	12,12,12	0.50	0	11,11,11	0.20	0
7	PG4	A	615	-	12,12,12	0.50	0	11,11,11	0.32	0
7	PG4	A	613	-	12,12,12	0.46	0	11,11,11	0.31	0
2	FAD	A	601	-	53,58,58	1.14	4 (7%)	68,89,89	1.43	9 (13%)
7	PG4	A	611	-	12,12,12	0.42	0	11,11,11	0.42	0
6	PEG	A	608	-	6,6,6	0.45	0	5,5,5	0.37	0
6	PEG	A	607	-	6,6,6	0.46	0	5,5,5	0.21	0
6	PEG	A	610	-	6,6,6	0.46	0	5,5,5	0.35	0
7	PG4	A	614	-	12,12,12	0.52	0	11,11,11	0.26	0
4	GSH	A	604	1	18,19,19	2.77	2 (11%)	23,24,24	0.99	2 (8%)
3	NDP	A	602	-	45,52,52	1.64	5 (11%)	53,80,80	1.17	2 (3%)
6	PEG	A	609	-	6,6,6	0.51	0	5,5,5	0.79	0
4	GSH	A	603	-	18,19,19	3.06	2 (11%)	23,24,24	1.20	3 (13%)

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
6	PEG	A	606	-	-	0/4/4/4	-
6	PEG	A	616	-	-	2/4/4/4	-
7	PG4	A	612	-	-	4/10/10/10	-
7	PG4	A	615	-	-	3/10/10/10	-
7	PG4	A	613	-	-	0/10/10/10	-
7	PG4	A	611	-	-	2/10/10/10	-
6	PEG	A	608	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	607	-	-	1/4/4/4	-
6	PEG	A	610	-	-	0/4/4/4	-
4	GSH	A	604	1	1/1/6/8	11/24/24/24	-
7	PG4	A	614	-	-	6/10/10/10	-
2	FAD	A	601	-	-	3/30/50/50	0/6/6/6
3	NDP	A	602	-	-	13/30/77/77	0/5/5/5
6	PEG	A	609	-	-	4/4/4/4	-
4	GSH	A	603	-	-	9/24/24/24	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	GSH	OE1-CD1	9.07	1.41	1.23
4	A	603	GSH	O2-C2	8.81	1.40	1.23
4	A	604	GSH	O2-C2	8.13	1.39	1.23
4	A	604	GSH	OE1-CD1	7.66	1.38	1.23
3	A	602	NDP	O7N-C7N	7.37	1.41	1.24
2	A	601	FAD	C4X-N5	4.46	1.39	1.30
3	A	602	NDP	C2A-N3A	4.36	1.39	1.32
2	A	601	FAD	C2A-N3A	3.80	1.38	1.32
3	A	602	NDP	C6N-C5N	3.51	1.39	1.33
2	A	601	FAD	C10-N1	2.45	1.38	1.33
2	A	601	FAD	C2A-N1A	2.35	1.38	1.33
3	A	602	NDP	C2N-C3N	2.24	1.41	1.34
3	A	602	NDP	C2A-N1A	2.12	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-5.92	119.42	128.68
3	A	602	NDP	N3A-C2A-N1A	-5.82	119.58	128.68
2	A	601	FAD	C4-N3-C2	-3.17	119.79	125.64
2	A	601	FAD	C9A-C5X-N5	-2.70	119.50	122.43
2	A	601	FAD	C4X-C4-N3	2.70	120.05	113.19
2	A	601	FAD	C4X-C10-N10	2.69	120.41	116.48
2	A	601	FAD	C10-C4X-N5	-2.68	119.18	124.86
3	A	602	NDP	C3D-C2D-C1D	2.53	106.23	101.43
4	A	603	GSH	O32-C3-CA3	2.49	121.39	112.74
4	A	603	GSH	CA2-CB2-SG2	-2.36	111.54	114.19
2	A	601	FAD	O4-C4-C4X	-2.27	120.57	126.60
2	A	601	FAD	C4-C4X-N5	2.27	121.47	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604	GSH	O32-C3-CA3	2.14	120.19	112.74
2	A	601	FAD	C4X-C10-N1	-2.06	119.94	124.73
4	A	604	GSH	O12-C1-O11	-2.05	119.43	124.09
4	A	603	GSH	O12-C1-CA1	2.04	120.33	113.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	604	GSH	CA1

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C5B-O5B-PA-O1A
3	A	602	NDP	C5D-O5D-PN-O3
3	A	602	NDP	C5D-O5D-PN-O1N
3	A	602	NDP	C5D-O5D-PN-O2N
3	A	602	NDP	O4D-C4D-C5D-O5D
4	A	603	GSH	N1-CA1-CB1-CG1
4	A	603	GSH	C1-CA1-CB1-CG1
4	A	603	GSH	CG1-CD1-N2-CA2
4	A	603	GSH	CA2-C2-N3-CA3
4	A	603	GSH	O2-C2-N3-CA3
4	A	604	GSH	N2-CA2-CB2-SG2
4	A	604	GSH	C2-CA2-CB2-SG2
4	A	604	GSH	CA2-C2-N3-CA3
4	A	603	GSH	OE1-CD1-N2-CA2
3	A	602	NDP	O4D-C1D-N1N-C2N
2	A	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NDP	C3D-C4D-C5D-O5D
4	A	604	GSH	O2-C2-N3-CA3
4	A	603	GSH	O31-C3-CA3-N3
7	A	614	PG4	O1-C1-C2-O2
7	A	615	PG4	O1-C1-C2-O2
6	A	616	PEG	O2-C3-C4-O4
4	A	604	GSH	N2-CD1-CG1-CB1
4	A	604	GSH	OE1-CD1-CG1-CB1
7	A	614	PG4	O2-C3-C4-O3
4	A	603	GSH	O32-C3-CA3-N3
6	A	609	PEG	O2-C3-C4-O4
2	A	601	FAD	C3B-C4B-C5B-O5B
6	A	609	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	608	PEG	O2-C3-C4-O4
7	A	615	PG4	O3-C5-C6-O4
6	A	616	PEG	O1-C1-C2-O2
7	A	614	PG4	O4-C7-C8-O5
3	A	602	NDP	C2B-O2B-P2B-O1X
7	A	611	PG4	O1-C1-C2-O2
4	A	604	GSH	O12-C1-CA1-CB1
6	A	609	PEG	C1-C2-O2-C3
7	A	612	PG4	C3-C4-O3-C5
7	A	614	PG4	C8-C7-O4-C6
3	A	602	NDP	C5B-O5B-PA-O3
7	A	615	PG4	C4-C3-O2-C2
3	A	602	NDP	PN-O3-PA-O1A
6	A	609	PEG	C4-C3-O2-C2
4	A	604	GSH	O11-C1-CA1-CB1
7	A	611	PG4	C4-C3-O2-C2
7	A	614	PG4	C3-C4-O3-C5
7	A	612	PG4	C8-C7-O4-C6
7	A	614	PG4	C1-C2-O2-C3
6	A	607	PEG	C1-C2-O2-C3
4	A	604	GSH	O2-C2-CA2-N2
2	A	601	FAD	P-O3P-PA-O1A
6	A	608	PEG	O1-C1-C2-O2
7	A	612	PG4	C6-C5-O3-C4
4	A	603	GSH	O12-C1-CA1-N1
3	A	602	NDP	PN-O3-PA-O2A
3	A	602	NDP	C2N-C3N-C7N-N7N
3	A	602	NDP	O4B-C4B-C5B-O5B
4	A	604	GSH	N1-CA1-CB1-CG1
4	A	604	GSH	N3-C2-CA2-N2
7	A	612	PG4	O3-C5-C6-O4

There are no ring outliers.

8 monomers are involved in 17 short contacts:

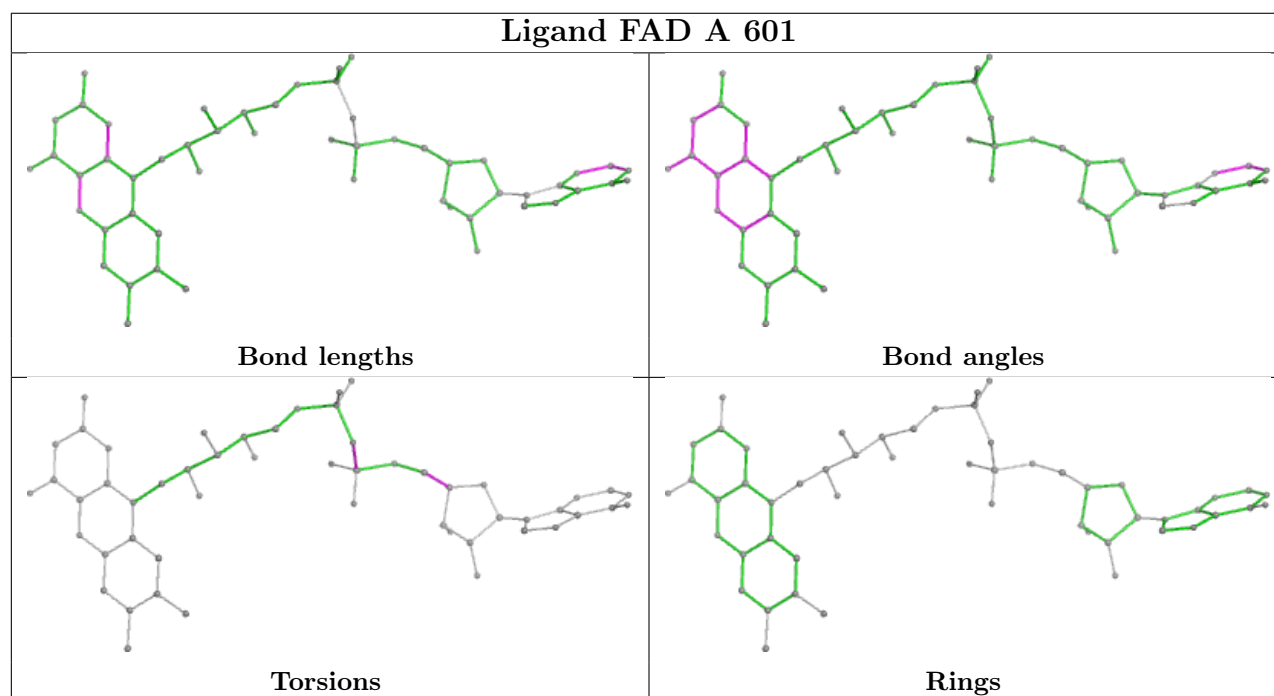
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	615	PG4	1	0
7	A	613	PG4	1	0
2	A	601	FAD	1	0
7	A	614	PG4	3	0
4	A	604	GSH	2	0
3	A	602	NDP	10	0

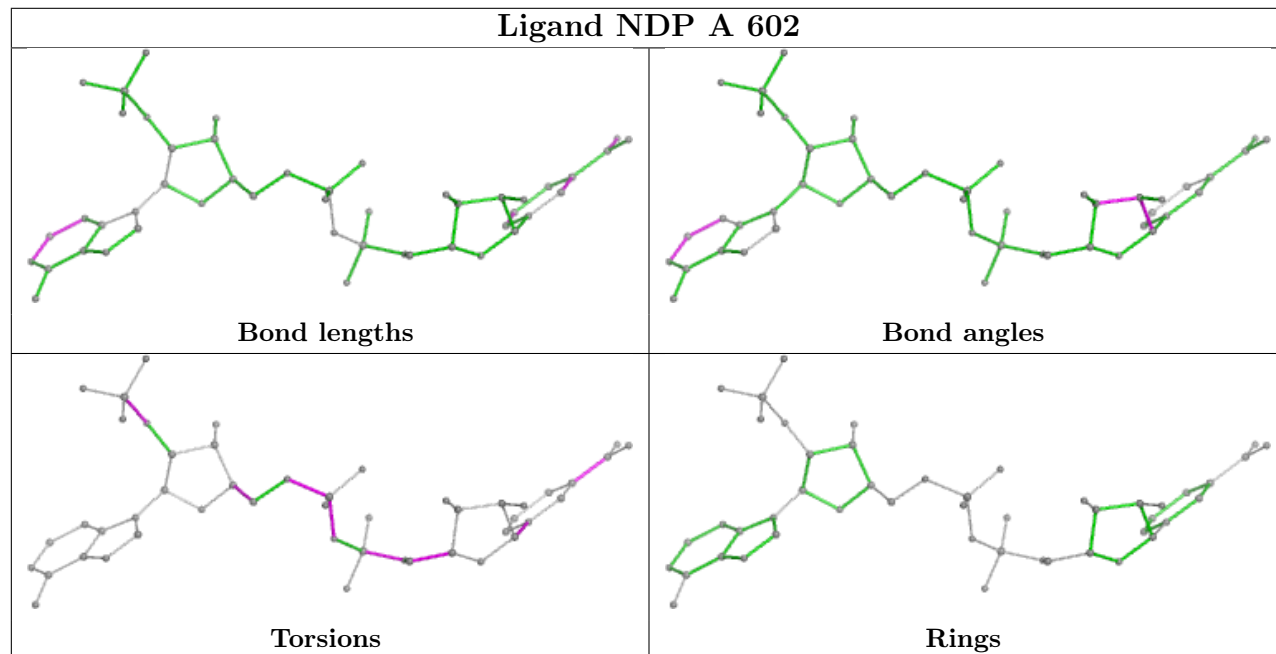
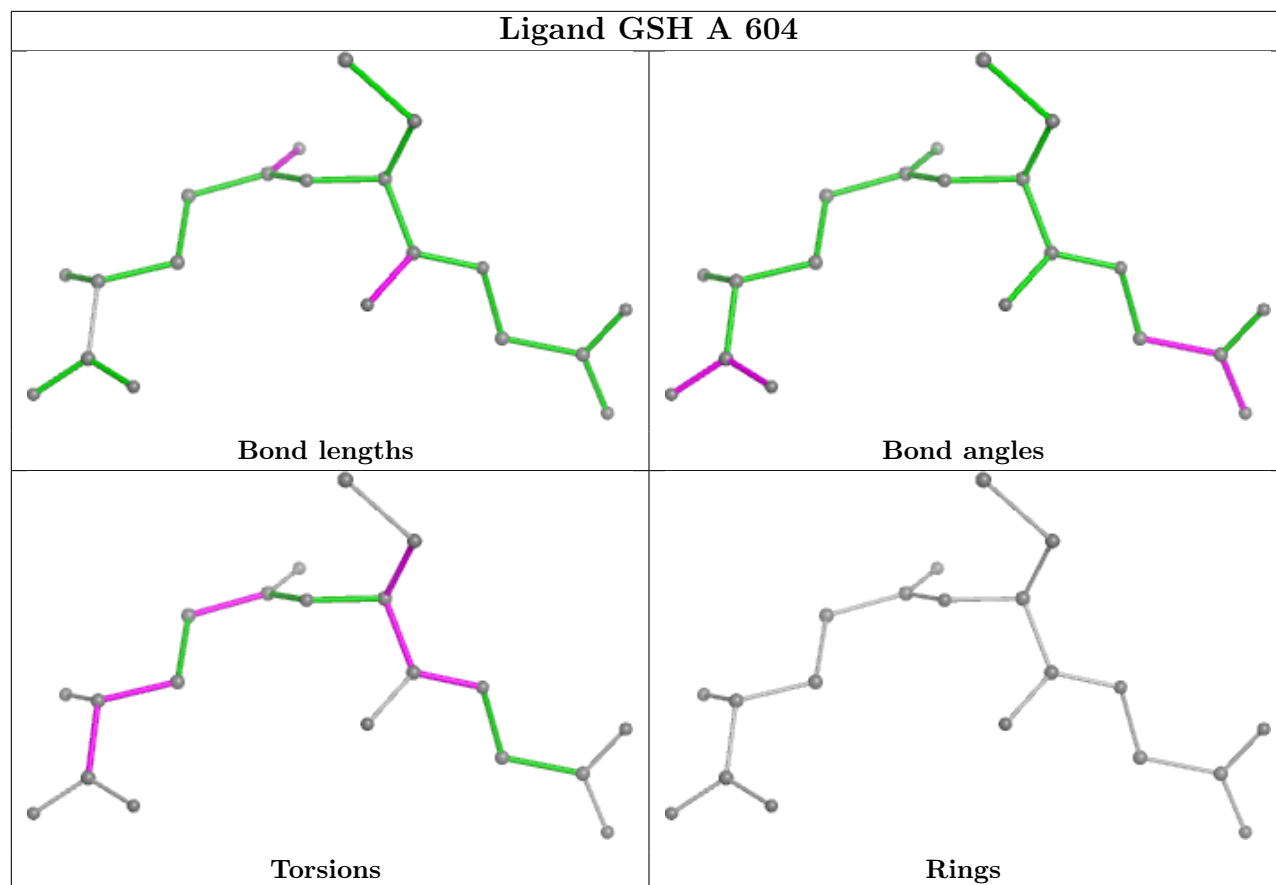
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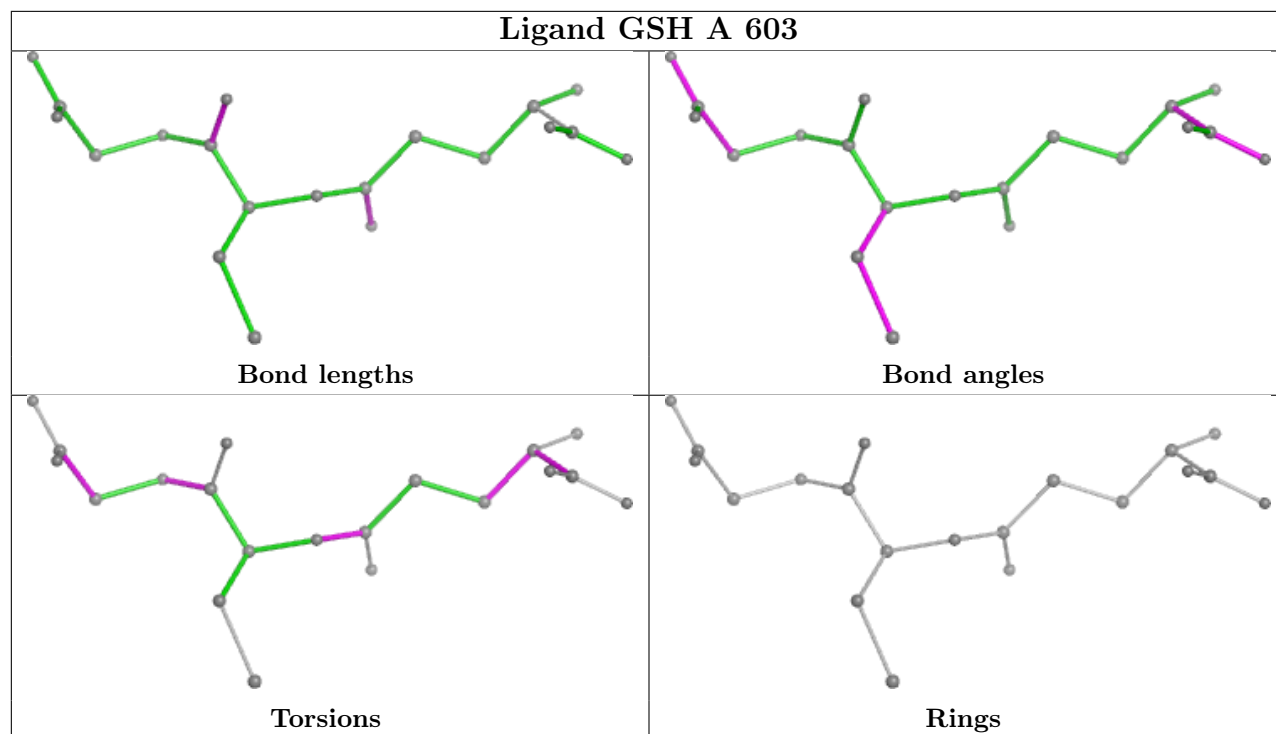
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	609	PEG	1	0
4	A	603	GSH	1	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	587/598 (98%)	-0.15	15 (2%) 57 58	19, 30, 54, 64	3 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	4.7
1	A	399	LYS	4.4
1	A	398	SER	4.3
1	A	592	ILE	3.8
1	A	397	LEU	3.8
1	A	402	CYS	3.1
1	A	400	VAL	2.7
1	A	6	GLY	2.6
1	A	591	PRO	2.5
1	A	241	LYS	2.5
1	A	403	GLU	2.4
1	A	375	THR	2.3
1	A	590	SER	2.3
1	A	285	PHE	2.2
1	A	360	THR	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

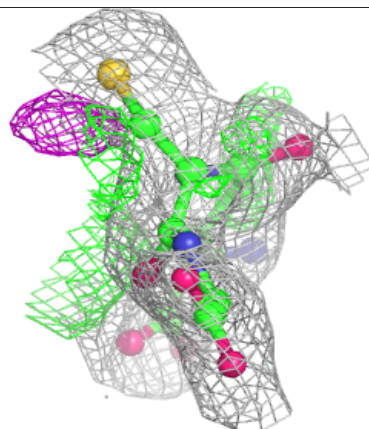
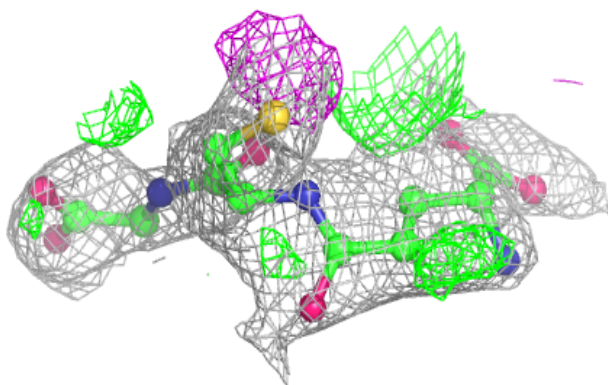
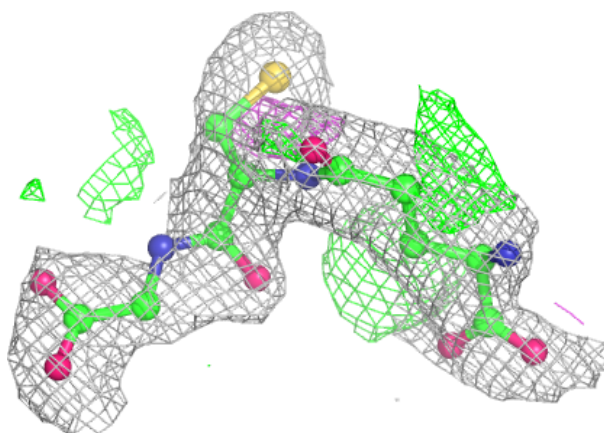
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GSH	A	604	20/20	0.73	0.19	64,68,72,72	0
4	GSH	A	603	20/20	0.84	0.14	56,58,62,62	0
6	PEG	A	608	7/7	0.85	0.18	45,47,50,51	0
7	PG4	A	612	13/13	0.85	0.18	62,64,71,71	0
6	PEG	A	610	7/7	0.87	0.13	48,49,51,51	0
6	PEG	A	607	7/7	0.87	0.15	57,58,60,62	0
7	PG4	A	614	13/13	0.87	0.15	53,54,56,57	0
3	NDP	A	602	48/48	0.88	0.14	29,43,57,57	48
6	PEG	A	606	7/7	0.88	0.16	40,41,45,45	0
6	PEG	A	609	7/7	0.88	0.14	29,33,35,36	0
7	PG4	A	615	13/13	0.88	0.16	56,60,66,66	0
5	CA	A	605	1/1	0.90	0.16	71,71,71,71	0
7	PG4	A	613	13/13	0.90	0.14	63,66,70,70	0
6	PEG	A	616	7/7	0.92	0.13	56,59,61,62	0
7	PG4	A	611	13/13	0.93	0.10	37,39,42,43	0
2	FAD	A	601	53/53	0.95	0.08	24,28,38,40	0

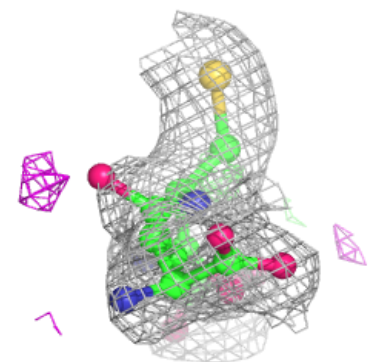
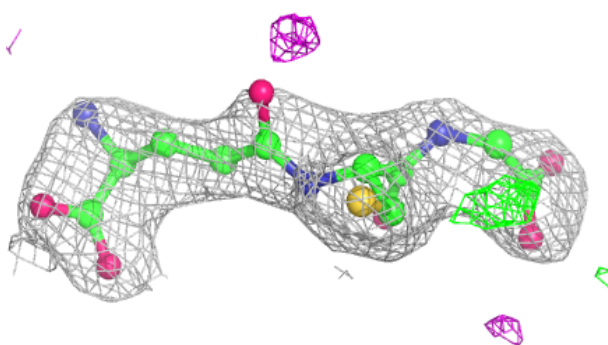
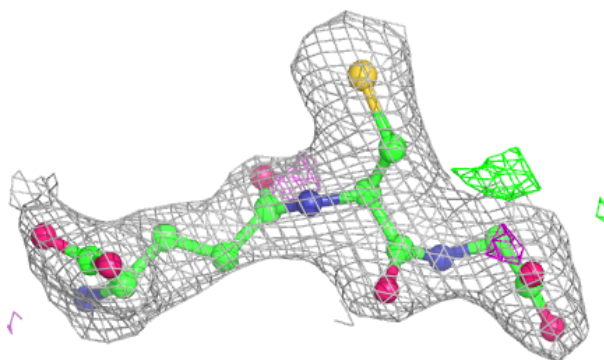
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around GSH A 604:**

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

**Electron density around GSH A 603:**

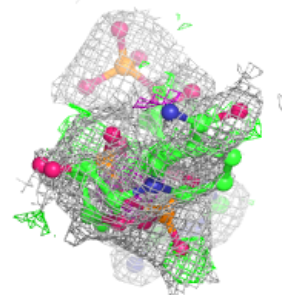
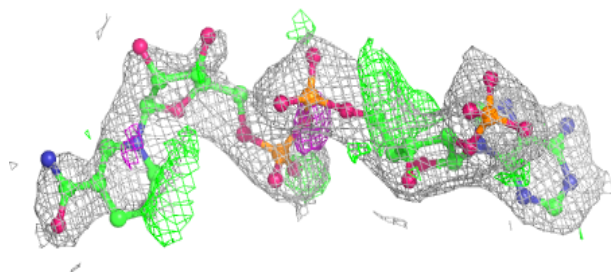
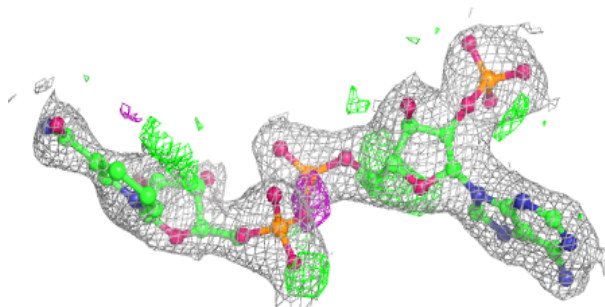
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



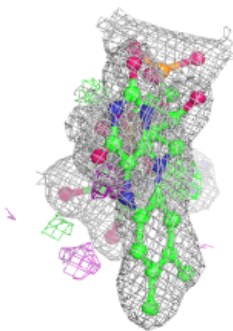
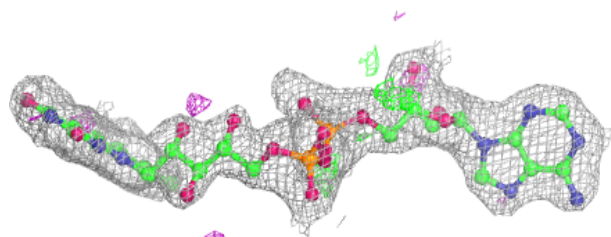
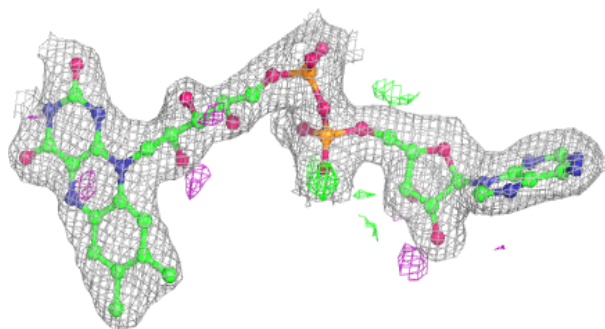


**Electron density around NDP A 602:**

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

**Electron density around FAD A 601:**

$2mF_o-DF_c$  (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.