WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2024 – 10:41 AM EST

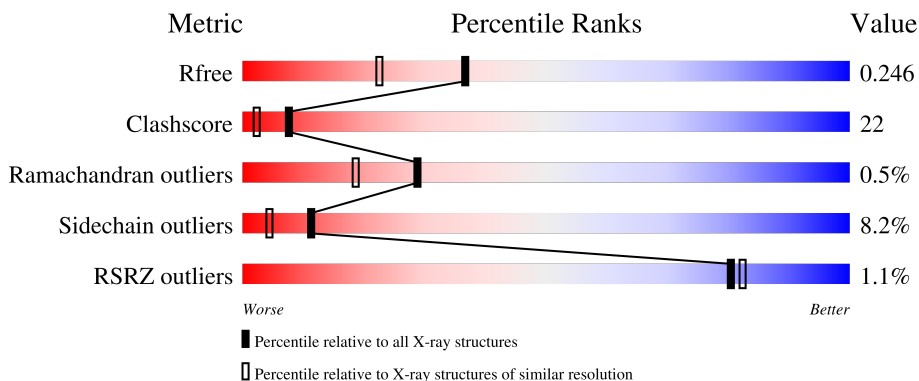|		
PDB ID	:	3KAL
Title	:	Structure of homoglutathione synthetase from Glycine max in closed conformation with homoglutathione, ADP, a sulfate ion, and three magnesium ions bound
Authors	:	Galant, A.; Arkus, K.A.J.; Zubieta, C.; Cahoon, R.E.; Jez, J.M.
Deposited on	:	2009-10-19
Resolution	:	1.90 Å(reported)

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.246
Clashscore		22
Ramachandran outliers		0.5%
Sidechain outliers		8.2%
RSRZ outliers		1.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	499	53% / 30% / 10% · 6%
1	B	499	48% / 33% / 11% · 6%

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
3	HGS	A	501	-	X	X	-
3	HGS	A	506	-	X	-	-
3	HGS	B	501	-	X	X	-
3	HGS	B	506	-	X	-	-
5	SO4	A	505	-	-	X	-
5	SO4	B	505	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8571 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 homoglutathione synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	14	0
			3828	2423	667	720	18			
1	B	468	Total	C	N	O	S	0	19	0
			3855	2434	676	728	17			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
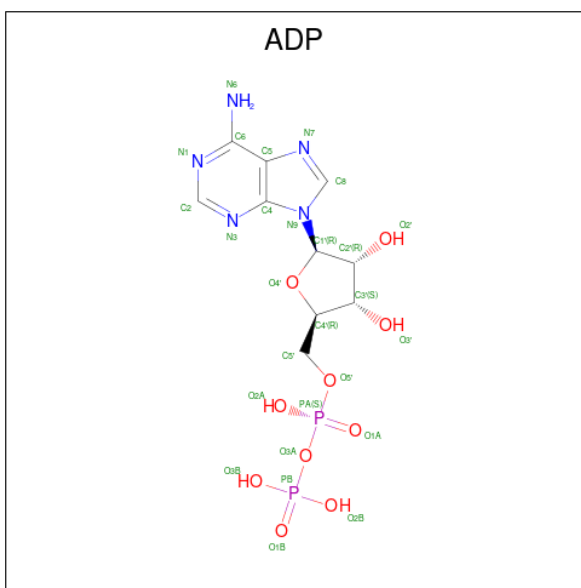
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is D-gamma-glutamyl-L-cysteinyl-beta-alanine (three-letter code: HGS) (formula: $C_{11}H_{19}N_3O_6S$).

HGS
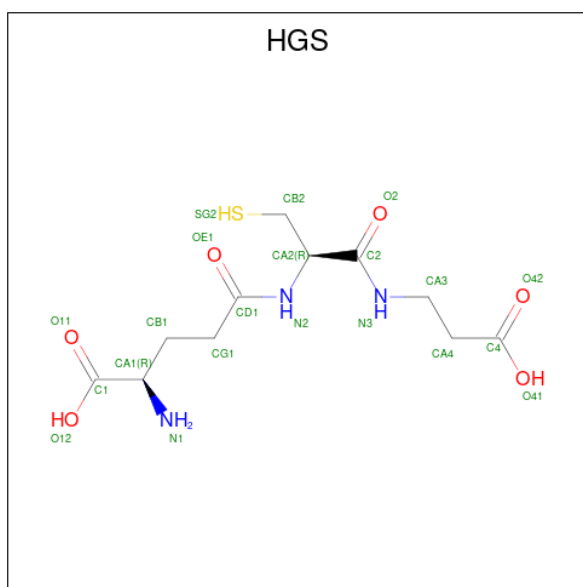
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			21	11	3	6	1		
3	A	1	Total	C	N	O	S	0	0
			21	11	3	6	1		
3	B	1	Total	C	N	O	S	0	0
			21	11	3	6	1		
3	B	1	Total	C	N	O	S	0	0
			21	11	3	6	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	B	3	Total	Mg	0	0
			3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3   O⁻ — S — O⁻ O4

      S

O2

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	371	Total 371	O 371	0	0
6	B	363	Total 363	O 363	0	0

3 Residue-property plots ⓘ

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: homoglutathione synthetase
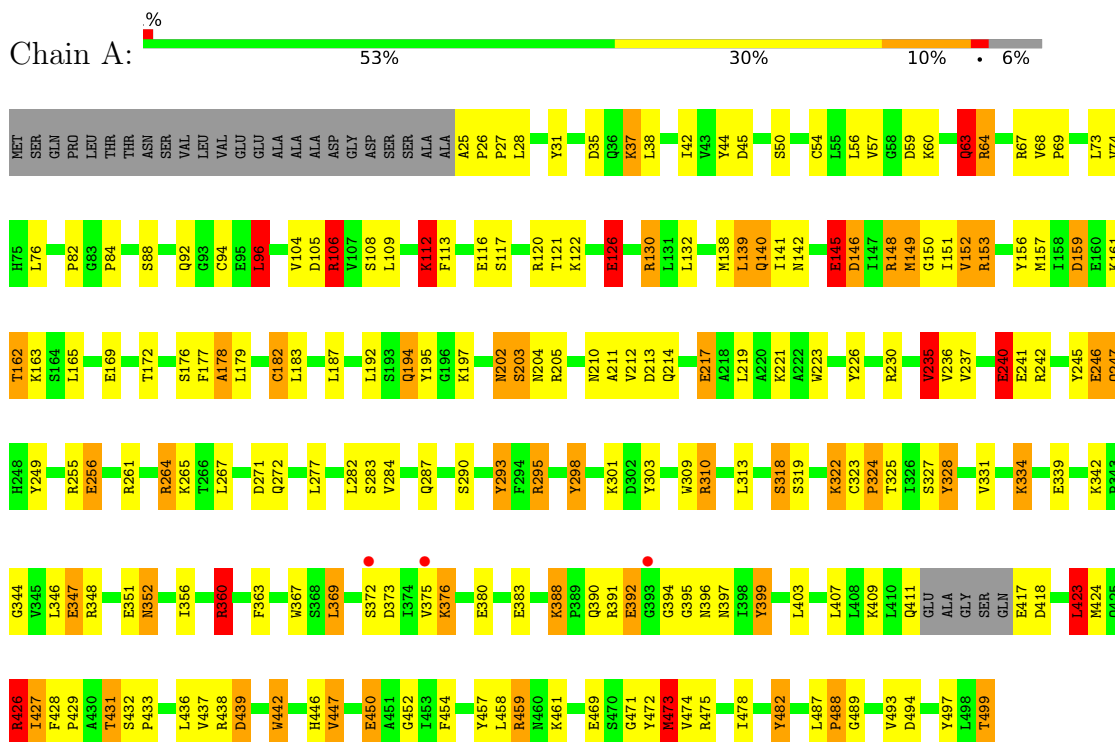
• Molecule 1: homoglutathione synthetase
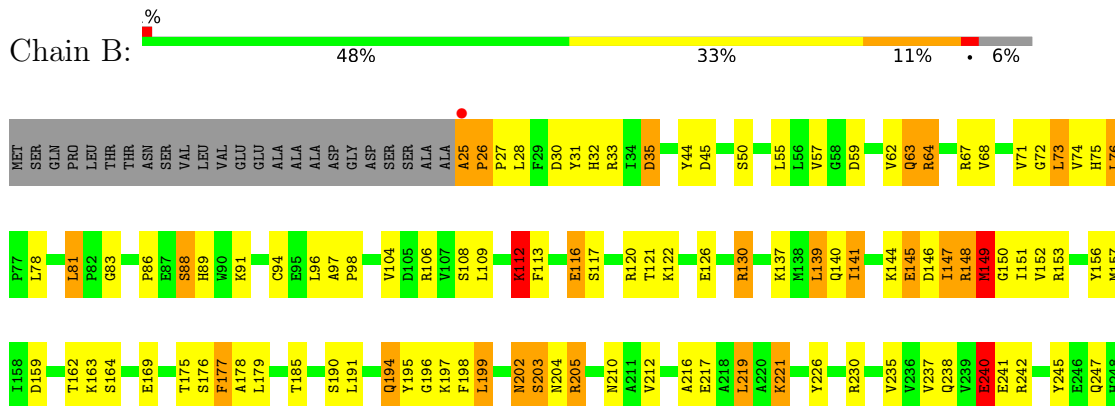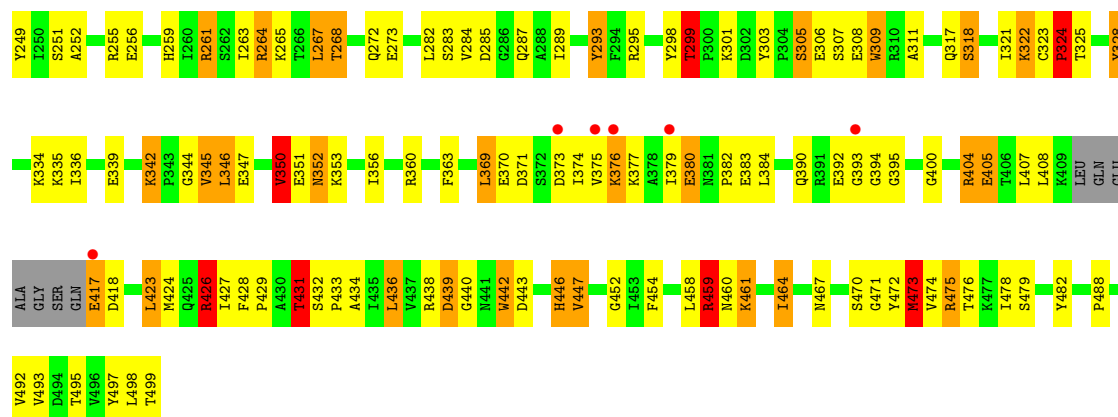
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	115.70Å 115.70Å 101.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.26 – 1.90 28.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.26-1.90) 99.8 (28.09-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.250 0.198 , 0.246	Depositor DCC
R_{free} test set	5992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l 0.488 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8571	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, SO4, HGS, MG

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	2.09	125/3901 (3.2%)	1.72	74/5269 (1.4%)
1	B	2.08	109/3927 (2.8%)	1.71	75/5303 (1.4%)
All	All	2.09	234/7828 (3.0%)	1.72	149/10572 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	B	0	5
All	All	1	8

The worst 5 of 234 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	GLU	CB-CG	12.81	1.76	1.52
1	A	240	GLU	CB-CG	11.81	1.74	1.52
1	B	245	TYR	CG-CD2	11.19	1.53	1.39
1	B	226	TYR	CG-CD1	10.67	1.53	1.39
1	A	126	GLU	CG-CD	10.20	1.67	1.51

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ARG	NE-CZ-NH1	-29.96	105.32	120.30
1	B	264	ARG	NE-CZ-NH1	-20.81	109.89	120.30
1	A	264	ARG	NE-CZ-NH2	17.19	128.90	120.30
1	B	130	ARG	NE-CZ-NH2	-16.69	111.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	475	ARG	NE-CZ-NH2	-15.43	112.58	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	431	THR	CB

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	372	SER	Peptide
1	A	392	GLU	Peptide
1	A	417	GLU	Peptide
1	B	148	ARG	Mainchain,Peptide
1	B	317	GLN	Mainchain

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	3828	0	3850	149	0
1	B	3855	0	3864	178	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	42	0	33	18	0
3	B	42	0	30	28	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	5	0	0	4	0
5	B	5	0	0	5	0
6	A	371	0	0	35	0
6	B	363	0	0	30	0
All	All	8571	0	7801	346	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 22.

The worst 5 of 346 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:96:LEU:CD1	1:A:96:LEU:CG	1.74	1.62
1:B:459[B]:ARG:CB	1:B:459[B]:ARG:CG	1.81	1.59
1:B:240:GLU:CG	1:B:240:GLU:CB	1.76	1.58
1:A:240:GLU:CG	1:A:240:GLU:CB	1.74	1.57
1:A:264:ARG:CD	1:A:264:ARG:CG	1.77	1.56

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	480/499 (96%)	458 (95%)	21 (4%)	1 (0%)	47	38
1	B	483/499 (97%)	448 (93%)	28 (6%)	7 (1%)	11	3
All	All	963/998 (96%)	906 (94%)	49 (5%)	8 (1%)	29	9

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149[A]	MET
1	B	149[B]	MET
1	B	439[A]	ASP
1	B	439[B]	ASP
1	B	369	LEU

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	424/431 (98%)	391 (92%)	33 (8%)	12	5
1	B	427/431 (99%)	388 (91%)	39 (9%)	9	3
All	All	851/862 (99%)	779 (92%)	72 (8%)	11	4

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	350	VAL
1	B	474	VAL
1	B	376	LYS
1	B	426	ARG
1	A	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	GLN
1	B	287	GLN
1	B	468	ASN
1	B	352	ASN
1	B	238	GLN

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 ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	SO4	A	505	4	4,4,4	1.67	1 (25%)	6,6,6	1.28	0
3	HGS	A	501	-	19,20,20	4.27	11 (57%)	24,25,25	6.75	16 (66%)
2	ADP	A	500	4	24,29,29	2.00	7 (29%)	29,45,45	1.65	6 (20%)
3	HGS	B	501	-	19,20,20	3.46	7 (36%)	24,25,25	6.33	17 (70%)
3	HGS	A	506	-	19,20,20	2.95	7 (36%)	24,25,25	3.36	12 (50%)
3	HGS	B	506	-	19,20,20	2.19	5 (26%)	24,25,25	3.00	11 (45%)
5	SO4	B	505	4	4,4,4	1.49	1 (25%)	6,6,6	1.54	1 (16%)
2	ADP	B	500	4	24,29,29	1.68	7 (29%)	29,45,45	1.50	5 (17%)

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	HGS	A	501	-	-	12/25/25/25	-
2	ADP	A	500	4	-	2/12/32/32	0/3/3/3
3	HGS	B	501	-	-	12/25/25/25	-
3	HGS	A	506	-	-	10/25/25/25	-
3	HGS	B	506	-	-	14/25/25/25	-
2	ADP	B	500	4	-	3/12/32/32	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HGS	CB2-CA2	9.86	1.63	1.53
3	B	501	HGS	CB2-CA2	8.28	1.62	1.53
3	A	501	HGS	CA4-C4	8.01	1.69	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	HGS	O2-C2	7.82	1.38	1.23
3	A	501	HGS	CA3-N3	6.65	1.61	1.46

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	HGS	CA3-N3-C2	18.29	155.21	122.59
3	B	501	HGS	CA3-N3-C2	18.07	154.82	122.59
3	A	501	HGS	CA2-CB2-SG2	-16.08	96.12	114.19
3	B	501	HGS	CA2-CB2-SG2	-13.00	99.58	114.19
3	B	501	HGS	CA2-C2-N3	9.86	136.43	116.54

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	HGS	O11-C1-CA1-N1
3	A	501	HGS	N1-CA1-CB1-CG1
3	A	501	HGS	N2-CA2-CB2-SG2
3	A	506	HGS	O11-C1-CA1-N1
3	A	506	HGS	C1-CA1-CB1-CG1

There are no ring outliers.

7 monomers are involved in 47 short contacts:

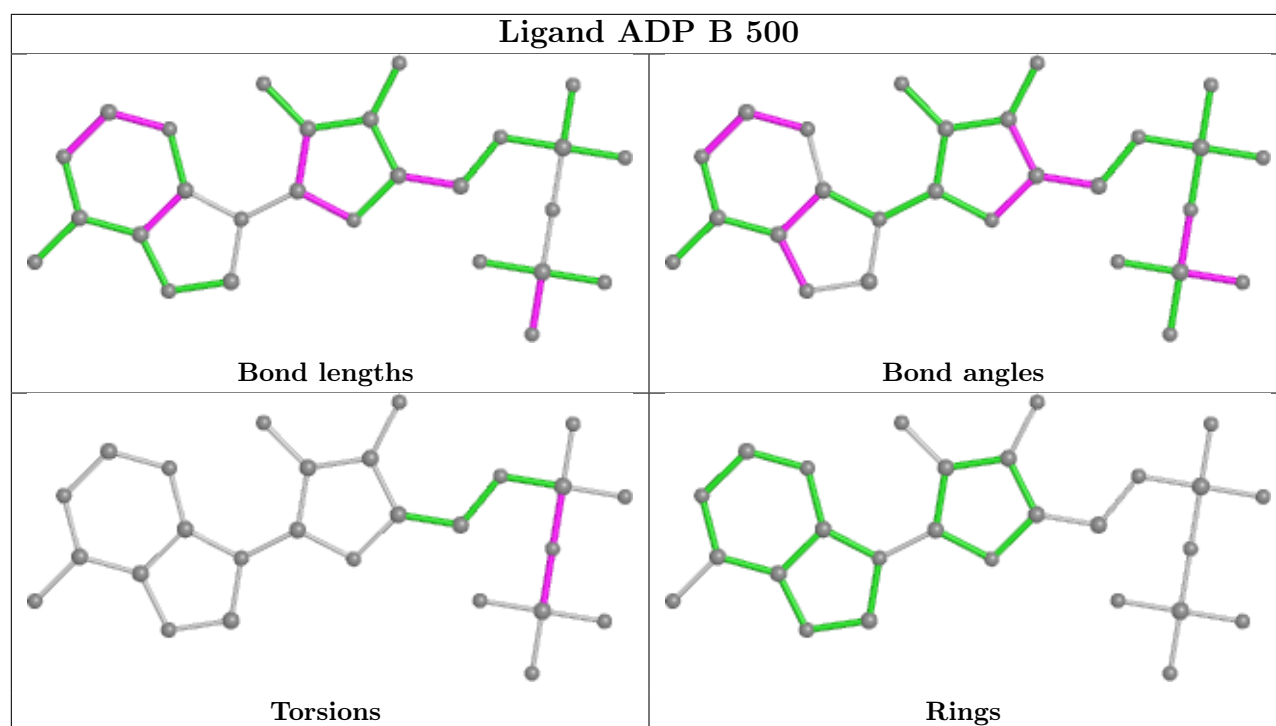| Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	SO4	4	0
3	A	501	HGS	12	0
2	A	500	ADP	1	0
3	B	501	HGS	21	0
3	A	506	HGS	6	0
3	B	506	HGS	7	0
5	B	505	SO4	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HGS A 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand ADP A 500	
Bond lengths	Bond angles
Torsions	Rings

Ligand HGS B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand HGS A 506

Bond lengths

Bond angles

Torsions

Rings

Ligand HGS B 506

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 500

Bond lengths

Bond angles

Torsions

Rings
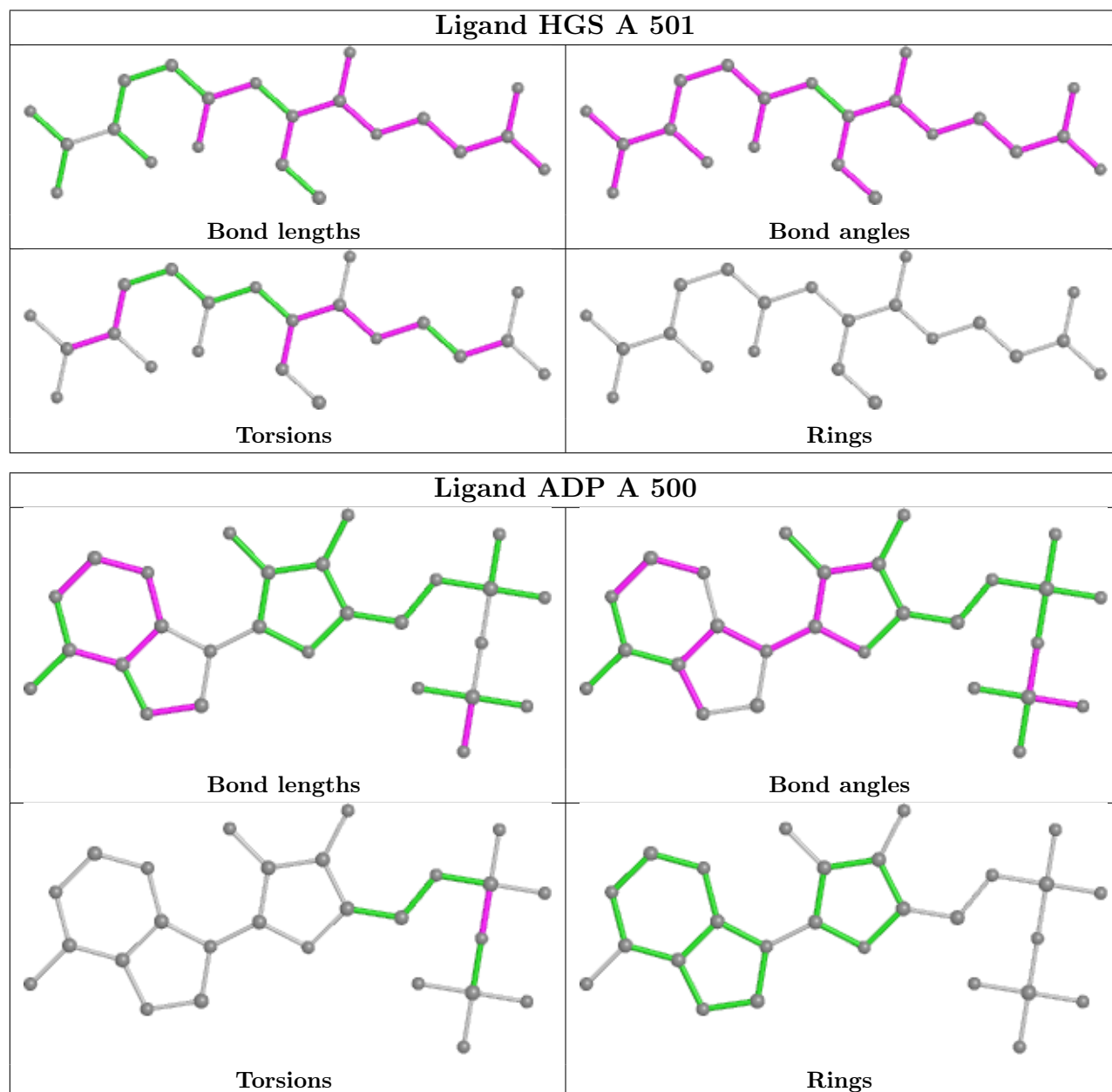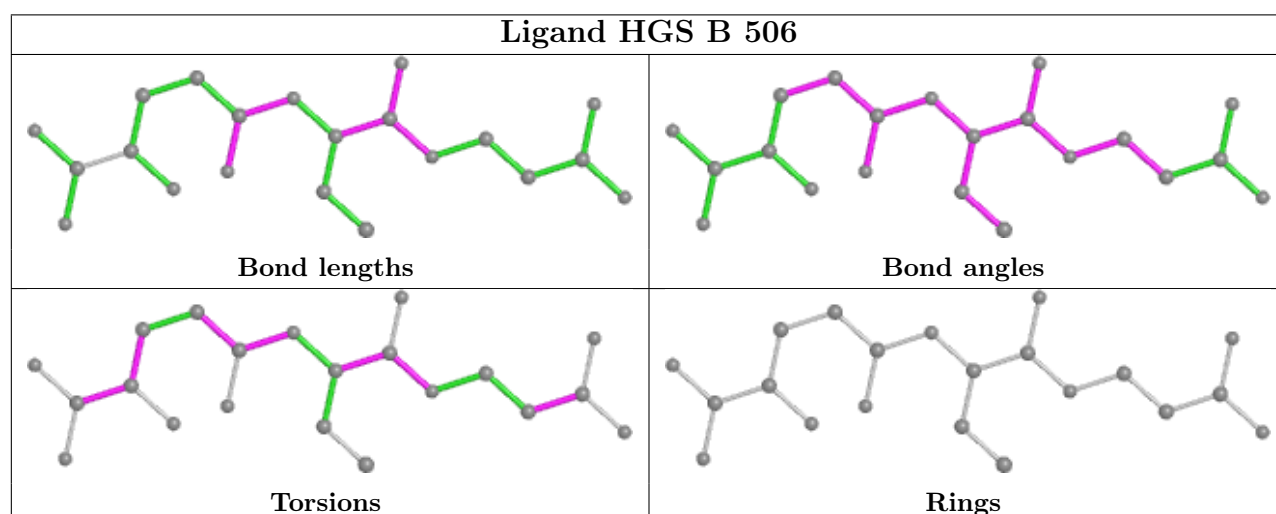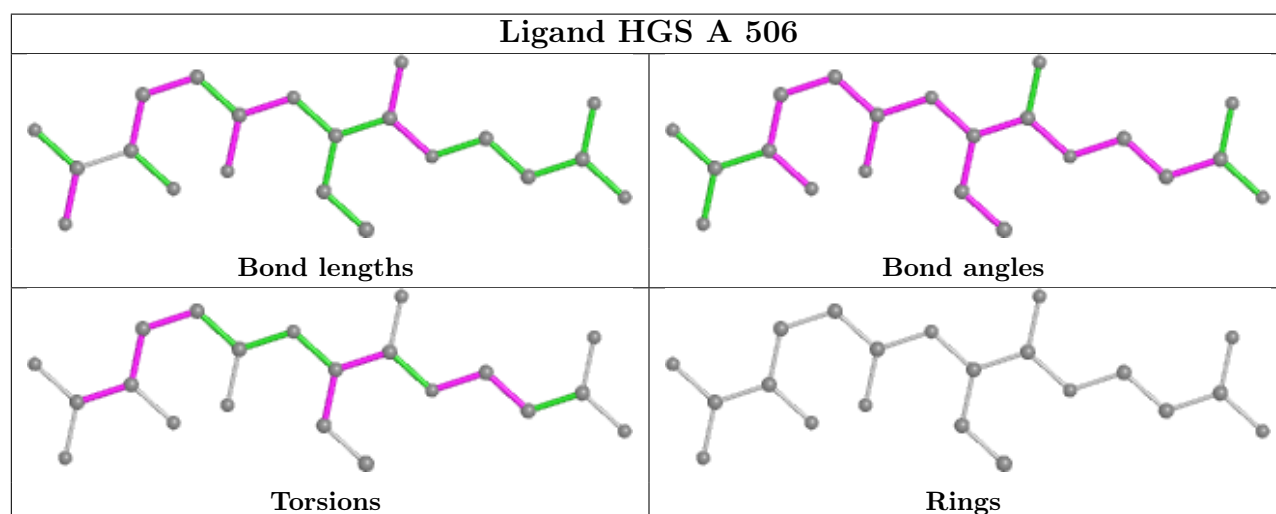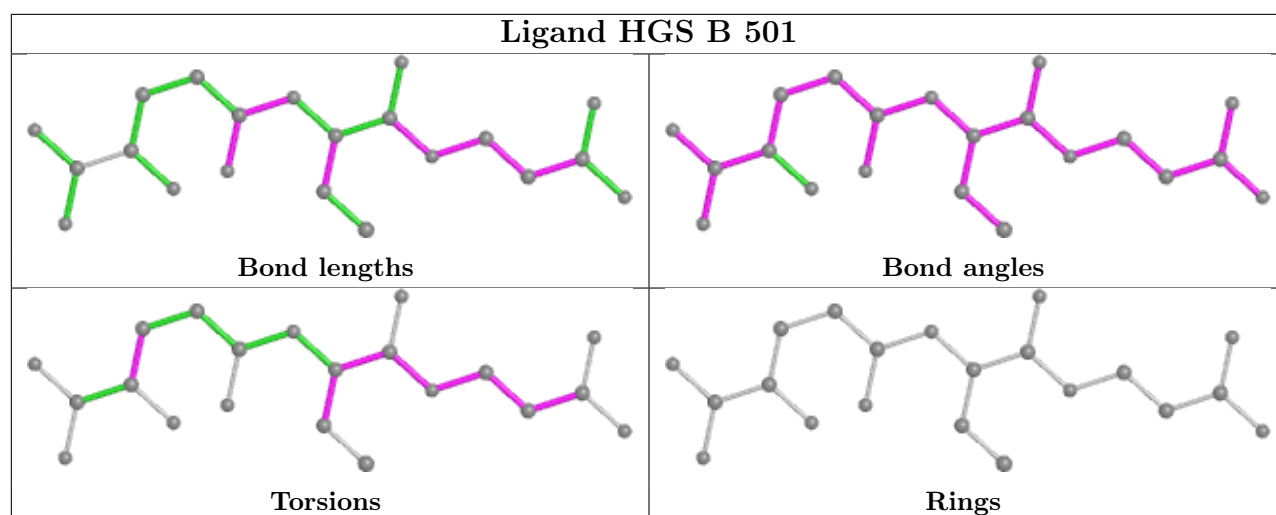
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	470/499 (94%)	-0.19	3 (0%)	89	90	18, 31, 64, 84	0
1	B	468/499 (93%)	-0.14	7 (1%)	73	76	20, 31, 65, 89	0
All	All	938/998 (93%)	-0.17	10 (1%)	80	82	18, 31, 66, 89	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	ILE	3.2
1	B	25	ALA	3.1
1	B	393	GLY	2.8
1	A	372	SER	2.7
1	B	376	LYS	2.6

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3   Carbohydrates ⓘ

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, 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
3	HGS	B	506	21/21	0.76	0.26	34,42,50,52	21
3	HGS	A	501	21/21	0.87	0.18	25,51,57,61	0
3	HGS	B	501	21/21	0.89	0.17	27,52,57,64	0
3	HGS	A	506	21/21	0.90	0.23	14,27,56,59	21
4	MG	B	504	1/1	0.97	0.06	36,36,36,36	0
5	SO4	A	505	5/5	0.97	0.08	29,37,46,49	0
4	MG	A	504	1/1	0.98	0.07	36,36,36,36	0
4	MG	A	502	1/1	0.98	0.07	39,39,39,39	0
4	MG	A	503	1/1	0.98	0.07	27,27,27,27	0
5	SO4	B	505	5/5	0.98	0.10	31,35,42,45	0
4	MG	B	503	1/1	0.99	0.06	29,29,29,29	0
2	ADP	B	500	27/27	0.99	0.09	27,33,37,39	0
2	ADP	A	500	27/27	0.99	0.08	24,31,37,37	0
4	MG	B	502	1/1	0.99	0.07	34,34,34,34	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.
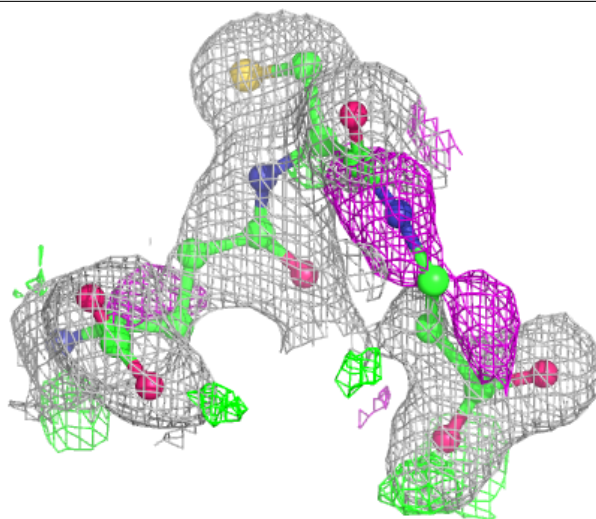
Electron density around HGS B 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
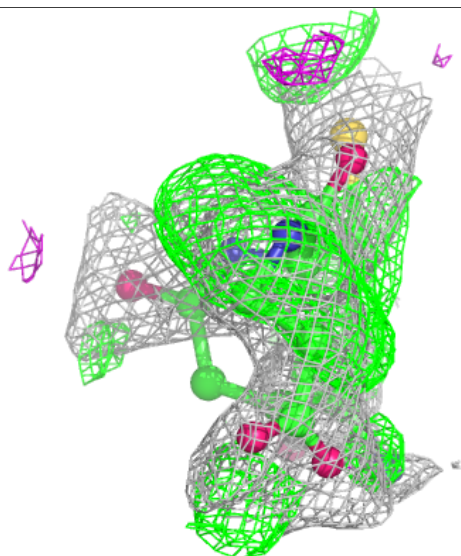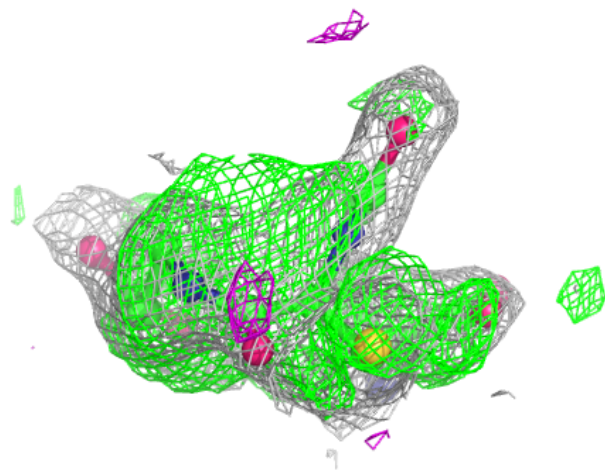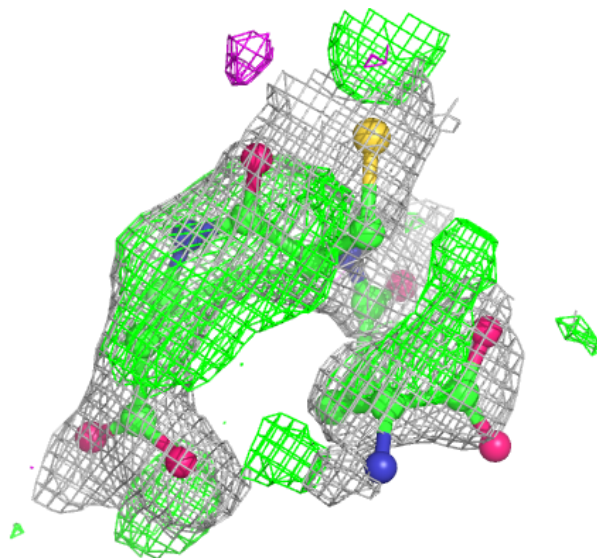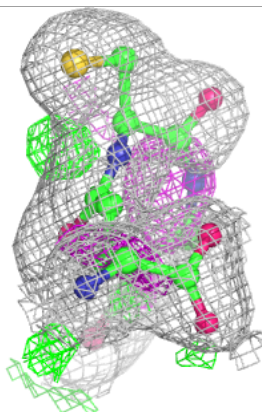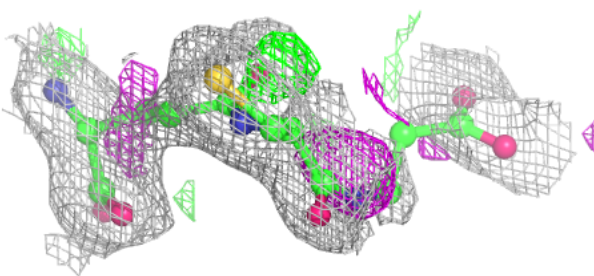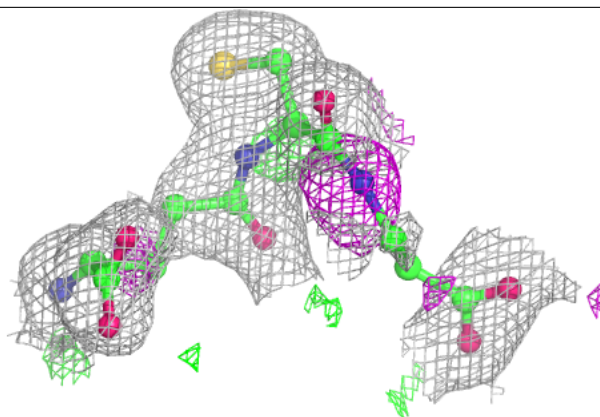
Electron density around HGS A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
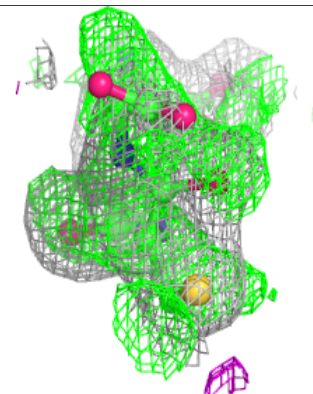mF_o-DF_c (at 3 rmsd) in purple (negative)
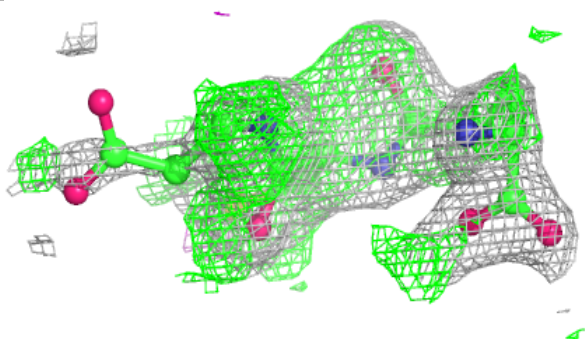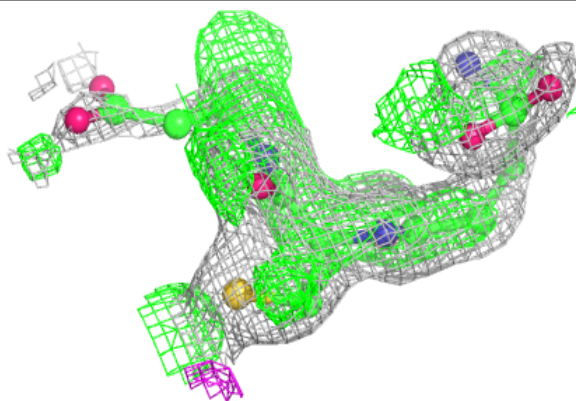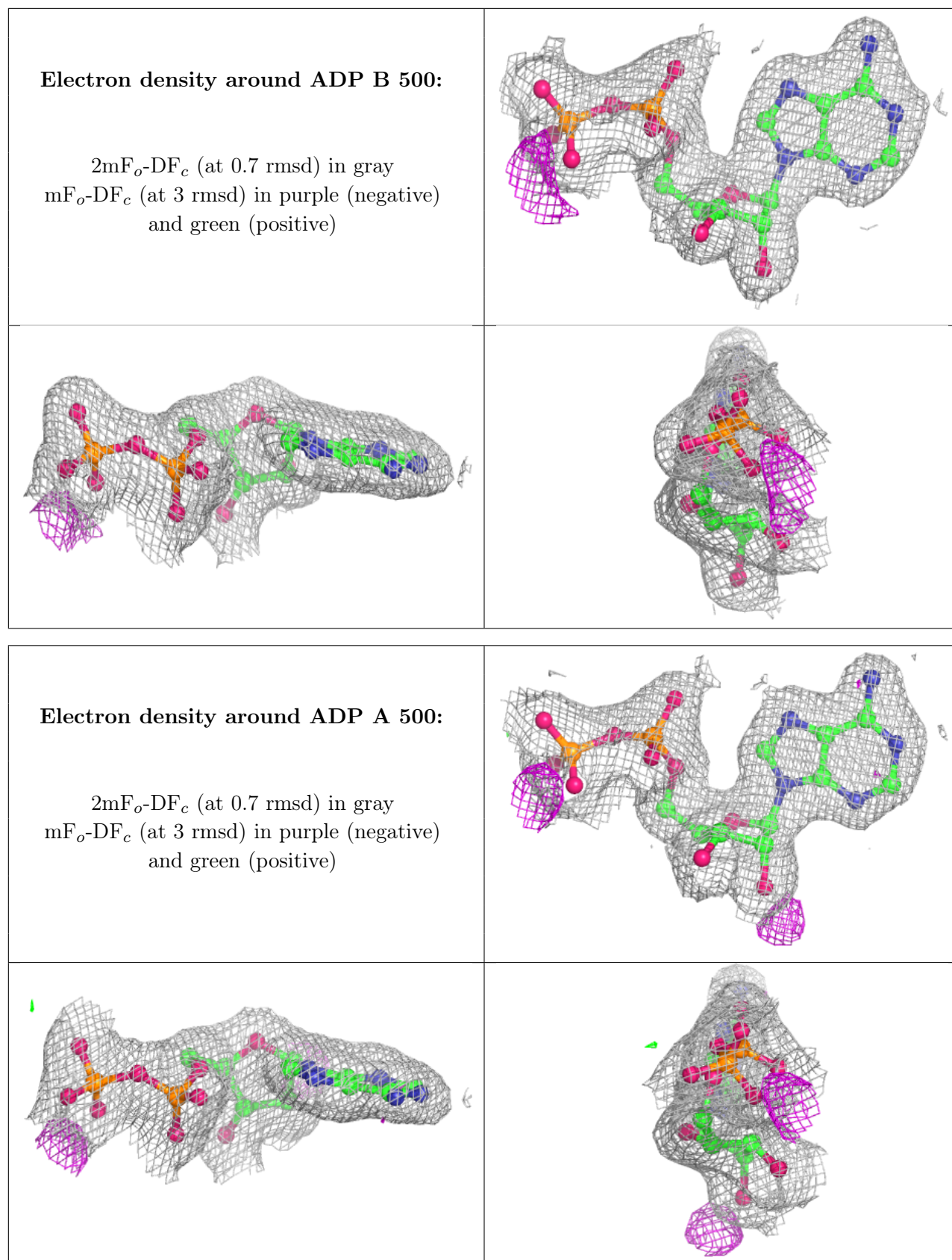and green (positive)
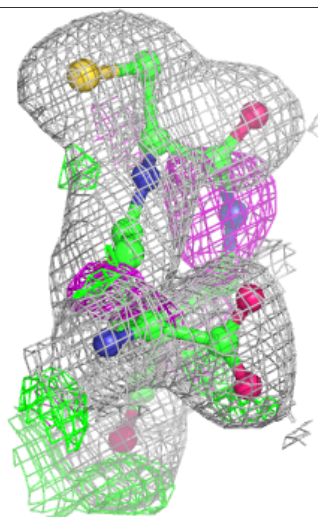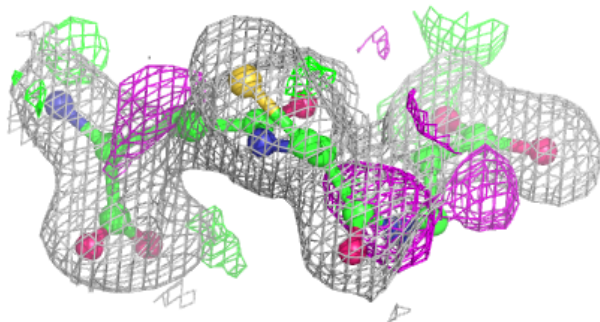
Electron density around HGS B 501:

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

Electron density around HGS A 506:

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

Electron density around ADP B 500:

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

Electron density around ADP A 500:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.