



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:54 AM BST

PDB ID : 2HQM
Title : Crystal Structure of Glutathione Reductase Glr1 from the Yeast *Saccharomyces cerevisiae*
Authors : Yu, J.; Zhou, C.Z.
Deposited on : 2006-07-19
Resolution : 2.40 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 : 2.13.1
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) : 2.13.1

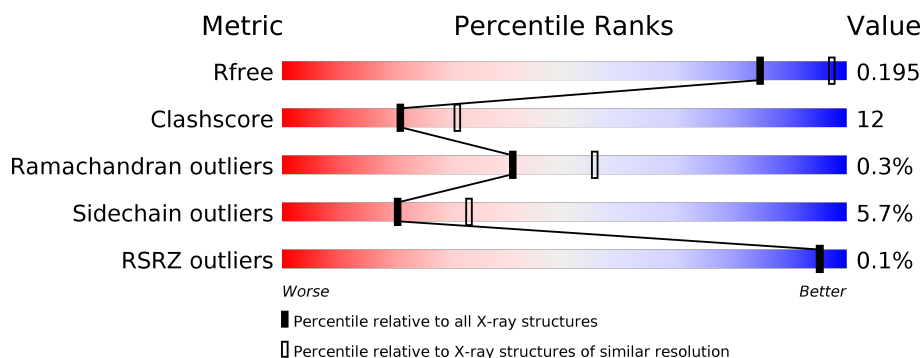
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	479	
1	B	479	

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
5	GSH	A	3001	-	-	X	-
5	GSH	B	4001	-	-	X	-
6	GOL	A	6001	-	X	X	-
6	GOL	A	6006	-	X	X	-
6	GOL	B	6003	-	X	-	-
6	GOL	B	6004	-	X	X	-
6	GOL	B	6007	-	X	X	-
6	GOL	B	6009	-	X	X	-
6	GOL	B	6010	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8152 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 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3588	2277	620	679	12			
1	B	461	Total	C	N	O	S	0	0	0
			3588	2277	620	679	12			

There are 24 discrepancies between the modelled and reference sequences:

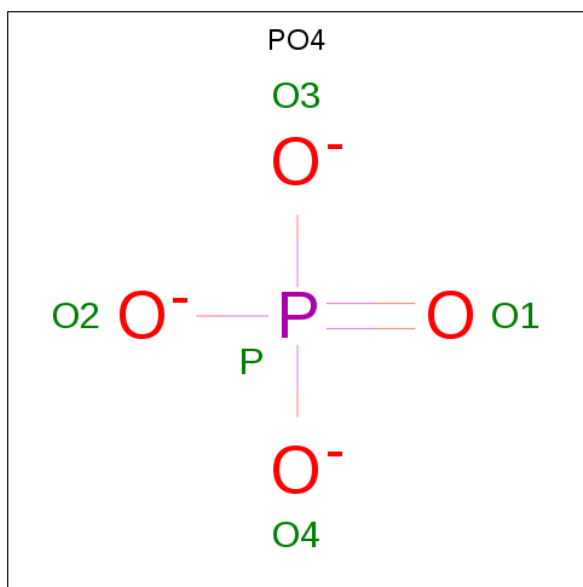
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	TYR	-	cloning artifact	UNP P41921
A	14	VAL	-	cloning artifact	UNP P41921
A	15	GLU	-	cloning artifact	UNP P41921
A	16	PHE	-	cloning artifact	UNP P41921
A	484	GLY	-	cloning artifact	UNP P41921
A	485	SER	-	cloning artifact	UNP P41921
A	486	HIS	-	cloning artifact	UNP P41921
A	487	HIS	-	cloning artifact	UNP P41921
A	488	HIS	-	cloning artifact	UNP P41921
A	489	HIS	-	cloning artifact	UNP P41921
A	490	HIS	-	cloning artifact	UNP P41921
A	491	HIS	-	cloning artifact	UNP P41921
B	13	TYR	-	cloning artifact	UNP P41921
B	14	VAL	-	cloning artifact	UNP P41921
B	15	GLU	-	cloning artifact	UNP P41921
B	16	PHE	-	cloning artifact	UNP P41921
B	484	GLY	-	cloning artifact	UNP P41921
B	485	SER	-	cloning artifact	UNP P41921
B	486	HIS	-	cloning artifact	UNP P41921
B	487	HIS	-	cloning artifact	UNP P41921
B	488	HIS	-	cloning artifact	UNP P41921
B	489	HIS	-	cloning artifact	UNP P41921
B	490	HIS	-	cloning artifact	UNP P41921
B	491	HIS	-	cloning artifact	UNP P41921

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



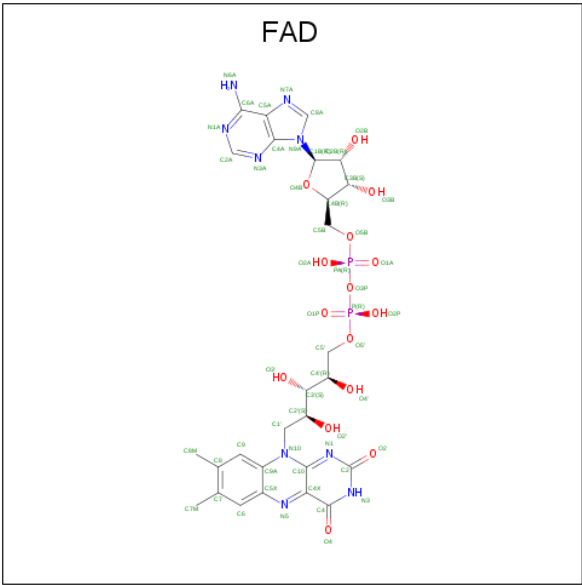
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



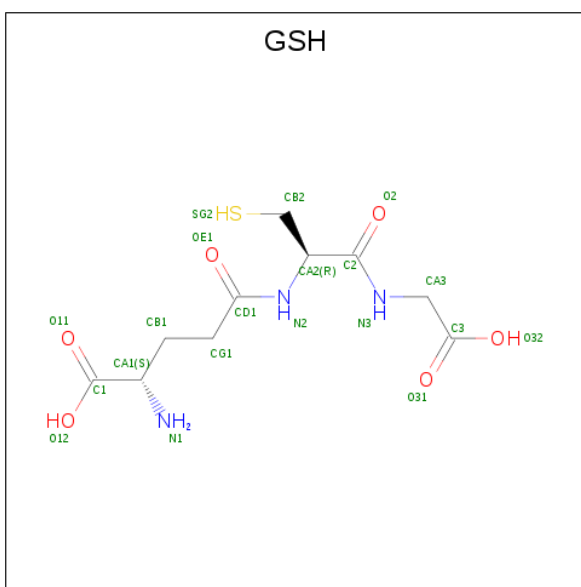
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



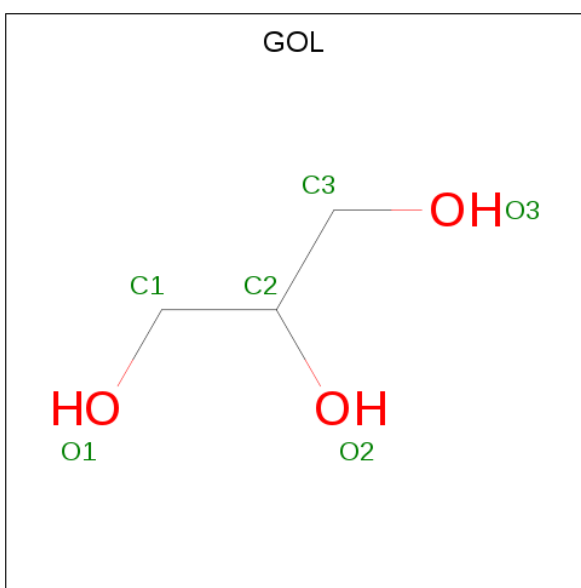
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

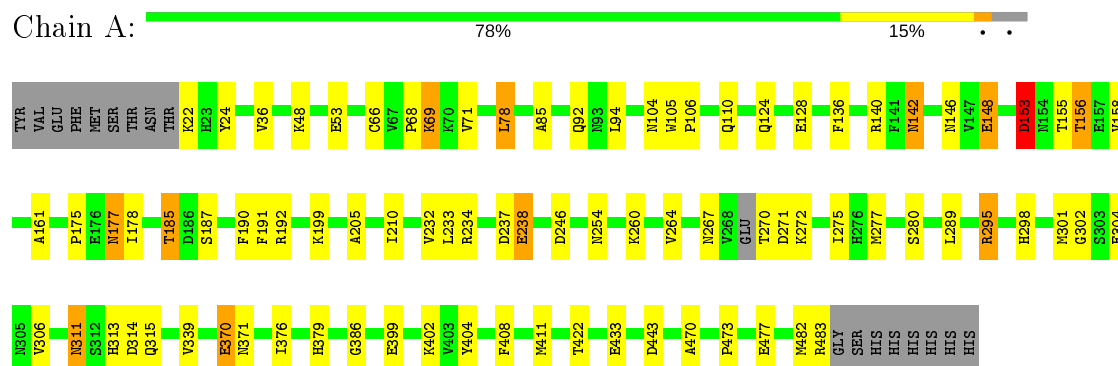
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	377	Total	O	0	0
			377	377		
7	B	349	Total	O	0	0
			349	349		

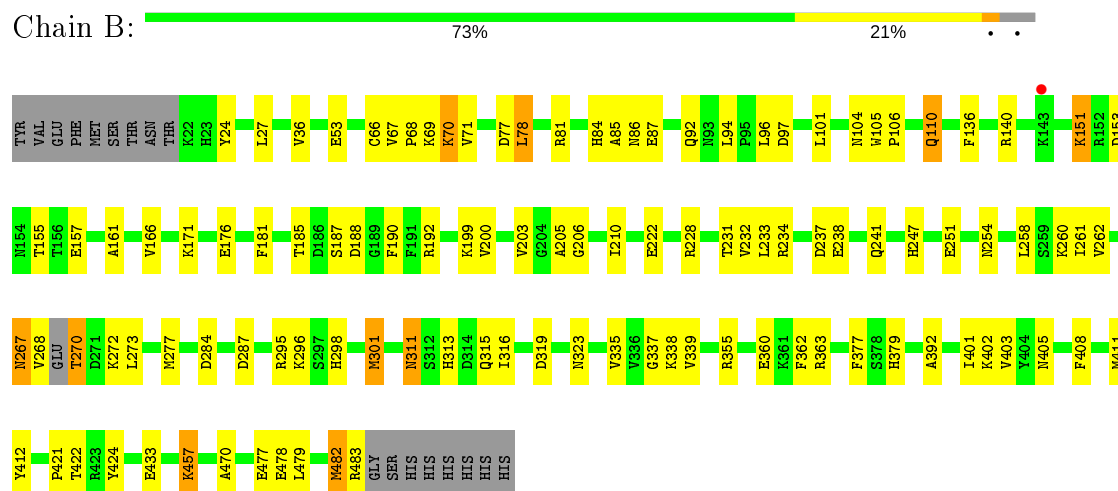
3 Residue-property plots [i](#)

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: Glutathione reductase



• Molecule 1: Glutathione reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	116.97Å 116.97Å 85.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.05 – 2.40 21.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (21.05-2.40) 92.9 (21.05-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.205 0.192 , 0.195	Depositor DCC
R_{free} test set	2118 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8152	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, NAG, FAD, 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	0.55	0/3658	0.75	5/4939 (0.1%)
1	B	0.57	2/3658 (0.1%)	0.74	3/4939 (0.1%)
All	All	0.56	2/7316 (0.0%)	0.74	8/9878 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	482	MET	C-N	5.33	1.46	1.34
1	B	87	GLU	CA-CB	-5.20	1.42	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	ASP	N-CA-C	-5.85	95.20	111.00
1	B	237	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	97	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	148	GLU	CA-CB-CG	5.40	125.27	113.40
1	A	271	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	237	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	87	GLU	CB-CG-CD	-5.18	100.21	114.20
1	A	295	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3588	0	3579	78	0
1	B	3588	0	3579	95	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	53	0	31	2	0
4	B	53	0	31	0	0
5	A	20	0	14	8	0
5	B	20	0	14	8	0
6	A	30	0	40	15	0
6	B	36	0	44	20	0
7	A	377	0	0	16	0
7	B	349	0	0	11	0
All	All	8152	0	7358	181	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 12.

All (181) 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)
6:B:6009:GOL:C2	6:B:6009:GOL:O2	1.63	1.46
6:A:6001:GOL:O2	6:A:6001:GOL:C2	1.64	1.43
6:A:6006:GOL:O2	6:A:6006:GOL:C2	1.67	1.40
6:B:6004:GOL:O2	6:B:6004:GOL:C2	1.73	1.37
1:B:110:GLN:HE21	1:B:110:GLN:HA	1.23	1.03
1:A:270:THR:HG22	1:A:272:LYS:H	1.32	0.93
1:A:205:ALA:HB3	7:A:6384:HOH:O	1.71	0.89
1:A:470:ALA:HB1	1:A:477:GLU:HG3	1.56	0.88
1:B:470:ALA:HB1	1:B:477:GLU:HG3	1.56	0.86
1:A:370:GLU:HG3	7:A:6323:HOH:O	1.75	0.84
1:A:104:ASN:HD22	1:B:92:GLN:HE22	1.26	0.84
6:B:6004:GOL:O2	6:B:6004:GOL:C1	2.26	0.83
1:A:473:PRO:HG2	1:B:70:LYS:HG3	1.61	0.82
1:A:36:VAL:HG12	3:A:5001:PO4:O3	1.81	0.80
6:B:6004:GOL:O2	6:B:6004:GOL:C3	2.31	0.79
1:B:337:GLY:C	6:B:6010:GOL:O1	2.21	0.79
1:B:238:GLU:HG3	5:B:4001:GSH:HA1	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:6001:GOL:O2	6:A:6001:GOL:C1	2.32	0.78
1:A:402:LYS:HD3	1:A:433:GLU:OE2	1.84	0.78
1:A:177:ASN:H	1:A:177:ASN:HD22	1.31	0.78
1:A:411:MET:CE	1:B:70:LYS:HB3	2.14	0.77
1:A:379:HIS:HD2	7:A:6234:HOH:O	1.68	0.75
1:A:142:ASN:C	1:A:142:ASN:HD22	1.91	0.73
1:A:238:GLU:CB	5:A:3001:GSH:HA1	2.19	0.73
6:A:6006:GOL:O2	6:A:6006:GOL:C1	2.37	0.72
1:B:36:VAL:HG12	3:B:5002:PO4:O2	1.90	0.72
6:A:6001:GOL:O2	6:A:6001:GOL:C3	2.37	0.72
1:A:411:MET:HE2	1:B:70:LYS:HB3	1.71	0.71
1:B:295:ARG:NE	7:B:6347:HOH:O	2.22	0.71
6:B:6009:GOL:C1	6:B:6009:GOL:O2	2.37	0.71
1:A:238:GLU:HB3	5:A:3001:GSH:HA1	1.72	0.71
6:A:6006:GOL:O2	6:A:6006:GOL:C3	2.37	0.71
1:B:110:GLN:HE21	1:B:110:GLN:CA	2.02	0.71
1:B:110:GLN:NE2	1:B:110:GLN:HA	2.01	0.70
1:A:148:GLU:HB3	1:A:158:VAL:HG22	1.72	0.70
1:A:92:GLN:HE22	1:B:104:ASN:HD22	1.39	0.69
1:A:311:ASN:ND2	1:A:315:GLN:H	1.91	0.69
1:A:175:PRO:HB2	1:A:178:ILE:HD12	1.74	0.68
1:A:233:LEU:HD13	1:A:376:ILE:HD13	1.76	0.67
1:A:275:ILE:HD11	1:A:289:LEU:HD22	1.77	0.67
1:B:238:GLU:CB	5:B:4001:GSH:HA1	2.25	0.67
1:B:238:GLU:CG	5:B:4001:GSH:HA1	2.25	0.66
1:B:360:GLU:O	1:B:363:ARG:HG3	1.95	0.66
5:A:3001:GSH:HB13	7:A:6247:HOH:O	1.96	0.66
1:B:205:ALA:HB3	7:B:6257:HOH:O	1.97	0.65
6:B:6009:GOL:C3	6:B:6009:GOL:O2	2.44	0.65
1:A:295:ARG:NH2	7:A:6380:HOH:O	2.30	0.64
1:B:268:VAL:HG12	1:B:268:VAL:O	1.97	0.64
1:A:155:THR:HG22	1:A:156:THR:N	2.11	0.64
1:B:479:LEU:HD23	1:B:482:MET:HE1	1.79	0.64
1:B:311:ASN:ND2	1:B:315:GLN:H	1.97	0.62
1:A:238:GLU:CG	5:A:3001:GSH:HA1	2.30	0.62
1:A:185:THR:HG22	7:A:6330:HOH:O	1.99	0.61
1:B:251:GLU:OE1	1:B:379:HIS:HD2	1.84	0.61
1:B:379:HIS:HB2	7:B:6205:HOH:O	2.01	0.60
1:A:178:ILE:HD11	6:A:6005:GOL:H11	1.84	0.59
1:B:402:LYS:HD3	1:B:433:GLU:OE1	2.03	0.59
6:B:6009:GOL:HO2	6:B:6009:GOL:C2	2.07	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:HE3	1:B:296:LYS:HE3	1.85	0.59
6:A:6001:GOL:HO2	6:A:6001:GOL:C2	2.08	0.58
1:A:192:ARG:NH2	6:A:6011:GOL:O3	2.36	0.58
1:B:151:LYS:HE3	1:B:157:GLU:HB2	1.84	0.58
1:B:228:ARG:HG2	6:B:6003:GOL:H12	1.84	0.58
1:A:443:ASP:CG	7:A:6293:HOH:O	2.42	0.57
1:B:295:ARG:NH2	7:B:6347:HOH:O	2.37	0.57
1:B:86:ASN:HD21	1:B:96:LEU:H	1.53	0.57
1:B:238:GLU:HB2	5:B:4001:GSH:HA1	1.87	0.57
6:A:6006:GOL:C2	6:A:6006:GOL:HO2	2.11	0.56
1:B:166:VAL:HG11	1:B:301:MET:CE	2.35	0.56
1:A:205:ALA:CB	6:A:6001:GOL:H2	2.36	0.56
1:B:254:ASN:HB3	7:B:6248:HOH:O	2.05	0.56
1:B:231:THR:HG21	1:B:241:GLN:OE1	2.06	0.56
1:A:205:ALA:HB3	6:A:6001:GOL:H2	1.88	0.55
1:B:205:ALA:HB3	6:B:6003:GOL:O2	2.06	0.55
1:B:166:VAL:HG11	1:B:301:MET:HE3	1.89	0.55
1:A:443:ASP:CB	7:A:6293:HOH:O	2.55	0.54
1:B:295:ARG:CZ	7:B:6347:HOH:O	2.56	0.54
1:B:408:PHE:CE1	1:B:478:GLU:HG3	2.42	0.54
1:A:254:ASN:HB3	7:A:6163:HOH:O	2.08	0.53
1:A:177:ASN:H	1:A:177:ASN:ND2	2.04	0.53
1:B:479:LEU:HD23	1:B:482:MET:CE	2.38	0.53
1:B:311:ASN:ND2	1:B:313:HIS:H	2.07	0.53
1:A:275:ILE:CD1	1:A:289:LEU:HD22	2.39	0.53
1:B:392:ALA:HB1	1:B:401:ILE:HD12	1.90	0.53
1:B:247:HIS:HA	6:B:6007:GOL:H32	1.91	0.53
1:A:311:ASN:HD21	1:A:315:GLN:H	1.54	0.53
1:B:338:LYS:N	6:B:6010:GOL:O1	2.42	0.53
1:B:192:ARG:NH2	6:B:6009:GOL:O1	2.42	0.52
1:A:411:MET:HE1	1:B:70:LYS:HB3	1.89	0.52
1:A:205:ALA:HB3	6:A:6001:GOL:C2	2.39	0.52
1:A:238:GLU:HG3	5:A:3001:GSH:HA1	1.91	0.52
1:A:379:HIS:CD2	7:A:6234:HOH:O	2.53	0.52
1:B:323:ASN:ND2	6:B:6002:GOL:O3	2.39	0.52
1:B:206:GLY:O	1:B:210:ILE:HD13	2.10	0.51
1:A:199:LYS:NZ	7:A:6314:HOH:O	2.24	0.51
1:B:228:ARG:CG	6:B:6003:GOL:H12	2.40	0.51
1:B:234:ARG:HG2	7:B:6257:HOH:O	2.10	0.51
1:A:71:VAL:HG23	1:B:411:MET:HE3	1.92	0.51
6:B:6004:GOL:H31	7:B:6106:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:HD21	1:A:146:ASN:H	1.58	0.50
1:B:267:ASN:ND2	1:B:268:VAL:H	2.08	0.50
1:A:192:ARG:NH1	7:A:6286:HOH:O	2.44	0.50
1:A:267:ASN:HB3	1:A:270:THR:HG21	1.94	0.50
1:B:238:GLU:HB2	5:B:4001:GSH:CA1	2.42	0.50
1:A:443:ASP:HB2	7:A:6293:HOH:O	2.12	0.50
1:B:405:ASN:ND2	5:B:4001:GSH:O2	2.44	0.50
1:B:24:TYR:O	1:B:161:ALA:HA	2.13	0.49
1:B:421:PRO:HG3	6:B:6007:GOL:H12	1.94	0.49
1:B:203:VAL:HG21	1:B:261:ILE:HD12	1.94	0.49
1:A:153:ASP:HB3	1:A:155:THR:OG1	2.13	0.48
1:A:238:GLU:HB3	5:A:3001:GSH:CB1	2.43	0.48
1:A:205:ALA:CB	7:A:6384:HOH:O	2.44	0.48
1:A:371:ASN:ND2	1:A:386:GLY:HA2	2.28	0.48
1:A:78:LEU:HD13	1:B:85:ALA:HA	1.95	0.48
1:A:142:ASN:C	1:A:142:ASN:ND2	2.65	0.48
1:B:77:ASP:O	1:B:81:ARG:HG3	2.13	0.48
1:B:424:TYR:HB3	1:B:482:MET:HE1	1.96	0.48
1:A:105:TRP:HB3	1:A:106:PRO:HD3	1.95	0.48
1:A:238:GLU:HB3	5:A:3001:GSH:CA1	2.44	0.47
1:B:153:ASP:OD2	1:B:155:THR:HG23	2.15	0.47
1:B:176:GLU:HG2	1:B:181:PHE:CZ	2.49	0.47
1:B:27:LEU:C	1:B:27:LEU:HD23	2.35	0.47
1:A:238:GLU:HB3	5:A:3001:GSH:HB12	1.96	0.47
1:A:205:ALA:HB1	1:A:232:VAL:HA	1.95	0.47
1:B:105:TRP:HB3	1:B:106:PRO:HD3	1.97	0.47
1:B:392:ALA:HB1	1:B:401:ILE:CD1	2.45	0.47
1:A:124:GLN:O	1:A:128:GLU:HG2	2.15	0.46
1:A:399:GLU:H	1:A:399:GLU:CD	2.19	0.46
1:A:71:VAL:CG2	1:B:411:MET:HE3	2.45	0.46
1:A:246:ASP:OD2	7:A:6108:HOH:O	2.21	0.45
1:A:411:MET:HE3	1:B:71:VAL:HG23	1.97	0.45
1:A:311:ASN:HD22	1:A:311:ASN:C	2.19	0.45
1:A:311:ASN:ND2	1:A:313:HIS:H	2.14	0.45
1:B:166:VAL:CG1	1:B:301:MET:HE3	2.46	0.45
6:B:6007:GOL:O2	7:B:6120:HOH:O	2.21	0.45
1:B:228:ARG:O	1:B:258:LEU:HA	2.16	0.45
5:B:4001:GSH:HG12	7:B:6252:HOH:O	2.16	0.45
1:B:153:ASP:OD2	1:B:153:ASP:C	2.55	0.45
1:B:270:THR:HG22	1:B:272:LYS:H	1.81	0.45
1:B:234:ARG:HG3	1:B:234:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:HA	1:B:78:LEU:HD13	1.98	0.44
1:B:110:GLN:NE2	1:B:110:GLN:CA	2.69	0.44
1:B:311:ASN:C	1:B:311:ASN:HD22	2.20	0.44
1:B:311:ASN:HD21	1:B:315:GLN:H	1.66	0.44
1:B:238:GLU:HB2	5:B:4001:GSH:CB1	2.48	0.44
1:B:53:GLU:O	1:B:136:PHE:HA	2.18	0.43
1:B:408:PHE:CZ	1:B:422:THR:HG21	2.53	0.43
1:A:404:TYR:HD1	1:A:483:ARG:HB3	1.83	0.43
1:B:272:LYS:HE2	1:B:287:ASP:OD1	2.17	0.43
1:B:268:VAL:CG1	1:B:268:VAL:O	2.64	0.43
1:B:319:ASP:OD2	1:B:323:ASN:HB2	2.18	0.43
1:B:84:HIS:HD2	1:B:412:TYR:OH	2.02	0.43
1:B:171:LYS:CE	1:B:296:LYS:HE3	2.48	0.43
1:A:408:PHE:CZ	1:A:422:THR:HG21	2.53	0.42
1:B:233:LEU:HA	7:B:6063:HOH:O	2.18	0.42
1:A:24:TYR:O	1:A:161:ALA:HA	2.19	0.42
1:A:264:VAL:HG22	1:A:275:ILE:HD13	2.00	0.42
1:B:70:LYS:HE3	1:B:377:PHE:CZ	2.55	0.42
1:B:457:LYS:HD2	1:B:457:LYS:HA	1.84	0.42
1:A:140:ARG:HG3	1:A:302:GLY:N	2.33	0.42
1:A:199:LYS:CE	7:A:6314:HOH:O	2.68	0.42
1:B:403:VAL:O	1:B:483:ARG:CZ	2.68	0.42
1:A:68:PRO:HB2	1:A:191:PHE:CE1	2.54	0.42
1:A:260:LYS:HA	6:A:6005:GOL:O3	2.20	0.42
1:A:53:GLU:O	1:A:136:PHE:HA	2.20	0.41
1:B:188:ASP:HB2	6:B:6009:GOL:H2	2.01	0.41
1:A:234:ARG:NH2	6:A:6001:GOL:O1	2.48	0.41
1:B:187:SER:O	1:B:190:PHE:HB3	2.21	0.41
1:B:355:ARG:HA	1:B:362:PHE:O	2.21	0.41
1:A:187:SER:O	1:A:190:PHE:HB3	2.21	0.41
1:A:24:TYR:CD2	1:A:48:LYS:HG2	2.56	0.41
4:A:1001:FAD:H1'1	4:A:1001:FAD:H9	1.85	0.41
1:B:232:VAL:O	1:B:241:GLN:HG2	2.21	0.41
1:B:247:HIS:CA	6:B:6007:GOL:H32	2.50	0.41
1:B:199:LYS:HE3	1:B:222:GLU:OE2	2.21	0.40
1:B:316:ILE:HD12	1:B:335:VAL:CG2	2.52	0.40
1:B:67:VAL:HB	1:B:68:PRO:CD	2.51	0.40
1:A:233:LEU:CD1	1:A:376:ILE:HD13	2.50	0.40
1:A:69:LYS:NZ	4:A:1001:FAD:N5	2.69	0.40
1:A:411:MET:HE1	1:B:70:LYS:CB	2.52	0.40
1:B:231:THR:CG2	1:B:241:GLN:OE1	2.69	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	457/479 (95%)	438 (96%)	17 (4%)	2 (0%)	34	48
1	B	457/479 (95%)	438 (96%)	18 (4%)	1 (0%)	47	62
All	All	914/958 (95%)	876 (96%)	35 (4%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	THR
1	A	339	VAL
1	B	339	VAL

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	386/403 (96%)	364 (94%)	22 (6%)	20	33
1	B	386/403 (96%)	364 (94%)	22 (6%)	20	33
All	All	772/806 (96%)	728 (94%)	44 (6%)	20	33

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	66	CYS
1	A	69	LYS
1	A	78	LEU
1	A	94	LEU
1	A	110	GLN
1	A	142	ASN
1	A	153	ASP
1	A	177	ASN
1	A	185	THR
1	A	210	ILE
1	A	238	GLU
1	A	277	MET
1	A	280	SER
1	A	298	HIS
1	A	301	MET
1	A	304	GLU
1	A	306	VAL
1	A	311	ASN
1	A	314	ASP
1	A	370	GLU
1	A	482	MET
1	B	66	CYS
1	B	69	LYS
1	B	70	LYS
1	B	78	LEU
1	B	94	LEU
1	B	101	LEU
1	B	110	GLN
1	B	140	ARG
1	B	151	LYS
1	B	185	THR
1	B	200	VAL
1	B	260	LYS
1	B	262	VAL
1	B	267	ASN
1	B	270	THR
1	B	273	LEU
1	B	277	MET
1	B	284	ASP
1	B	298	HIS
1	B	301	MET
1	B	311	ASN

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Mol	Chain	Res	Type
1	B	457	LYS

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

Mol	Chain	Res	Type
1	A	92	GLN
1	A	93	ASN
1	A	117	HIS
1	A	126	ASN
1	A	142	ASN
1	A	146	ASN
1	A	177	ASN
1	A	242	ASN
1	A	276	HIS
1	A	298	HIS
1	A	311	ASN
1	A	323	ASN
1	A	371	ASN
1	A	432	ASN
1	B	84	HIS
1	B	86	ASN
1	B	92	GLN
1	B	110	GLN
1	B	267	ASN
1	B	298	HIS
1	B	311	ASN
1	B	371	ASN
1	B	405	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 ligands are modelled in this entry.

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	GOL	A	6005	-	5,5,5	0.35	0	5,5,5	1.02	0
6	GOL	B	6007	-	5,5,5	2.02	2 (40%)	5,5,5	3.29	3 (60%)
3	PO4	B	5002	-	4,4,4	1.47	1 (25%)	6,6,6	0.58	0
5	GSH	A	3001	1	12,19,19	1.29	2 (16%)	15,24,24	2.01	5 (33%)
6	GOL	B	6004	-	5,5,5	4.78	4 (80%)	5,5,5	3.95	4 (80%)
6	GOL	B	6003	-	5,5,5	4.92	4 (80%)	5,5,5	5.59	5 (100%)
6	GOL	B	6002	-	5,5,5	1.00	1 (20%)	5,5,5	1.21	1 (20%)
6	GOL	A	6011	-	5,5,5	1.73	1 (20%)	5,5,5	1.87	1 (20%)
4	FAD	A	1001	-	51,58,58	1.53	4 (7%)	60,89,89	1.58	9 (15%)
6	GOL	B	6009	-	5,5,5	3.57	3 (60%)	5,5,5	3.24	5 (100%)
2	NAG	A	1301	1	14,14,15	0.57	0	17,19,21	0.68	0
2	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	0.85	1 (5%)
4	FAD	B	2001	-	51,58,58	1.53	4 (7%)	60,89,89	1.53	8 (13%)
5	GSH	B	4001	1	12,19,19	1.62	3 (25%)	15,24,24	2.42	5 (33%)
6	GOL	B	6010	-	5,5,5	2.37	1 (20%)	5,5,5	2.74	4 (80%)
6	GOL	A	6008	-	5,5,5	1.31	1 (20%)	5,5,5	1.77	2 (40%)
6	GOL	A	6006	-	5,5,5	4.44	3 (60%)	5,5,5	4.09	5 (100%)
3	PO4	A	5001	-	4,4,4	1.39	1 (25%)	6,6,6	0.45	0
6	GOL	A	6001	-	5,5,5	3.58	3 (60%)	5,5,5	4.01	5 (100%)

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	GOL	A	6005	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	6007	-	-	4/4/4/4	-
6	GOL	A	6001	-	-	3/4/4/4	-
5	GSH	A	3001	1	-	3/18/24/24	-
6	GOL	B	6004	-	-	2/4/4/4	-
6	GOL	B	6003	-	-	2/4/4/4	-
6	GOL	A	6011	-	-	3/4/4/4	-
4	FAD	A	1001	-	-	4/30/50/50	0/6/6/6
6	GOL	B	6009	-	-	4/4/4/4	-
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	FAD	B	2001	-	-	4/30/50/50	0/6/6/6
5	GSH	B	4001	1	-	2/18/24/24	-
6	GOL	B	6010	-	-	4/4/4/4	-
6	GOL	A	6008	-	-	2/4/4/4	-
6	GOL	A	6006	-	-	4/4/4/4	-
6	GOL	B	6002	-	-	2/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6004	GOL	O2-C2	10.00	1.73	1.43
6	B	6003	GOL	O2-C2	-8.86	1.17	1.43
6	A	6006	GOL	O2-C2	8.11	1.67	1.43
6	A	6001	GOL	O2-C2	7.04	1.64	1.43
6	B	6009	GOL	O2-C2	6.76	1.63	1.43
4	B	2001	FAD	C10-N1	5.77	1.40	1.33
4	A	1001	FAD	C10-N1	5.76	1.40	1.33
4	A	1001	FAD	C4X-N5	4.83	1.40	1.33
6	B	6010	GOL	O2-C2	4.78	1.57	1.43
4	B	2001	FAD	C4X-N5	4.68	1.40	1.33
6	B	6003	GOL	O3-C3	4.56	1.61	1.42
4	B	2001	FAD	C4-N3	4.18	1.40	1.33
4	A	1001	FAD	C4-N3	4.13	1.40	1.33
6	B	6003	GOL	O1-C1	3.82	1.58	1.42
6	A	6006	GOL	O1-C1	3.68	1.57	1.42
6	A	6006	GOL	O3-C3	3.66	1.57	1.42
6	A	6011	GOL	O2-C2	3.55	1.54	1.43
5	B	4001	GSH	CA1-N1	-3.47	1.39	1.47
6	B	6007	GOL	O2-C2	-3.31	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	FAD	C5X-N5	3.09	1.40	1.35
4	A	1001	FAD	C5X-N5	2.97	1.40	1.35
6	A	6001	GOL	O1-C1	2.86	1.54	1.42
6	B	6009	GOL	O3-C3	2.79	1.54	1.42
6	A	6008	GOL	O2-C2	2.74	1.51	1.43
6	B	6009	GOL	O1-C1	2.62	1.53	1.42
6	B	6007	GOL	O1-C1	-2.53	1.31	1.42
3	B	5002	PO4	P-O2	-2.52	1.47	1.54
5	A	3001	GSH	O2-C2	2.50	1.28	1.23
5	B	4001	GSH	OE1-CD1	2.48	1.28	1.23
6	A	6001	GOL	O3-C3	2.46	1.52	1.42
5	B	4001	GSH	O2-C2	2.36	1.28	1.23
6	B	6004	GOL	O1-C1	2.29	1.52	1.42
6	B	6004	GOL	C1-C2	2.21	1.60	1.51
5	A	3001	GSH	OE1-CD1	2.17	1.27	1.23
6	B	6003	GOL	C3-C2	2.08	1.60	1.51
6	B	6004	GOL	C3-C2	2.05	1.60	1.51
3	A	5001	PO4	P-O3	-2.05	1.48	1.54
6	B	6002	GOL	O2-C2	2.01	1.49	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6003	GOL	O2-C2-C1	6.36	137.15	109.12
4	B	2001	FAD	C4-N3-C2	6.36	120.51	115.14
4	A	1001	FAD	C4-N3-C2	6.20	120.38	115.14
6	B	6007	GOL	C3-C2-C1	-6.05	88.18	111.70
6	B	6003	GOL	C3-C2-C1	-5.96	88.54	111.70
6	B	6003	GOL	O2-C2-C3	5.65	134.01	109.12
6	A	6006	GOL	C3-C2-C1	-5.42	90.62	111.70
6	B	6004	GOL	O2-C2-C1	-5.37	85.47	109.12
5	A	3001	GSH	CA3-N3-C2	-5.16	114.91	122.34
6	B	6003	GOL	O3-C3-C2	-4.92	86.60	110.20
5	B	4001	GSH	CG1-CD1-N2	4.92	124.36	115.83
6	B	6003	GOL	O1-C1-C2	-4.91	86.67	110.20
6	B	6004	GOL	O2-C2-C3	-4.83	87.85	109.12
6	A	6001	GOL	C3-C2-C1	-4.83	92.94	111.70
6	A	6001	GOL	O1-C1-C2	-4.65	87.90	110.20
4	A	1001	FAD	N3A-C2A-N1A	-4.63	121.45	128.68
5	B	4001	GSH	CA3-N3-C2	-4.48	115.89	122.34
5	B	4001	GSH	OE1-CD1-CG1	-4.48	113.82	122.02
4	B	2001	FAD	N3A-C2A-N1A	-4.40	121.80	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6009	GOL	C3-C2-C1	-4.32	94.92	111.70
6	B	6004	GOL	C3-C2-C1	-4.31	94.96	111.70
6	A	6006	GOL	O1-C1-C2	-3.96	91.20	110.20
6	A	6001	GOL	O3-C3-C2	-3.95	91.25	110.20
4	A	1001	FAD	O4B-C1B-C2B	-3.81	101.35	106.93
6	A	6006	GOL	O3-C3-C2	-3.66	92.65	110.20
6	A	6006	GOL	O2-C2-C1	-3.65	93.05	109.12
6	B	6009	GOL	O1-C1-C2	-3.58	93.05	110.20
6	B	6010	GOL	C3-C2-C1	-3.56	97.87	111.70
5	A	3001	GSH	CA2-CB2-SG2	-3.52	110.24	114.19
4	A	1001	FAD	C4X-N5-C5X	3.52	120.29	116.77
6	A	6011	GOL	C3-C2-C1	-3.49	98.15	111.70
6	A	6001	GOL	O2-C2-C1	-3.47	93.83	109.12
6	A	6006	GOL	O2-C2-C3	-3.41	94.10	109.12
6	B	6010	GOL	O1-C1-C2	-3.11	95.29	110.20
6	B	6009	GOL	O2-C2-C1	-2.95	96.11	109.12
4	B	2001	FAD	O4B-C1B-C2B	-2.95	102.61	106.93
6	A	6008	GOL	C3-C2-C1	-2.94	100.27	111.70
4	B	2001	FAD	C1'-N10-C9A	2.94	120.61	118.29
4	B	2001	FAD	C4X-N5-C5X	2.92	119.69	116.77
4	B	2001	FAD	C4X-C4-N3	-2.88	119.50	123.43
6	A	6001	GOL	O2-C2-C3	-2.79	96.84	109.12
6	B	6007	GOL	O2-C2-C1	2.77	121.33	109.12
4	B	2001	FAD	C10-C4X-N5	-2.77	119.34	121.26
5	B	4001	GSH	CA2-CB2-SG2	-2.77	111.08	114.19
6	B	6007	GOL	O2-C2-C3	2.76	121.30	109.12
6	B	6009	GOL	O3-C3-C2	-2.72	97.14	110.20
6	B	6004	GOL	O1-C1-C2	-2.68	97.35	110.20
4	A	1001	FAD	C4X-C4-N3	-2.59	119.90	123.43
4	A	1001	FAD	C10-C4X-N5	-2.54	119.50	121.26
4	A	1001	FAD	C1'-N10-C9A	2.51	120.27	118.29
6	B	6010	GOL	O2-C2-C1	-2.51	98.08	109.12
4	A	1001	FAD	P-O3P-PA	-2.47	124.35	132.83
5	B	4001	GSH	CB2-CA2-C2	-2.37	104.88	109.76
4	B	2001	FAD	P-O3P-PA	-2.30	124.93	132.83
5	A	3001	GSH	C3-CA3-N3	-2.28	106.03	110.43
6	B	6009	GOL	O2-C2-C3	-2.25	99.22	109.12
6	B	6010	GOL	O3-C3-C2	-2.24	99.44	110.20
5	A	3001	GSH	CG1-CD1-N2	2.19	119.63	115.83
6	A	6008	GOL	O2-C2-C1	-2.15	99.65	109.12
2	B	1303	NAG	C8-C7-N2	2.12	119.68	116.10
4	A	1001	FAD	C5X-C9A-N10	2.07	119.22	117.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6002	GOL	C3-C2-C1	-2.05	103.75	111.70
5	A	3001	GSH	OE1-CD1-CG1	-2.00	118.36	122.02

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	6007	GOL	O1-C1-C2-C3
5	A	3001	GSH	N1-CA1-CB1-CG1
5	A	3001	GSH	C1-CA1-CB1-CG1
6	B	6003	GOL	C1-C2-C3-O3
6	B	6002	GOL	O1-C1-C2-O2
6	B	6002	GOL	O1-C1-C2-C3
6	A	6011	GOL	O1-C1-C2-C3
6	A	6008	GOL	C1-C2-C3-O3
6	B	6009	GOL	O1-C1-C2-C3
6	B	6009	GOL	C1-C2-C3-O3
2	B	1303	NAG	C8-C7-N2-C2
6	B	6010	GOL	O1-C1-C2-C3
6	B	6010	GOL	C1-C2-C3-O3
6	B	6010	GOL	O2-C2-C3-O3
6	A	6006	GOL	O1-C1-C2-C3
6	A	6006	GOL	C1-C2-C3-O3
6	A	6001	GOL	C1-C2-C3-O3
2	B	1303	NAG	O7-C7-N2-C2
6	B	6009	GOL	O1-C1-C2-O2
6	B	6007	GOL	C1-C2-C3-O3
6	B	6003	GOL	O1-C1-C2-C3
6	A	6001	GOL	O1-C1-C2-C3
6	B	6007	GOL	O1-C1-C2-O2
6	A	6011	GOL	O1-C1-C2-O2
6	A	6008	GOL	O2-C2-C3-O3
6	B	6009	GOL	O2-C2-C3-O3
6	B	6010	GOL	O1-C1-C2-O2
6	A	6001	GOL	O2-C2-C3-O3
6	B	6007	GOL	O2-C2-C3-O3
6	A	6006	GOL	O1-C1-C2-O2
4	A	1001	FAD	PA-O3P-P-O5'
4	B	2001	FAD	PA-O3P-P-O5'
4	A	1001	FAD	P-O3P-PA-O1A
4	B	2001	FAD	P-O3P-PA-O1A
5	A	3001	GSH	C2-CA2-CB2-SG2

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Mol	Chain	Res	Type	Atoms
5	B	4001	GSH	C2-CA2-CB2-SG2
6	A	6006	GOL	O2-C2-C3-O3
6	B	6004	GOL	O1-C1-C2-O2
4	A	1001	FAD	P-O3P-PA-O2A
4	B	2001	FAD	P-O3P-PA-O2A
4	A	1001	FAD	O4B-C4B-C5B-O5B
4	B	2001	FAD	O4B-C4B-C5B-O5B
5	B	4001	GSH	N1-CA1-CB1-CG1
6	B	6004	GOL	O2-C2-C3-O3
6	A	6011	GOL	O2-C2-C3-O3

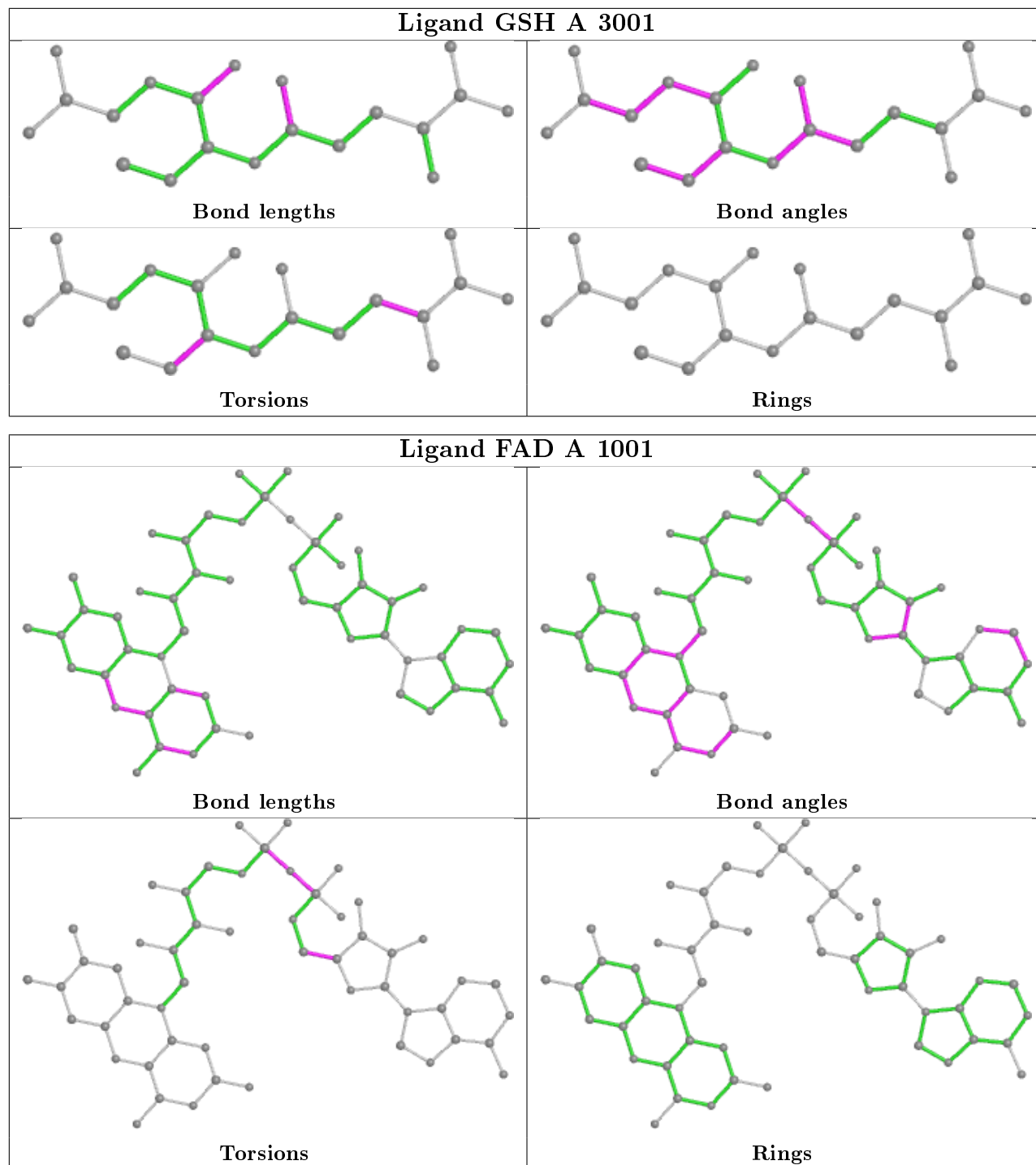
There are no ring outliers.

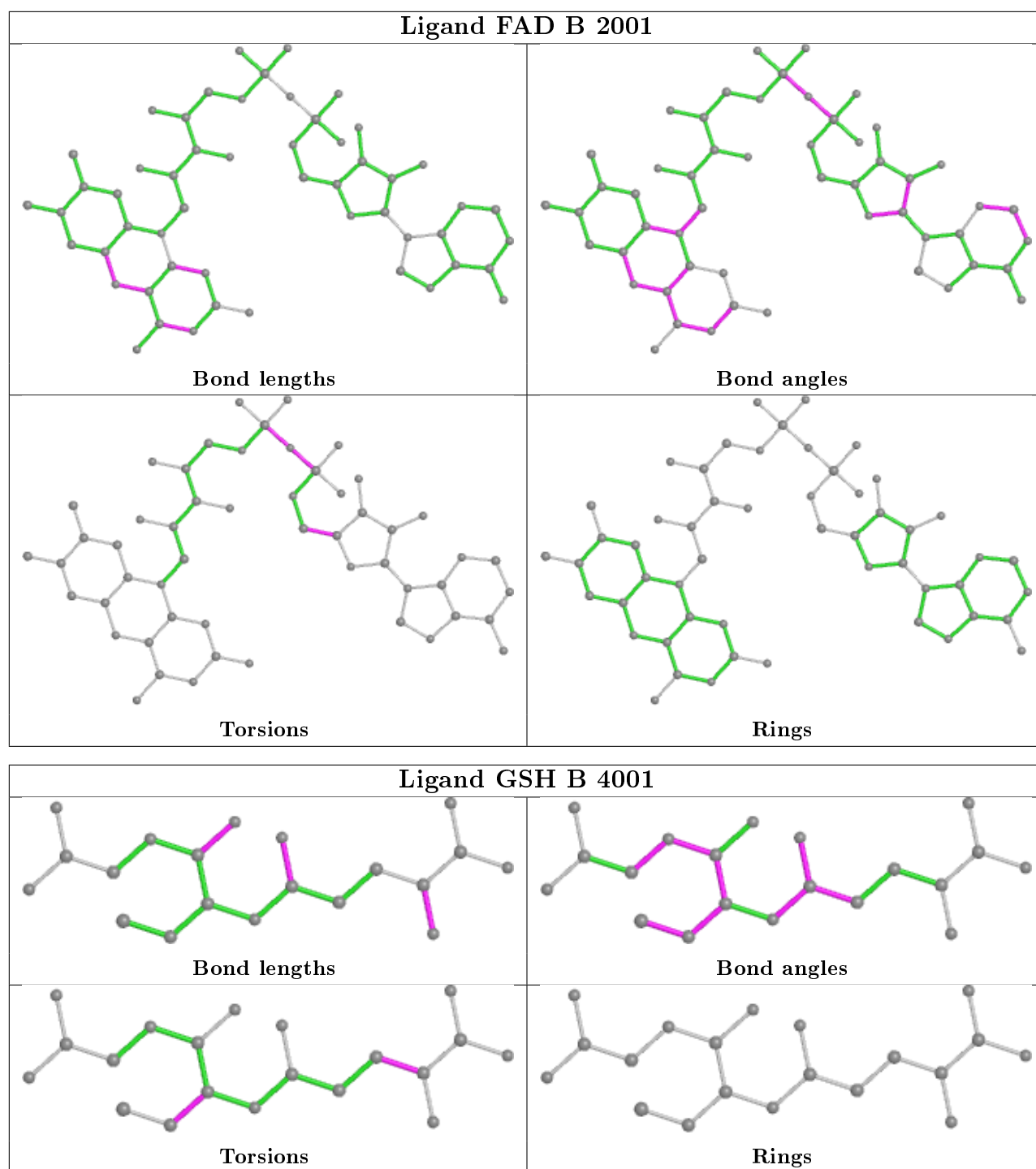
15 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6005	GOL	2	0
6	B	6007	GOL	4	0
3	B	5002	PO4	1	0
5	A	3001	GSH	8	0
6	B	6004	GOL	4	0
6	B	6003	GOL	3	0
6	B	6002	GOL	1	0
6	A	6011	GOL	1	0
4	A	1001	FAD	2	0
6	B	6009	GOL	6	0
5	B	4001	GSH	8	0
6	B	6010	GOL	2	0
6	A	6006	GOL	4	0
3	A	5001	PO4	1	0
6	A	6001	GOL	8	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	461/479 (96%)	-0.80	0	100	100	12, 22, 48, 73	0
1	B	461/479 (96%)	-0.78	1 (0%)	95	94	13, 22, 47, 68	0
All	All	922/958 (96%)	-0.79	1 (0%)	95	95	12, 22, 48, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	LYS	2.3

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
5	GSH	A	3001	20/20	0.82	0.33	27,43,54,54	20
6	GOL	A	6001	6/6	0.82	0.31	33,36,39,42	6
6	GOL	A	6008	6/6	0.83	0.25	41,46,47,49	6
6	GOL	B	6003	6/6	0.85	0.39	28,30,33,35	6

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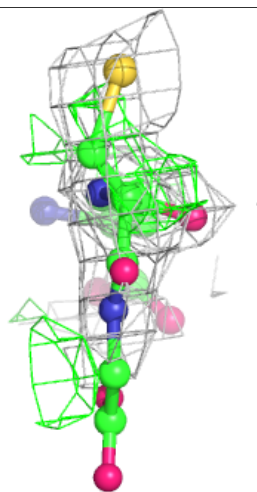
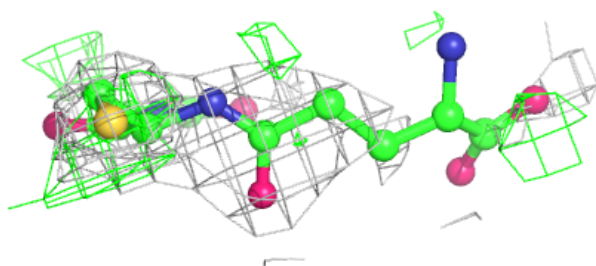
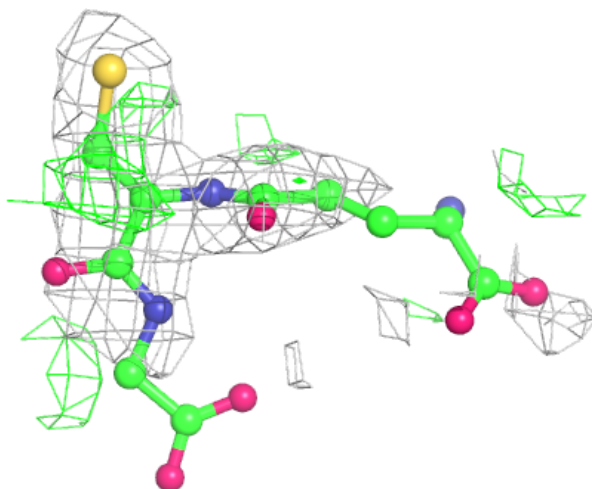
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	6002	6/6	0.85	0.23	39,43,44,45	6
5	GSH	B	4001	20/20	0.86	0.32	23,40,49,49	20
6	GOL	B	6010	6/6	0.87	0.29	46,47,48,48	6
6	GOL	A	6006	6/6	0.89	0.23	38,38,39,41	6
6	GOL	A	6011	6/6	0.90	0.19	39,41,42,44	6
6	GOL	A	6005	6/6	0.92	0.24	32,33,33,34	6
6	GOL	B	6009	6/6	0.92	0.17	40,42,43,43	6
6	GOL	B	6007	6/6	0.92	0.17	29,30,32,33	6
6	GOL	B	6004	6/6	0.93	0.17	25,30,31,35	6
2	NAG	B	1303	14/15	0.94	0.14	31,35,38,40	0
2	NAG	A	1301	14/15	0.95	0.13	30,33,36,36	0
3	PO4	A	5001	5/5	0.95	0.15	41,42,43,44	5
3	PO4	B	5002	5/5	0.96	0.17	40,40,41,41	5
4	FAD	B	2001	53/53	0.98	0.09	12,16,22,24	0
4	FAD	A	1001	53/53	0.98	0.09	10,17,24,26	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.

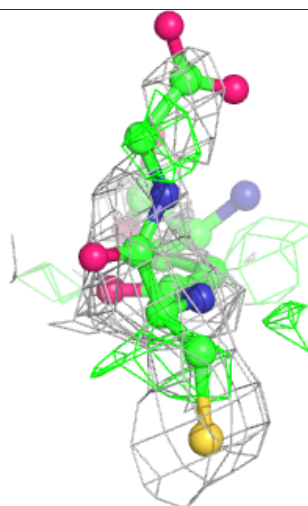
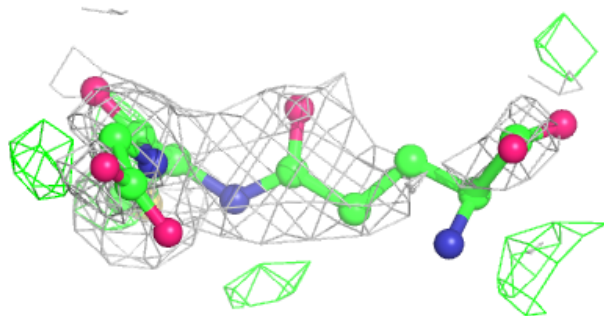
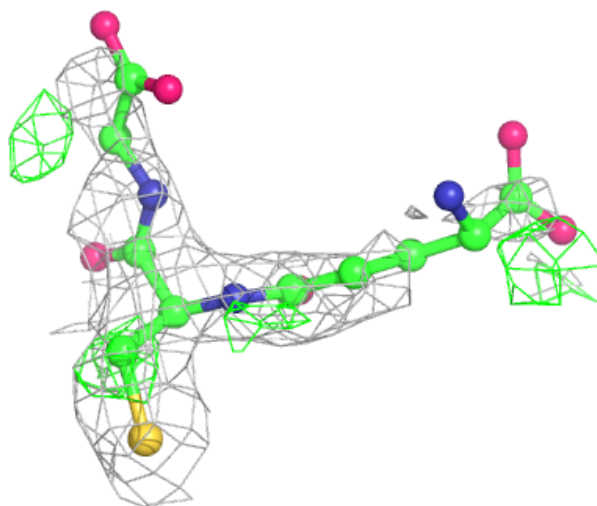
Electron density around GSH A 3001:

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



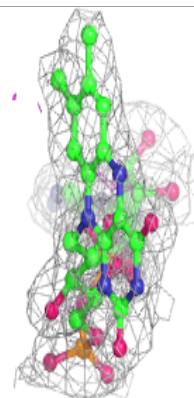
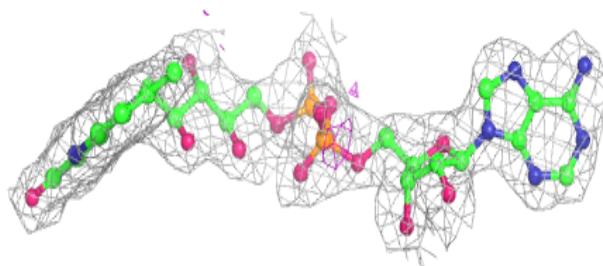
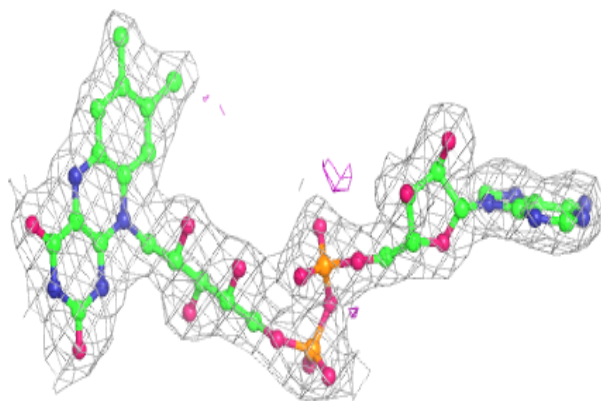
Electron density around GSH B 4001:

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

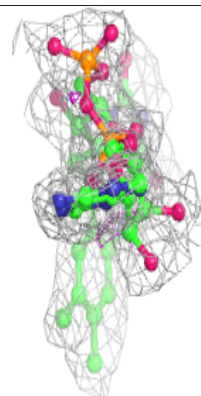
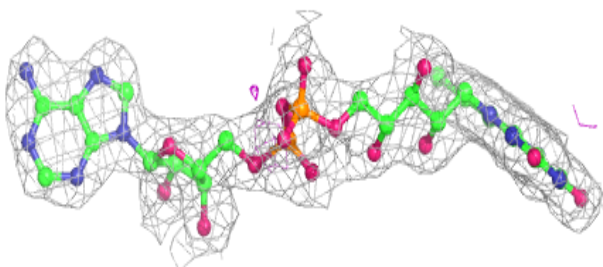
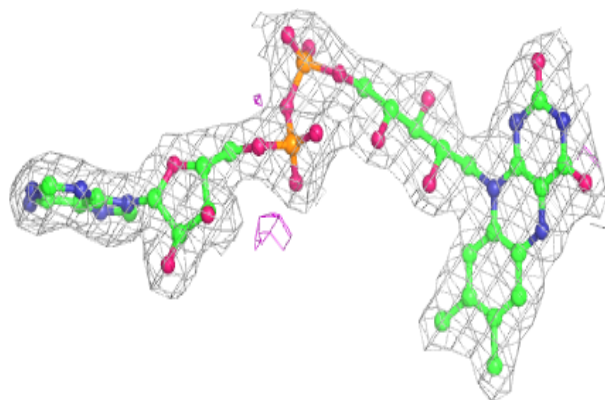


Electron density around FAD B 2001:

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

**Electron density around FAD A 1001:**

$2mF_o-DF_c$ (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.