



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:12 PM UTC

PDB ID : 3L9W / pdb_00003l9w
Title : KefC C-terminal domain in complex with KefF and GSH
Authors : Roosild, T.P.
Deposited on : 2010-01-05
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

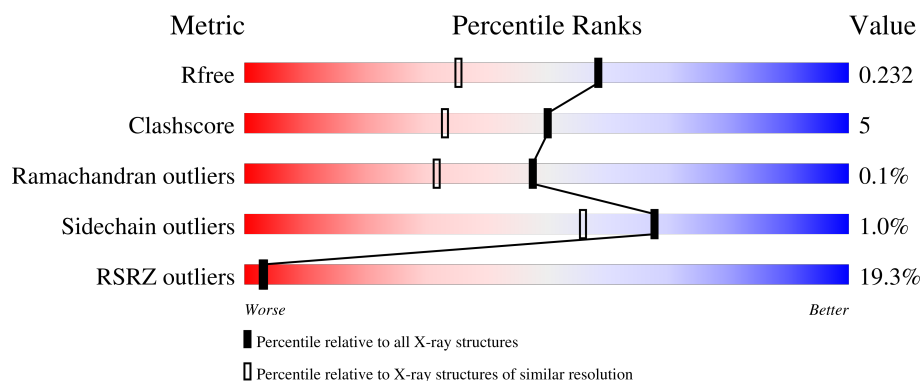
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	413	17% 73% 9% 18%
1	B	413	15% 75% 11% 14%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5981 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-regulated potassium-efflux system protein kefC, linker, ancillary protein kefF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2707	1732	480	480	15			
1	B	357	Total	C	N	O	S	0	0	0
			2853	1820	508	509	16			

There are 34 discrepancies between the modelled and reference sequences:

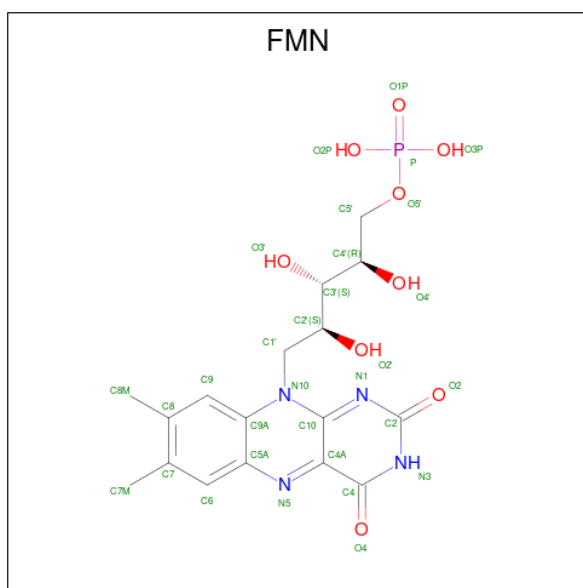
Chain	Residue	Modelled	Actual	Comment	Reference
A	396	GLY	-	expression tag	UNP P03819
A	397	SER	-	expression tag	UNP P03819
A	398	HIS	-	expression tag	UNP P03819
A	399	GLY	-	expression tag	UNP P03819
A	400	MET	-	expression tag	UNP P03819
A	989	THR	-	linker	UNP P03819
A	990	SER	-	linker	UNP P03819
A	991	GLY	-	linker	UNP P03819
A	992	GLY	-	linker	UNP P03819
A	993	LEU	-	linker	UNP P03819
A	994	VAL	-	linker	UNP P03819
A	995	PRO	-	linker	UNP P03819
A	996	ARG	-	linker	UNP P03819
A	997	GLY	-	linker	UNP P03819
A	998	SER	-	linker	UNP P03819
A	999	SER	-	linker	UNP P03819
A	1000	GLY	-	linker	UNP P03819
B	396	GLY	-	expression tag	UNP P03819
B	397	SER	-	expression tag	UNP P03819
B	398	HIS	-	expression tag	UNP P03819
B	399	GLY	-	expression tag	UNP P03819
B	400	MET	-	expression tag	UNP P03819
B	989	THR	-	linker	UNP P03819
B	990	SER	-	linker	UNP P03819

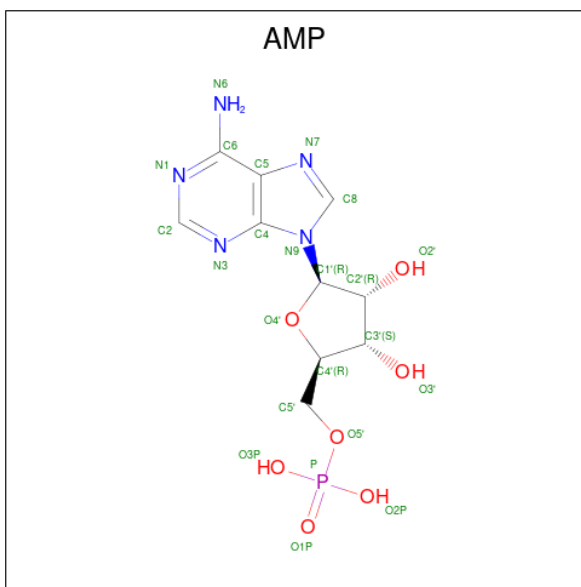
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Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLY	-	linker	UNP P03819
B	992	GLY	-	linker	UNP P03819
B	993	LEU	-	linker	UNP P03819
B	994	VAL	-	linker	UNP P03819
B	995	PRO	-	linker	UNP P03819
B	996	ARG	-	linker	UNP P03819
B	997	GLY	-	linker	UNP P03819
B	998	SER	-	linker	UNP P03819
B	999	SER	-	linker	UNP P03819
B	1000	GLY	-	linker	UNP P03819

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



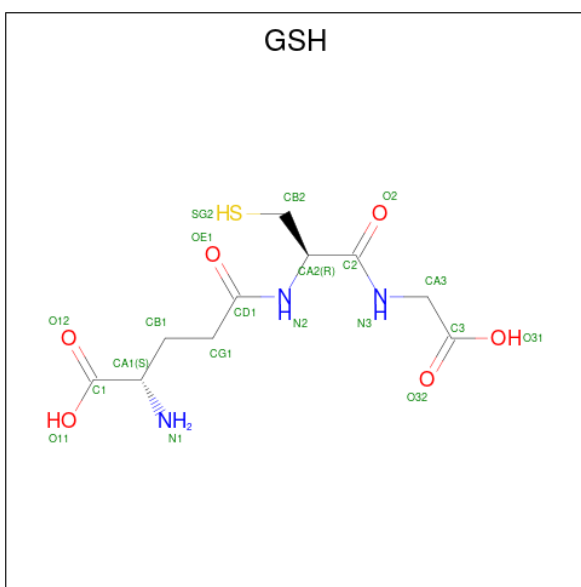


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

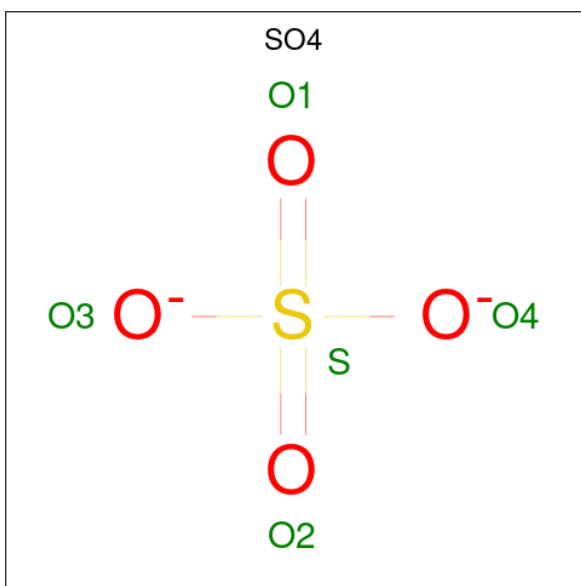
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

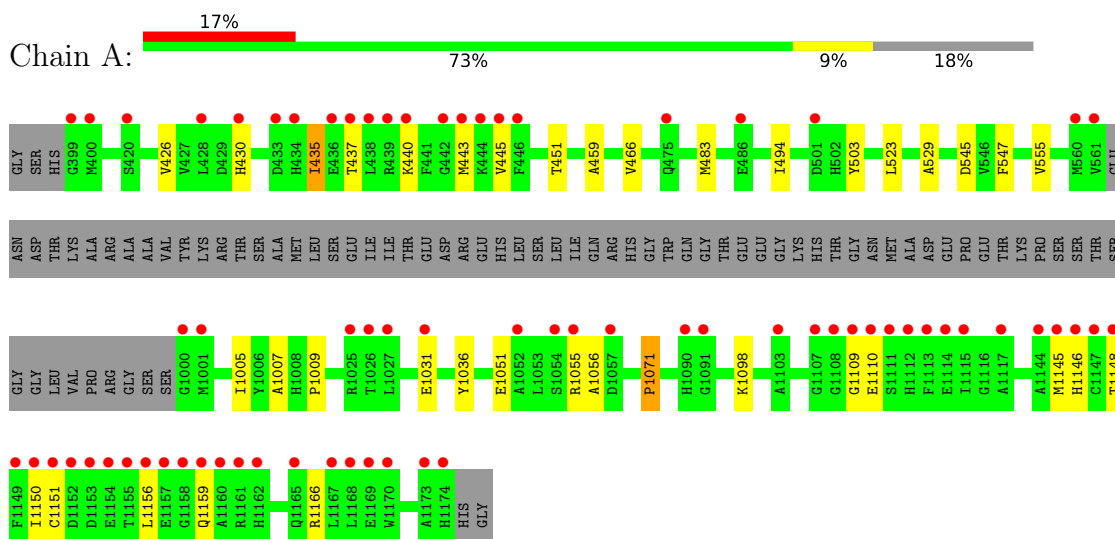
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total 142	O 142	0	0
7	B	144	Total 144	O 144	0	0

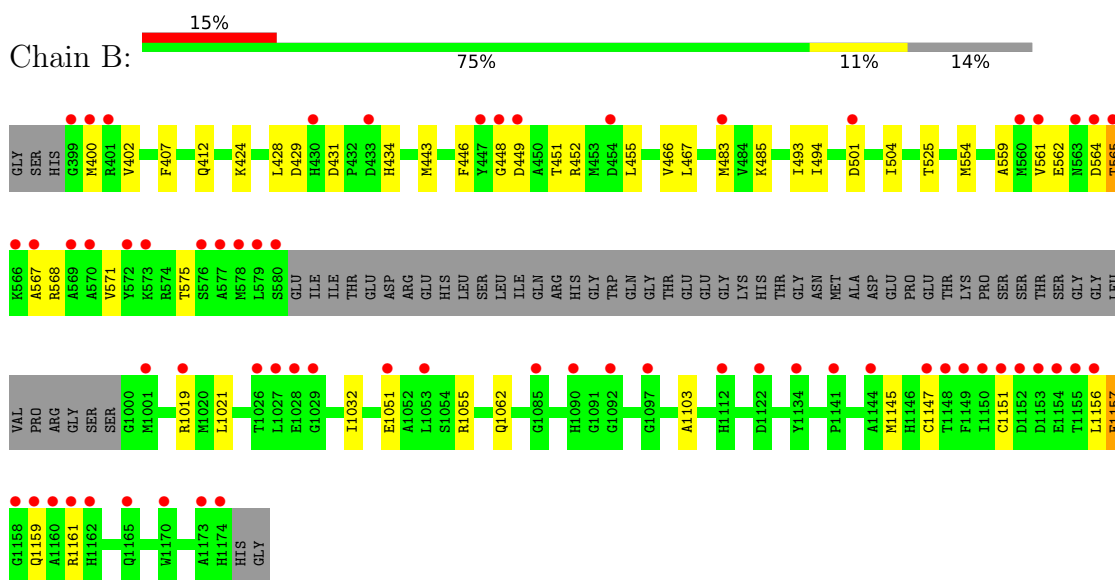
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutathione-regulated potassium-efflux system protein kefC, linker, ancillary protein kefF



- Molecule 1: Glutathione-regulated potassium-efflux system protein kefC, linker, ancillary protein kefF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.76Å 85.85Å 189.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.46 – 1.75 33.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	90.2 (33.46-1.75) 90.2 (33.46-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.234 0.206 , 0.232	Depositor DCC
R_{free} test set	4764 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5981	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: ZN, AMP, SO4, FMN, 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	1.06	3/2778 (0.1%)	1.06	0/3761
1	B	1.02	1/2925 (0.0%)	1.02	1/3958 (0.0%)
All	All	1.04	4/5703 (0.1%)	1.04	1/7719 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	ASP	N-CA	5.62	1.53	1.46
1	A	1005	ILE	CA-CB	5.06	1.58	1.53
1	B	402	VAL	N-CA	5.03	1.52	1.46
1	A	1071	PRO	CA-C	5.03	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	565	THR	N-CA-C	5.05	116.79	111.28

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	2707	0	2659	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2853	0	2809	38	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	20	0	14	0	0
6	B	5	0	0	0	0
7	A	142	0	0	0	0
7	B	144	0	0	2	0
All	All	5981	0	5544	59	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 5.

All (59) 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:1031:GLU:OE1	1:A:1055:ARG:NH2	2.07	0.88
1:B:485:LYS:HE2	1:B:493:ILE:HD12	1.69	0.73
1:B:501:ASP:OD1	1:B:568:ARG:NH1	2.22	0.73
1:B:1145:MET:HE2	1:B:1159:GLN:HB3	1.73	0.70
1:A:1148:THR:HA	1:A:1151:CYS:SG	2.32	0.69
1:B:451:THR:O	1:B:483:MET:SD	2.52	0.67
1:B:1019:ARG:HH11	1:B:1157:GLU:HG2	1.59	0.67
1:A:1056:ALA:O	1:A:1098:LYS:NZ	2.26	0.62
1:A:1051:GLU:OE1	1:A:1055:ARG:NH1	2.32	0.62
1:B:466:VAL:CG1	1:B:494:ILE:HD12	2.29	0.61
1:A:451:THR:O	1:A:483:MET:HE1	2.00	0.61
1:B:1019:ARG:HD2	1:B:1156:LEU:CD2	2.32	0.60
1:B:466:VAL:HG13	1:B:494:ILE:HD12	1.87	0.56
1:A:503:TYR:CE1	1:A:555:VAL:HG12	2.40	0.56
1:B:428:LEU:HD23	1:B:446:PHE:HB2	1.87	0.55
1:B:1157:GLU:O	1:B:1161:ARG:HG3	2.07	0.54
1:A:529:ALA:HA	1:B:494:ILE:CD1	2.38	0.54
1:B:431:ASP:HB3	1:B:434:HIS:CD2	2.44	0.53
1:B:1019:ARG:HD2	1:B:1156:LEU:HD23	1.91	0.52
1:A:440:LYS:HD3	1:B:565:THR:HG21	1.92	0.52
1:A:494:ILE:HG22	1:B:525:THR:HG23	1.92	0.52
1:B:400:MET:H	1:B:424:LYS:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HA	1:B:494:ILE:HD13	1.90	0.51
1:A:443:MET:HG3	1:A:445:VAL:HG23	1.94	0.50
1:A:1145:MET:HA	1:A:1159:GLN:HE21	1.77	0.50
1:B:448:GLY:HA3	1:B:455:LEU:HD11	1.94	0.49
1:B:561:VAL:HG12	1:B:562:GLU:H	1.76	0.49
1:B:1019:ARG:NH1	1:B:1157:GLU:HG2	2.27	0.49
1:B:1051:GLU:OE2	1:B:1055:ARG:HD3	2.12	0.49
1:A:1151:CYS:SG	1:A:1156:LEU:HD13	2.53	0.49
1:B:434:HIS:HE1	7:B:346:HOH:O	1.96	0.49
1:B:1062:GLN:HA	1:B:1103:ALA:O	2.13	0.48
1:B:554:MET:HG3	1:B:571:VAL:HG12	1.97	0.46
1:A:426:VAL:HG21	1:A:459:ALA:HB1	1.98	0.46
1:B:400:MET:H	1:B:424:LYS:CB	2.29	0.46
1:B:429:ASP:OD1	1:B:434:HIS:HD2	1.98	0.46
1:A:1145:MET:HG3	1:A:1159:GLN:HB3	1.97	0.46
1:A:1150:ILE:HD12	1:A:1150:ILE:O	2.16	0.46
1:A:435:ILE:HD13	1:A:445:VAL:HG12	1.98	0.45
1:B:1147:CYS:O	1:B:1151:CYS:HB3	2.16	0.45
1:B:1021:LEU:HD22	1:B:1032:ILE:HD13	1.99	0.45
1:A:1145:MET:CG	1:A:1159:GLN:HB3	2.46	0.45
1:B:407:PHE:CE1	1:B:412:GLN:HG2	2.52	0.45
1:B:449:ASP:O	1:B:455:LEU:HD12	2.18	0.44
1:A:1007:ALA:O	1:A:1071:PRO:HG2	2.17	0.44
1:B:485:LYS:NZ	7:B:198:HOH:O	2.49	0.44
1:A:466:VAL:CG1	1:A:494:ILE:HD12	2.48	0.43
1:A:1109:GLY:HA2	1:A:1146:HIS:HB3	2.01	0.43
1:B:562:GLU:C	1:B:564:ASP:H	2.27	0.43
1:A:1009:PRO:HA	1:A:1036:TYR:CG	2.53	0.43
1:A:437:THR:HA	1:A:440:LYS:HD2	2.00	0.43
1:B:561:VAL:HG11	1:B:567:ALA:HB1	2.01	0.42
1:B:1145:MET:HG3	1:B:1159:GLN:HG3	2.01	0.42
1:B:554:MET:HB2	1:B:575:THR:HG21	2.00	0.42
1:A:466:VAL:HG13	1:A:494:ILE:HD12	2.02	0.41
1:A:523:LEU:HD21	1:A:547:PHE:HD2	1.84	0.41
1:B:449:ASP:HB3	1:B:452:ARG:HG3	2.03	0.41
1:B:504:ILE:HG23	1:B:559:ALA:HA	2.02	0.40
1:A:529:ALA:CA	1:B:494:ILE:HD13	2.52	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	334/413 (81%)	326 (98%)	7 (2%)	1 (0%)	36	21
1	B	353/413 (86%)	345 (98%)	8 (2%)	0	100	100
All	All	687/826 (83%)	671 (98%)	15 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1110	GLU

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	279/340 (82%)	276 (99%)	3 (1%)	65	52
1	B	294/340 (86%)	291 (99%)	3 (1%)	68	56
All	All	573/680 (84%)	567 (99%)	6 (1%)	68	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	HIS
1	A	435	ILE
1	A	1166	ARG
1	B	443	MET
1	B	467	LEU

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Mol	Chain	Res	Type
1	B	1157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1165	GLN
1	B	490	HIS
1	B	1096	HIS
1	B	1159	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	AMP	A	2401	-	25,25,25	1.31	4 (16%)	37,38,38	2.14	14 (37%)
3	AMP	B	2401	-	25,25,25	1.61	3 (12%)	37,38,38	1.90	10 (27%)
2	FMN	B	2400	-	33,33,33	1.31	3 (9%)	48,50,50	1.17	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GSH	B	1	-	18,19,19	2.74	2 (11%)	21,24,24	2.28	5 (23%)
2	FMN	A	2400	-	33,33,33	1.15	2 (6%)	48,50,50	1.40	9 (18%)
6	SO4	B	1177	-	4,4,4	0.29	0	6,6,6	0.82	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
3	AMP	A	2401	-	-	0/10/26/26	0/3/3/3
3	AMP	B	2401	-	-	0/10/26/26	0/3/3/3
2	FMN	B	2400	-	-	0/18/18/18	0/3/3/3
5	GSH	B	1	-	-	3/24/24/24	-
2	FMN	A	2400	-	-	0/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1	GSH	OE1-CD1	8.71	1.40	1.23
5	B	1	GSH	O2-C2	6.83	1.36	1.23
3	B	2401	AMP	C5-C4	5.69	1.49	1.39
2	B	2400	FMN	C4A-N5	4.72	1.40	1.30
2	A	2400	FMN	C4A-N5	4.02	1.39	1.30
2	B	2400	FMN	C10-N1	3.54	1.40	1.33
3	A	2401	AMP	C5-C4	3.13	1.44	1.39
3	B	2401	AMP	C5-C6	2.75	1.48	1.41
3	B	2401	AMP	C8-N7	2.55	1.36	1.31
3	A	2401	AMP	C8-N7	2.53	1.36	1.31
3	A	2401	AMP	C5-C6	2.51	1.48	1.41
2	A	2400	FMN	C10-N1	2.26	1.37	1.33
3	A	2401	AMP	C2-N3	2.13	1.37	1.33
2	B	2400	FMN	C9-C9A	2.12	1.43	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	GSH	CA2-CB2-SG2	-6.57	106.75	114.16
3	A	2401	AMP	N3-C2-N1	-5.60	120.11	128.58
3	B	2401	AMP	C5-C4-N3	-5.12	119.67	126.72
3	B	2401	AMP	N3-C4-N9	4.54	134.88	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	GSH	CB1-CA1-N1	4.38	121.55	110.12
3	A	2401	AMP	C5-C4-N3	-4.25	120.87	126.72
5	B	1	GSH	CB1-CG1-CD1	-4.08	103.97	113.06
3	A	2401	AMP	C2-N3-C4	3.75	121.00	111.83
3	A	2401	AMP	O2P-P-O5'	-3.58	97.34	106.67
2	A	2400	FMN	C4A-C10-N10	3.55	121.56	116.48
3	B	2401	AMP	N3-C2-N1	-3.45	123.37	128.58
3	B	2401	AMP	C2-N3-C4	3.35	120.01	111.83
3	B	2401	AMP	C4-N9-C8	3.27	109.17	105.74
2	A	2400	FMN	C4-N3-C2	-3.24	119.89	125.64
3	A	2401	AMP	N3-C4-N9	3.22	132.64	127.17
3	A	2401	AMP	C2-N1-C6	3.22	124.01	118.73
5	B	1	GSH	CB1-CA1-C1	3.20	118.92	110.45
3	B	2401	AMP	C4-C5-N7	-3.14	106.99	110.58
3	A	2401	AMP	C4-C5-N7	-2.78	107.41	110.58
2	B	2400	FMN	C4A-C10-N10	2.76	120.43	116.48
2	A	2400	FMN	C4A-C4-N3	2.74	120.22	113.25
2	B	2400	FMN	O4-C4-N3	-2.71	115.01	120.11
2	B	2400	FMN	C10-C4A-N5	-2.62	119.46	124.81
2	A	2400	FMN	C10-C4A-N5	-2.62	119.46	124.81
3	B	2401	AMP	C5-N7-C8	2.47	107.33	103.45
3	A	2401	AMP	C4-N9-C8	2.42	108.28	105.74
3	A	2401	AMP	N9-C8-N7	-2.42	110.51	113.94
3	A	2401	AMP	C5-N7-C8	2.41	107.24	103.45
2	B	2400	FMN	C4A-C4-N3	2.28	119.07	113.25
2	B	2400	FMN	C4-N3-C2	-2.27	121.62	125.64
3	B	2401	AMP	C2-N1-C6	2.26	122.44	118.73
2	B	2400	FMN	C4'-C3'-C2'	-2.24	109.84	113.57
3	A	2401	AMP	O4'-C1'-C2'	-2.19	101.92	106.62
3	A	2401	AMP	C6-C5-N7	2.18	136.29	132.09
2	A	2400	FMN	C4-C4A-N5	2.16	121.19	118.21
3	A	2401	AMP	N6-C6-N1	2.15	123.17	118.38
3	B	2401	AMP	O4'-C1'-N9	2.14	112.19	108.09
3	A	2401	AMP	O3P-P-O2P	2.13	115.78	107.80
5	B	1	GSH	O31-C3-CA3	2.13	120.89	112.81
2	A	2400	FMN	C4A-C10-N1	-2.10	119.43	124.59
2	A	2400	FMN	C9A-C5A-N5	-2.06	120.27	122.45
2	A	2400	FMN	O2P-P-O1P	2.05	118.82	110.83
2	A	2400	FMN	C4'-C3'-C2'	-2.04	110.17	113.57
2	B	2400	FMN	C4-C4A-N5	2.04	121.03	118.21
3	B	2401	AMP	N9-C8-N7	-2.02	111.06	113.94

There are no chirality outliers.

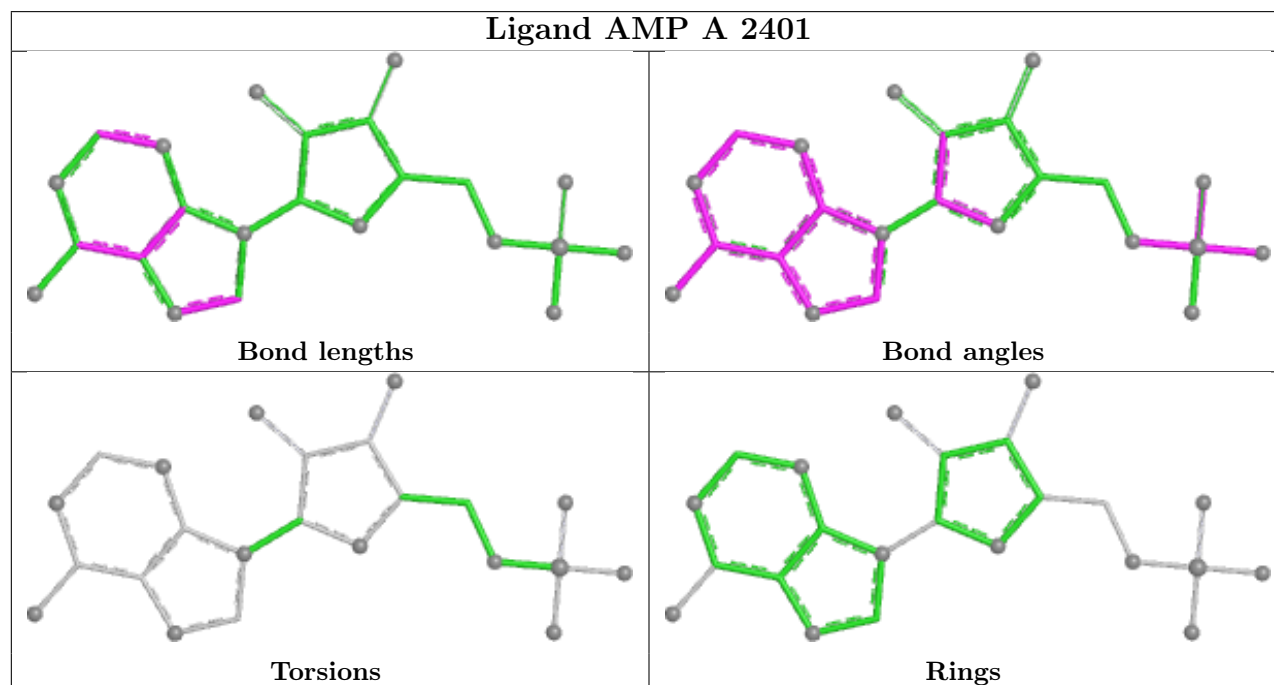
All (3) torsion outliers are listed below:

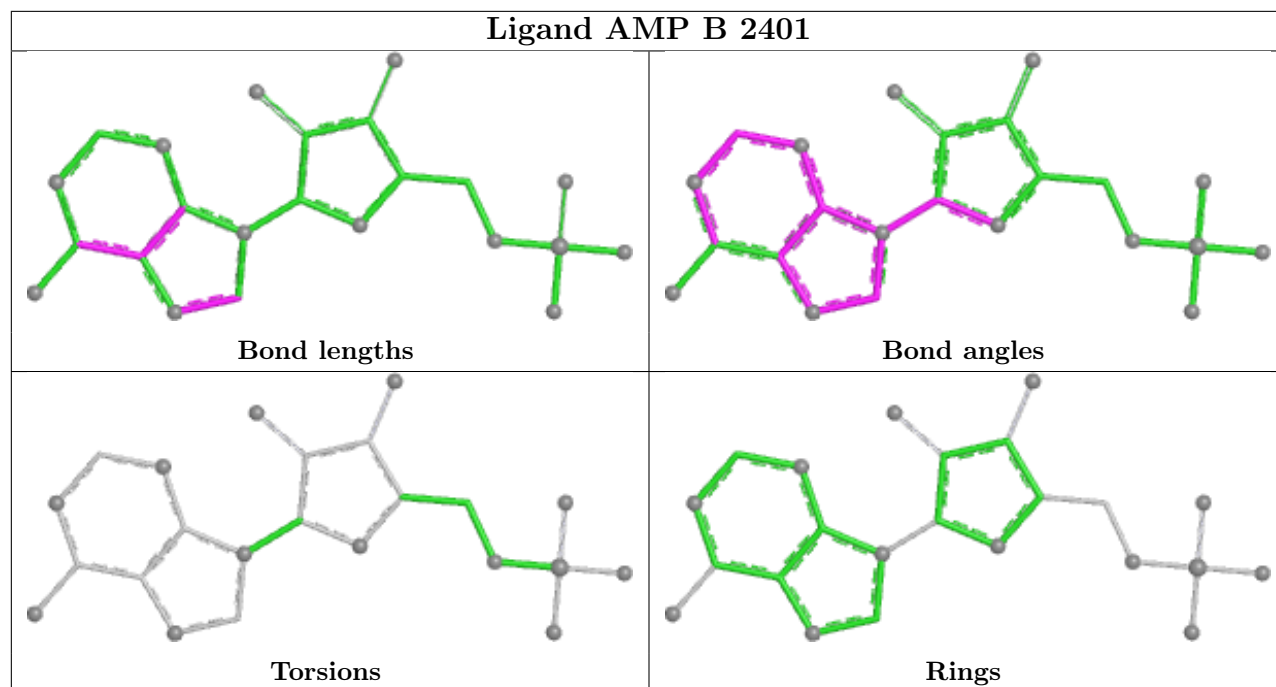
Mol	Chain	Res	Type	Atoms
5	B	1	GSH	N1-CA1-CB1-CG1
5	B	1	GSH	O11-C1-CA1-N1
5	B	1	GSH	O12-C1-CA1-N1

There are no ring outliers.

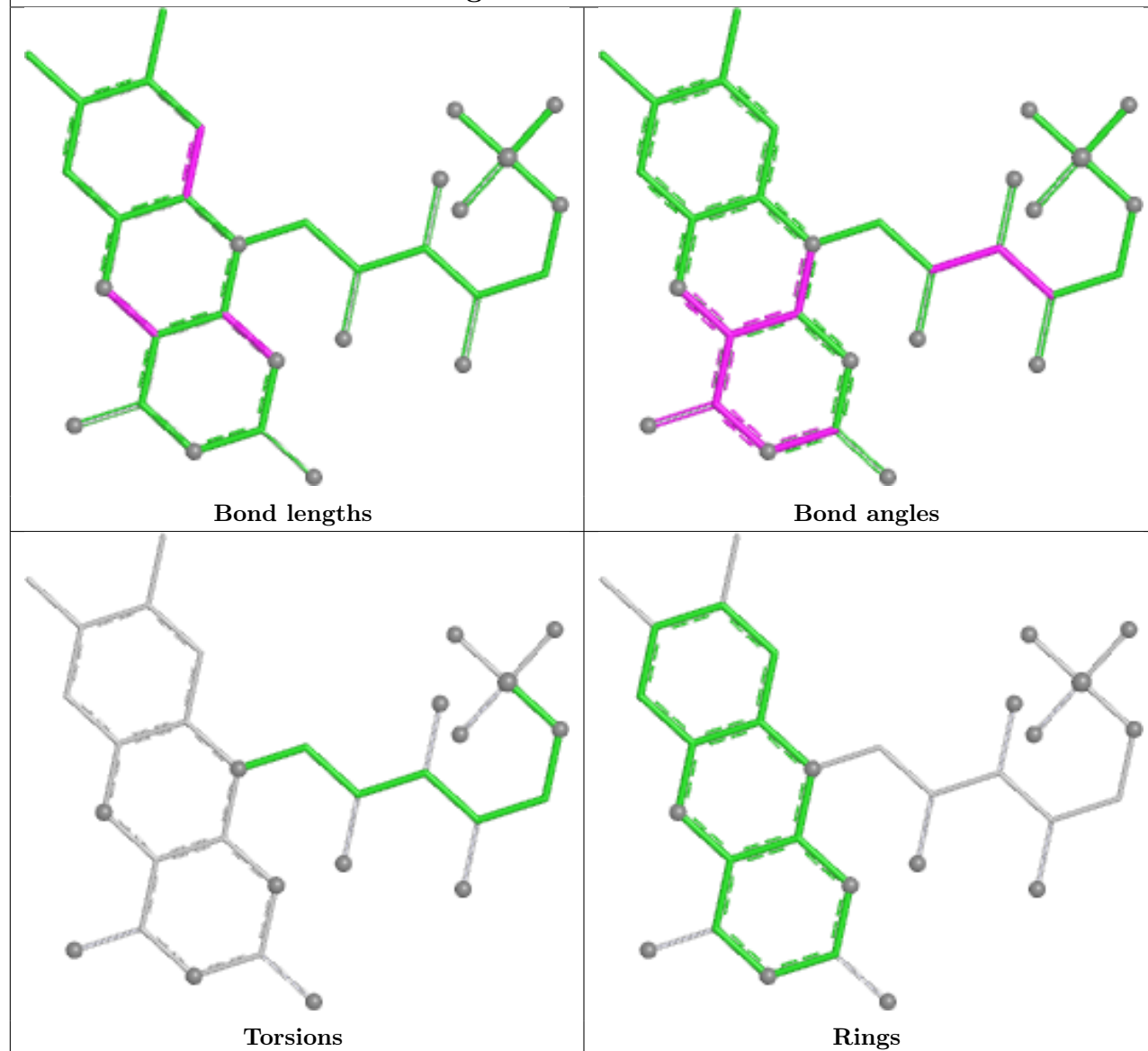
No monomer is involved in short contacts.

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.

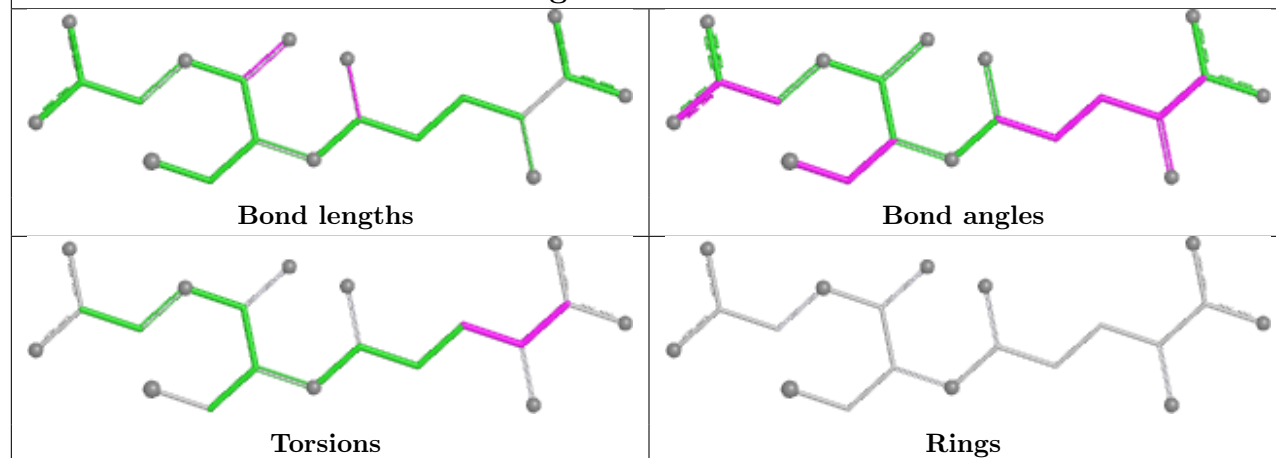


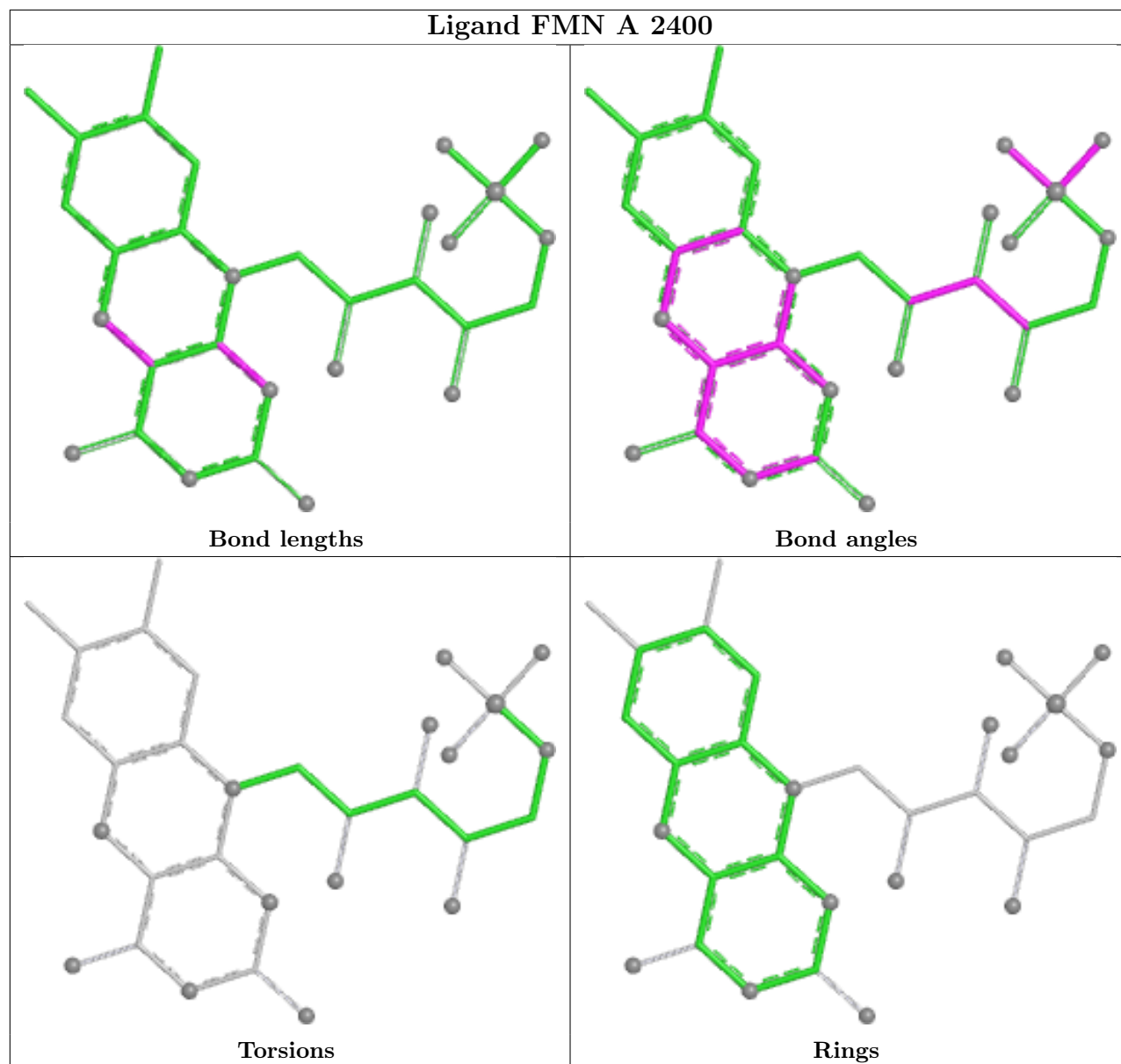


Ligand FMN B 2400



Ligand GSH B 1





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

6.1 Protein, DNA and RNA chains

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	338/413 (81%)	1.18	71 (21%) 2 2	18, 30, 61, 84	0
1	B	357/413 (86%)	0.94	63 (17%) 4 4	18, 30, 59, 83	0
All	All	695/826 (84%)	1.06	134 (19%) 3 3	18, 30, 61, 84	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1150	ILE	17.8
1	A	1147	CYS	13.0
1	A	1149	PHE	9.8
1	A	1148	THR	7.6
1	B	399	GLY	6.7
1	A	1108	GLY	6.2
1	A	1151	CYS	6.2
1	B	1150	ILE	6.2
1	A	561	VAL	6.1
1	B	1151	CYS	6.0
1	A	1162	HIS	5.8
1	B	1173	ALA	5.8
1	B	1147	CYS	5.6
1	B	1174	HIS	5.6
1	B	1149	PHE	5.5
1	A	1155	THR	5.5
1	B	1122	ASP	5.4
1	A	1146	HIS	5.1
1	B	1156	LEU	5.0
1	A	443	MET	5.0
1	A	1111	SER	4.9
1	A	400	MET	4.9
1	A	399	GLY	4.7
1	B	400	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	439	ARG	4.6
1	B	565	THR	4.6
1	A	1109	GLY	4.6
1	B	1155	THR	4.6
1	B	577	ALA	4.5
1	A	1159	GLN	4.5
1	A	560	MET	4.5
1	A	1107	GLY	4.4
1	B	561	VAL	4.4
1	A	1027	LEU	4.2
1	B	564	ASP	4.1
1	B	1152	ASP	4.1
1	A	1156	LEU	4.1
1	B	1158	GLY	4.0
1	A	1112	HIS	3.9
1	B	430	HIS	3.9
1	A	1115	ILE	3.8
1	A	444	LYS	3.7
1	B	1160	ALA	3.7
1	A	1157	GLU	3.7
1	B	567	ALA	3.7
1	A	1173	ALA	3.6
1	A	1160	ALA	3.6
1	A	1174	HIS	3.6
1	A	446	PHE	3.6
1	A	433	ASP	3.6
1	B	1148	THR	3.5
1	B	1159	GLN	3.5
1	A	1054	SER	3.4
1	A	1152	ASP	3.4
1	A	1158	GLY	3.4
1	A	1161	ARG	3.4
1	B	576	SER	3.3
1	A	1001	MET	3.3
1	A	1090	HIS	3.3
1	A	437	THR	3.2
1	A	1110	GLU	3.2
1	B	1162	HIS	3.2
1	B	1144	ALA	3.1
1	A	1154	GLU	3.1
1	B	1028	GLU	3.1
1	B	483	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1026	THR	3.1
1	A	1031	GLU	3.1
1	B	578	MET	3.0
1	A	1000	GLY	3.0
1	B	560	MET	3.0
1	A	1091	GLY	3.0
1	B	1153	ASP	2.8
1	A	438	LEU	2.8
1	A	501	ASP	2.8
1	A	445	VAL	2.8
1	B	1154	GLU	2.7
1	A	1144	ALA	2.7
1	A	1168	LEU	2.7
1	B	570	ALA	2.7
1	A	1170	TRP	2.7
1	B	433	ASP	2.7
1	B	572	TYR	2.6
1	B	573	LYS	2.6
1	B	447	TYR	2.6
1	B	563	ASN	2.6
1	A	1117	ALA	2.6
1	B	1161	ARG	2.6
1	A	1169	GLU	2.5
1	A	442	GLY	2.5
1	B	1134	TYR	2.5
1	A	436	GLU	2.5
1	B	1165	GLN	2.5
1	B	454	ASP	2.5
1	B	1090	HIS	2.5
1	A	1025	ARG	2.4
1	B	1029	GLY	2.4
1	B	580	SER	2.4
1	B	1026	THR	2.4
1	A	428	LEU	2.4
1	B	1027	LEU	2.4
1	B	1019	ARG	2.4
1	A	1165	GLN	2.3
1	A	1145	MET	2.3
1	B	1092	GLY	2.3
1	B	569	ALA	2.3
1	A	434	HIS	2.3
1	A	1114	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1153	ASP	2.3
1	A	1052	ALA	2.2
1	B	579	LEU	2.2
1	A	1103	ALA	2.2
1	B	1053	LEU	2.2
1	B	1097	GLY	2.2
1	B	1001	MET	2.2
1	B	1170	TRP	2.2
1	A	1113	PHE	2.2
1	A	420	SER	2.2
1	B	1112	HIS	2.1
1	B	566	LYS	2.1
1	B	1141	PRO	2.1
1	A	475	GLN	2.1
1	A	430	HIS	2.1
1	B	1085	GLY	2.1
1	A	1055	ARG	2.1
1	B	448	GLY	2.1
1	B	1051	GLU	2.1
1	A	1167	LEU	2.1
1	A	486	GLU	2.0
1	B	501	ASP	2.0
1	B	401	ARG	2.0
1	A	1057	ASP	2.0
1	B	449	ASP	2.0
1	A	440	LYS	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](#)

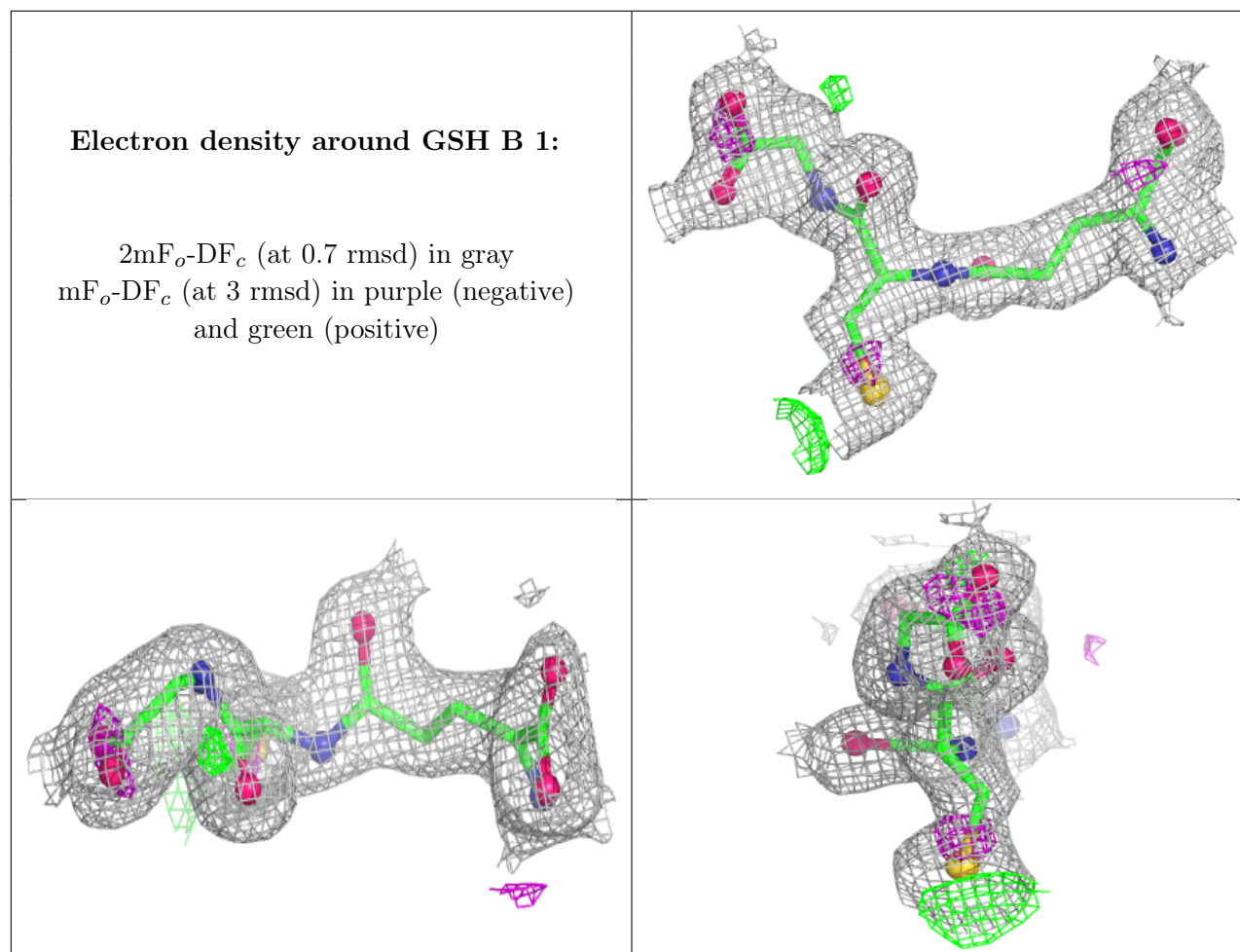
There are no oligosaccharides in this entry.

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.

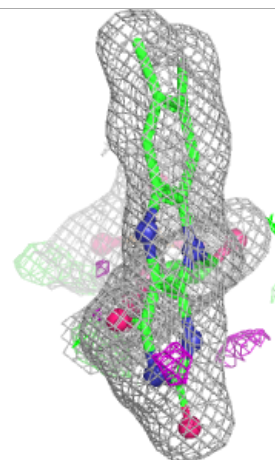
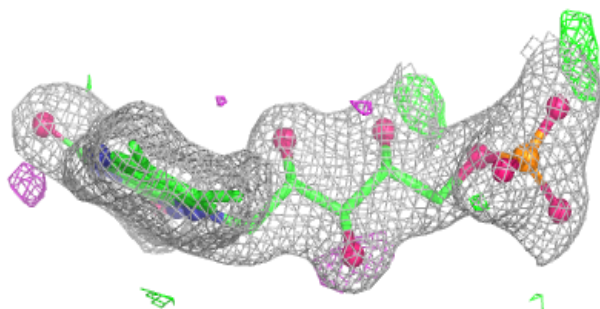
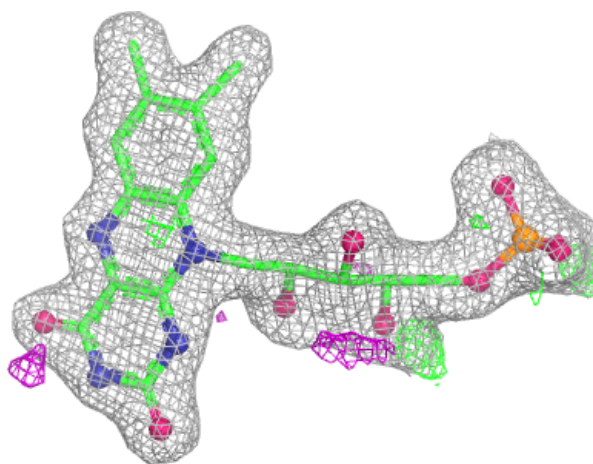
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	1177	5/5	0.76	0.20	67,68,71,72	0
5	GSH	B	1	20/20	0.92	0.10	25,38,48,49	0
2	FMN	A	2400	31/31	0.94	0.10	25,34,37,39	0
2	FMN	B	2400	31/31	0.94	0.11	24,32,34,35	0
3	AMP	B	2401	23/23	0.95	0.11	23,41,44,45	0
4	ZN	A	2402	1/1	0.97	0.18	45,45,45,45	0
3	AMP	A	2401	23/23	0.98	0.05	19,25,28,31	0
4	ZN	B	2402	1/1	0.98	0.19	44,44,44,44	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.



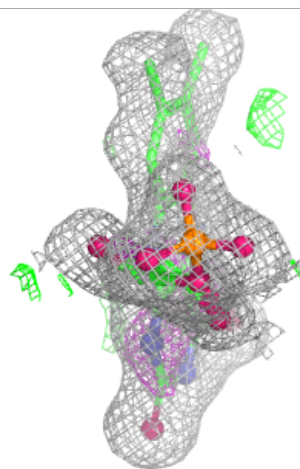
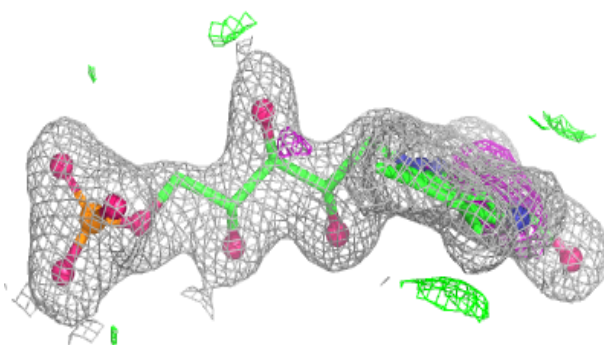
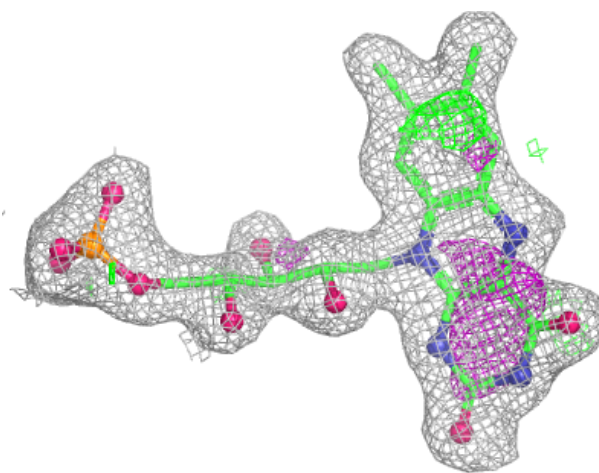
Electron density around FMN A 2400:

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



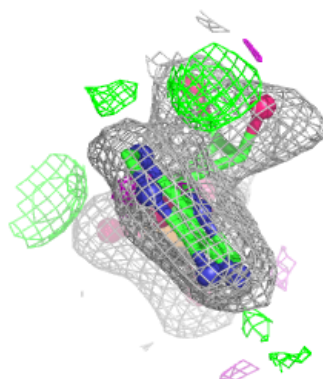
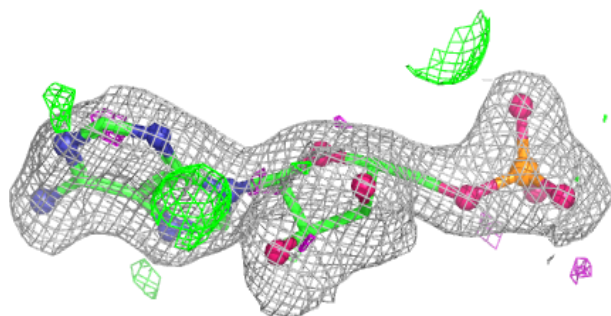
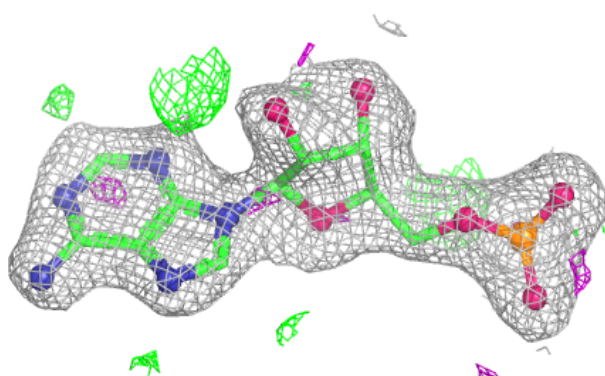
Electron density around FMN B 2400:

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

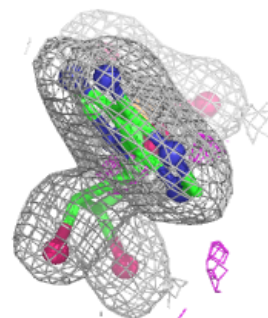
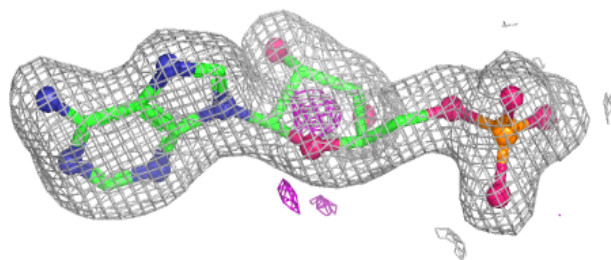
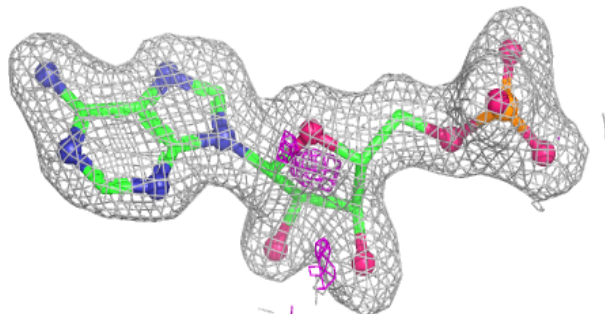


Electron density around AMP B 2401:

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

**Electron density around AMP A 2401:**

$2mF_o-DF_c$ (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.