



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:45 am BST

PDB ID : 2EL9
Title : Crystal structure of E.coli Histidyl-tRNA synthetase complexed with a histidyl-adenylate analogue
Authors : Yanagisawa, T.; Si, S.Y.; Matsuno, M.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-27
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

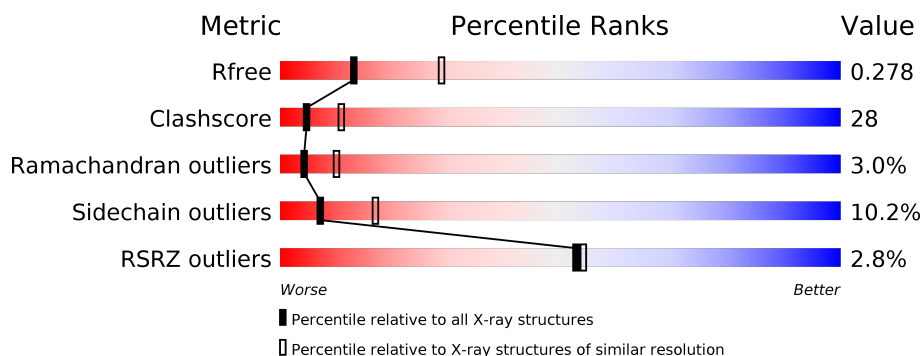
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	431	<div> <div>5%</div> <div> <div>41%</div> <div>39%</div> <div>6%</div> <div>14%</div> </div> </div>
1	B	431	<div> <div>52%</div> <div>30%</div> <div>5%</div> <div>13%</div> </div>
1	C	431	<div> <div>4%</div> <div> <div>44%</div> <div>36%</div> <div>6%</div> <div>14%</div> </div> </div>
1	D	431	<div> <div>48%</div> <div>35%</div> <div>6%</div> <div>11%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HSS	C	710	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12050 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 Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2903	1826	521	545	11			
1	B	376	Total	C	N	O	S	0	0	0
			2923	1837	525	550	11			
1	C	372	Total	C	N	O	S	0	0	0
			2899	1822	521	545	11			
1	D	385	Total	C	N	O	S	0	0	0
			2993	1883	535	564	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP P60906
A	-5	PRO	-	EXPRESSION TAG	UNP P60906
A	-4	GLY	-	EXPRESSION TAG	UNP P60906
A	-3	TYR	-	EXPRESSION TAG	UNP P60906
A	-2	GLN	-	EXPRESSION TAG	UNP P60906
A	-1	ASP	-	EXPRESSION TAG	UNP P60906
A	0	PRO	-	EXPRESSION TAG	UNP P60906
B	-6	GLY	-	EXPRESSION TAG	UNP P60906
B	-5	PRO	-	EXPRESSION TAG	UNP P60906
B	-4	GLY	-	EXPRESSION TAG	UNP P60906
B	-3	TYR	-	EXPRESSION TAG	UNP P60906
B	-2	GLN	-	EXPRESSION TAG	UNP P60906
B	-1	ASP	-	EXPRESSION TAG	UNP P60906
B	0	PRO	-	EXPRESSION TAG	UNP P60906
C	-6	GLY	-	EXPRESSION TAG	UNP P60906
C	-5	PRO	-	EXPRESSION TAG	UNP P60906
C	-4	GLY	-	EXPRESSION TAG	UNP P60906
C	-3	TYR	-	EXPRESSION TAG	UNP P60906
C	-2	GLN	-	EXPRESSION TAG	UNP P60906
C	-1	ASP	-	EXPRESSION TAG	UNP P60906
C	0	PRO	-	EXPRESSION TAG	UNP P60906

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	EXPRESSION TAG	UNP P60906
D	-5	PRO	-	EXPRESSION TAG	UNP P60906
D	-4	GLY	-	EXPRESSION TAG	UNP P60906
D	-3	TYR	-	EXPRESSION TAG	UNP P60906
D	-2	GLN	-	EXPRESSION TAG	UNP P60906
D	-1	ASP	-	EXPRESSION TAG	UNP P60906
D	0	PRO	-	EXPRESSION TAG	UNP P60906

- # HSS

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0



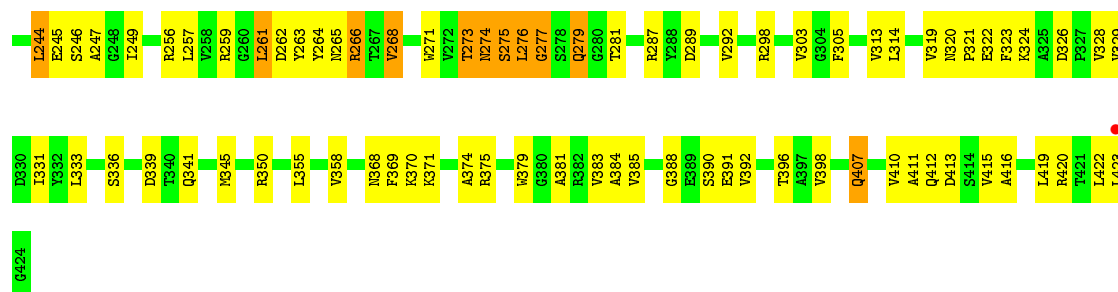
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	49	Total 49	O 49	0	0
3	C	45	Total 45	O 45	0	0
3	D	66	Total 66	O 66	0	0

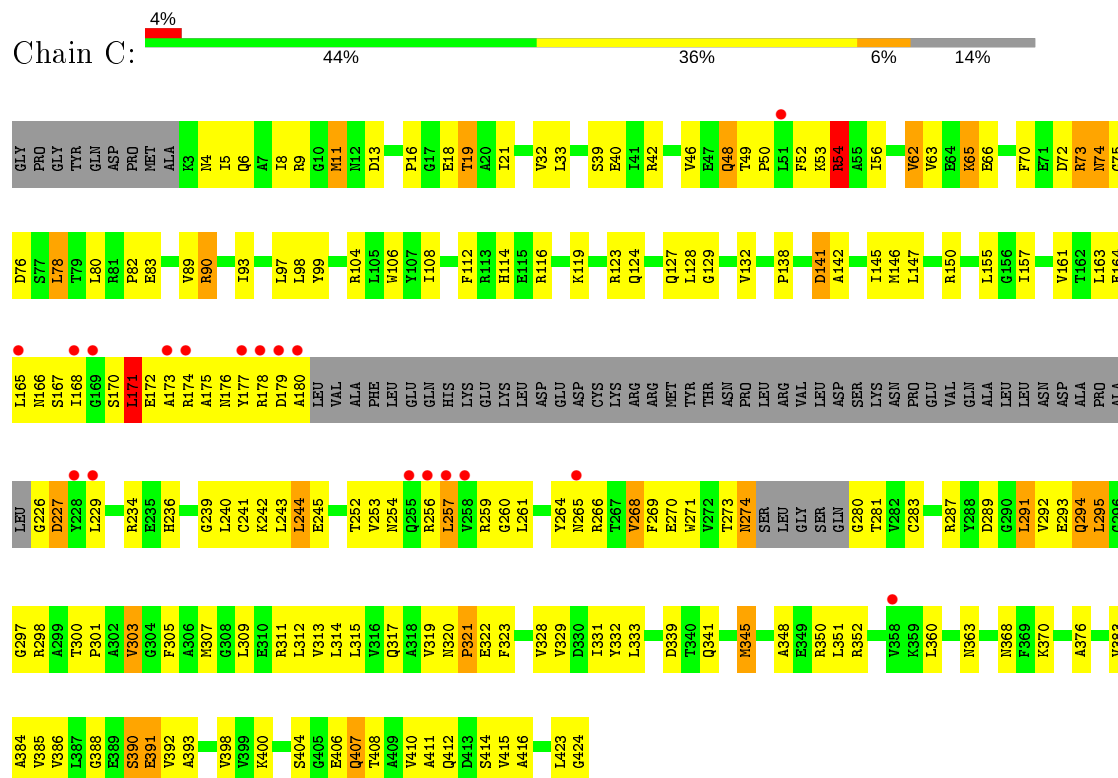
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 5% 41% 39% 6% 14%
- GLY PRO GLY TYR GLN ASP PRO MET MET K3 N4 I5 I8 R9 G10 M11 H12 D13 Y14 L15 P16 G17 E18 T19 A20 I21 V22 T28 V32 L33 Y38 S39 E40 I41 R42 R43 L43 P44 I45 V46 E47 Q48 T49 P50 L51 F52 K53 R54 A55 I56 V63 E64 K65 E66 M67 Y68 T69 D72 R73 I74 G75 D76 S77 L78 T79 L80 M81 R82 B83 R90 G96 L97 L98 E102 G103 R104 L105 W106 I107 I108 F112 R113 H114 E115 Q118 R121 Y122 R123 Q124 F125 L128 E131 V132 F133 Q136 G137 P138 D139 I140 D141 A142 M146 A149 Y150 W151 W152 L155 V161 T162 L163 E164 L165 M166 S167 L168 G169 S170 L171 E172 A173 R174 A175 N176 Y177 R178 D179 A180 VAL LEU ALA PHE LEU GLU GLN HIS LYS GLY LEU LYS LEU ASP GLU R254 Q255 R256 L257 V258 R259 G260 L261 Y264 H265 R266 T267 V268 F269 G270 W271 V272 ASP T273 I274 SER SER ASN LEU GLY PRO GLN SER SER E336 D339 T340 V345

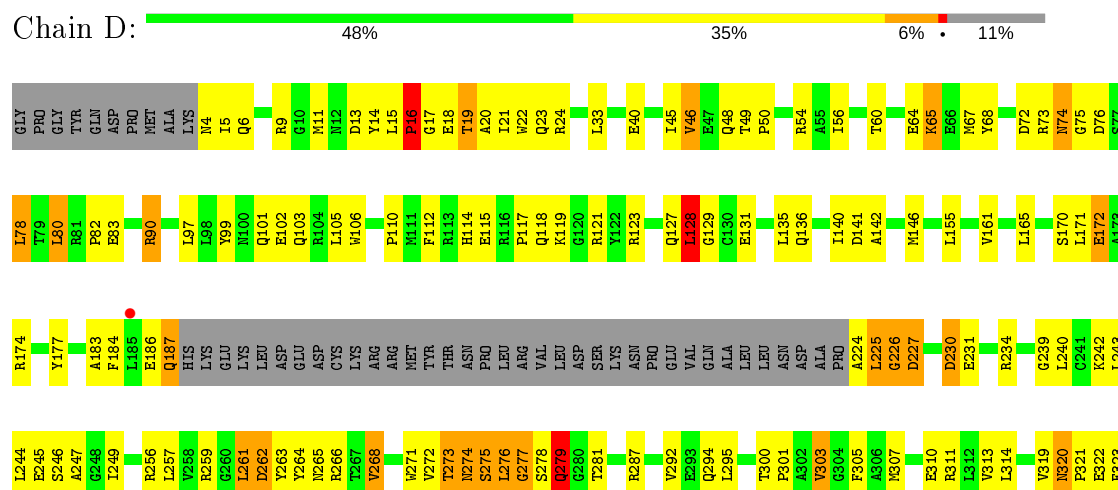
- [illegible]



• Molecule 1: Histidyl-tRNA synthetase



• Molecule 1: Histidyl-tRNA synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.11Å 108.34Å 193.65Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	48.80 – 2.70 48.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.80-2.70) 95.4 (48.80-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.285 0.220 , 0.278	Depositor DCC
R_{free} test set	6521 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8788e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HSS

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	0.48	0/2955	0.74	0/3995
1	B	0.50	1/2976 (0.0%)	0.74	0/4025
1	C	0.45	0/2951	0.71	2/3989 (0.1%)
1	D	0.50	0/3047	0.75	1/4122 (0.0%)
All	All	0.48	1/11929 (0.0%)	0.74	3/16131 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	CYS	CB-SG	-5.18	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	171	LEU	CA-CB-CG	5.14	127.12	115.30
1	D	128	LEU	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2903	0	2869	198	0
1	B	2923	0	2888	144	0
1	C	2899	0	2861	191	0
1	D	2993	0	2956	177	0
2	A	33	0	21	4	0
2	B	33	0	21	2	0
2	C	33	0	21	9	0
2	D	33	0	21	5	0
3	A	40	0	0	2	0
3	B	49	0	0	2	0
3	C	45	0	0	1	0
3	D	66	0	0	4	0
All	All	12050	0	11658	659	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 28.

The worst 5 of 659 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:287:ARG:HG2	1:A:303:VAL:HG13	1.32	1.06
1:C:127:GLN:HE22	2:C:710:HSS:H5'2	1.25	1.01
1:A:320:ASN:HD22	1:A:320:ASN:N	1.55	1.00
1:C:127:GLN:NE2	2:C:710:HSS:H5'2	1.79	0.97
1:C:74:ASN:ND2	1:C:76:ASP:H	1.60	0.97

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	366/431 (85%)	324 (88%)	31 (8%)	11 (3%)	4 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	372/431 (86%)	343 (92%)	18 (5%)	11 (3%)	4	10
1	C	366/431 (85%)	329 (90%)	26 (7%)	11 (3%)	4	10
1	D	381/431 (88%)	330 (87%)	39 (10%)	12 (3%)	4	9
All	All	1485/1724 (86%)	1326 (89%)	114 (8%)	45 (3%)	4	10

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	266	ARG
1	B	274	ASN
1	B	275	SER
1	C	4	ASN

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	297/347 (86%)	267 (90%)	30 (10%)	7	17
1	B	299/347 (86%)	267 (89%)	32 (11%)	6	15
1	C	296/347 (85%)	269 (91%)	27 (9%)	9	21
1	D	306/347 (88%)	273 (89%)	33 (11%)	6	15
All	All	1198/1388 (86%)	1076 (90%)	122 (10%)	7	17

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	303	VAL
1	C	65	LYS
1	D	268	VAL
1	B	314	LEU
1	B	407	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	274	ASN
1	C	127	GLN
1	D	236	HIS
1	B	279	GLN
1	B	320	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	HSS	A	510	-	29,36,36	2.99	6 (20%)	31,53,53	2.38	5 (16%)
2	HSS	B	610	-	29,36,36	3.01	6 (20%)	31,53,53	1.69	6 (19%)
2	HSS	C	710	-	29,36,36	3.01	6 (20%)	31,53,53	2.07	5 (16%)
2	HSS	D	810	-	29,36,36	3.00	6 (20%)	31,53,53	1.87	7 (22%)

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
2	HSS	A	510	-	-	2/18/39/39	0/4/4/4
2	HSS	B	610	-	-	4/18/39/39	0/4/4/4
2	HSS	C	710	-	-	7/18/39/39	0/4/4/4
2	HSS	D	810	-	-	5/18/39/39	0/4/4/4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	HSS	O2S-S	9.72	1.50	1.42
2	C	710	HSS	O2S-S	9.54	1.50	1.42
2	D	810	HSS	O2S-S	9.53	1.50	1.42
2	A	510	HSS	O3S-S	9.50	1.50	1.42
2	C	710	HSS	O3S-S	9.34	1.50	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	710	HSS	C-N1S-S	-8.66	110.59	124.61
2	A	510	HSS	C-N1S-S	-7.96	111.73	124.61
2	A	510	HSS	O3S-S-O2S	-7.38	109.26	120.76
2	D	810	HSS	C-N1S-S	-6.29	114.43	124.61
2	B	610	HSS	C-N1S-S	-4.91	116.66	124.61

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

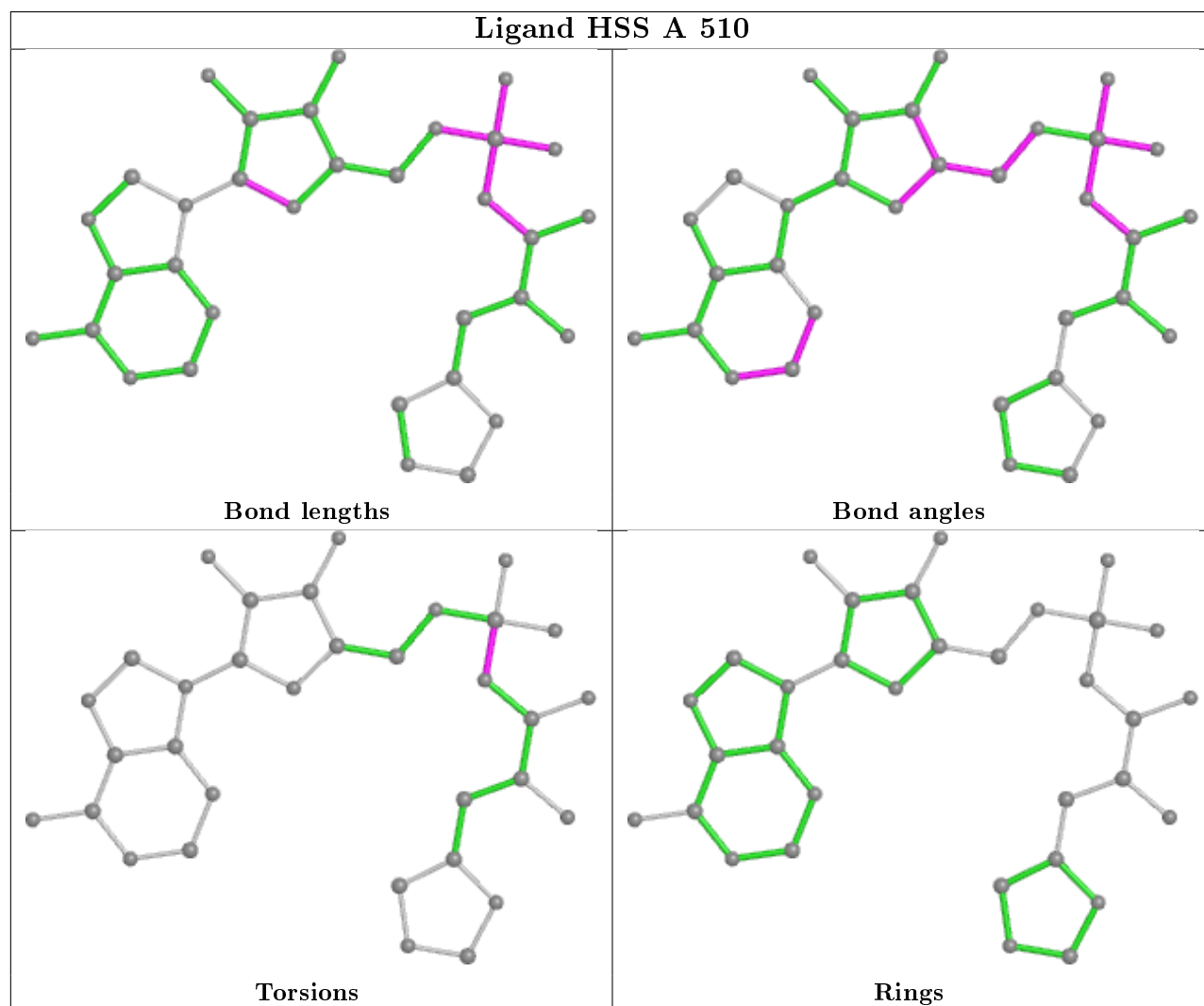
Mol	Chain	Res	Type	Atoms
2	A	510	HSS	C-N1S-S-O2S
2	A	510	HSS	C-N1S-S-O3S
2	B	610	HSS	N1S-C-CA-CB
2	C	710	HSS	CA-CB-CG-N11
2	D	810	HSS	C5'-O5'-S-N1S

There are no ring outliers.

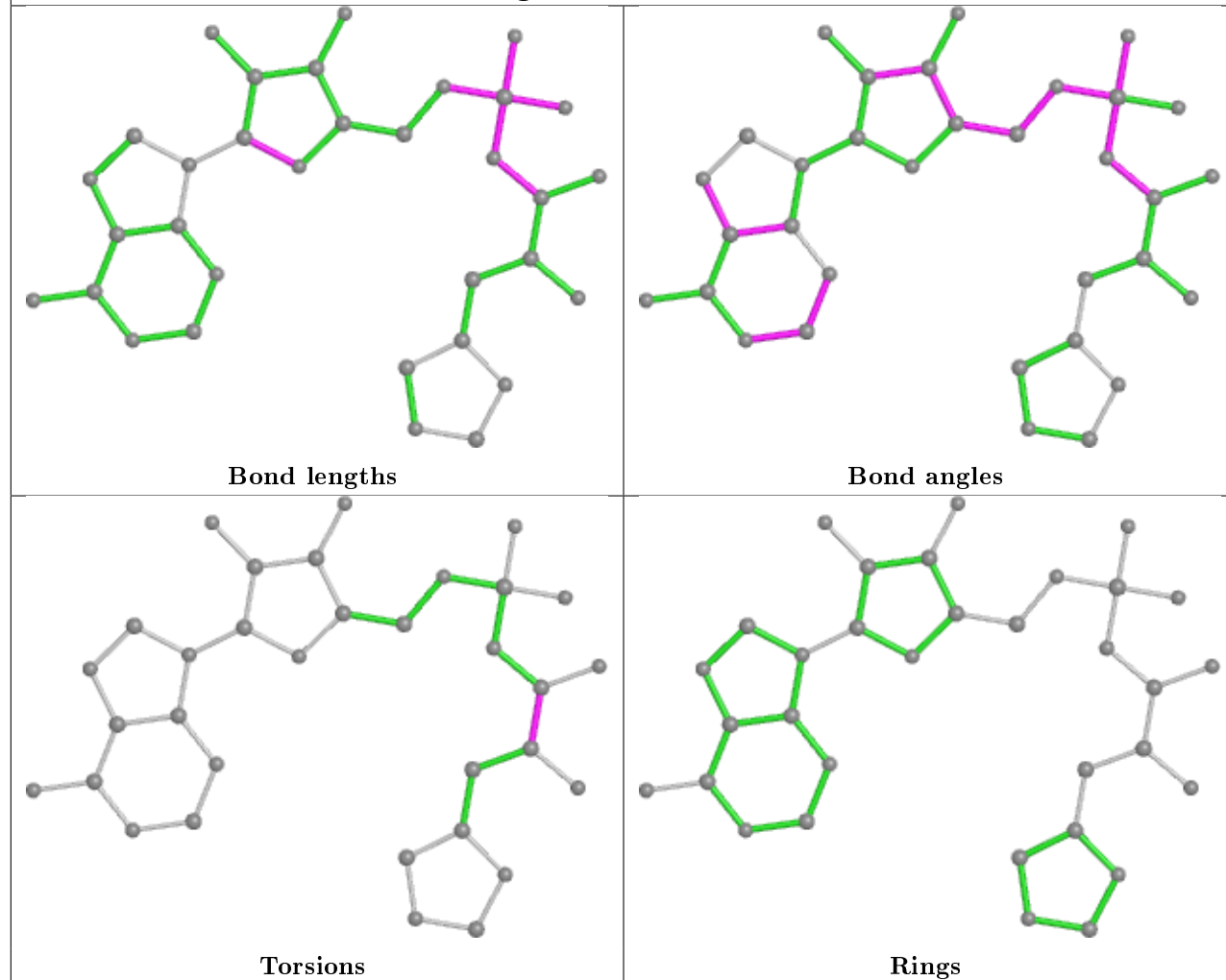
4 monomers are involved in 20 short contacts:

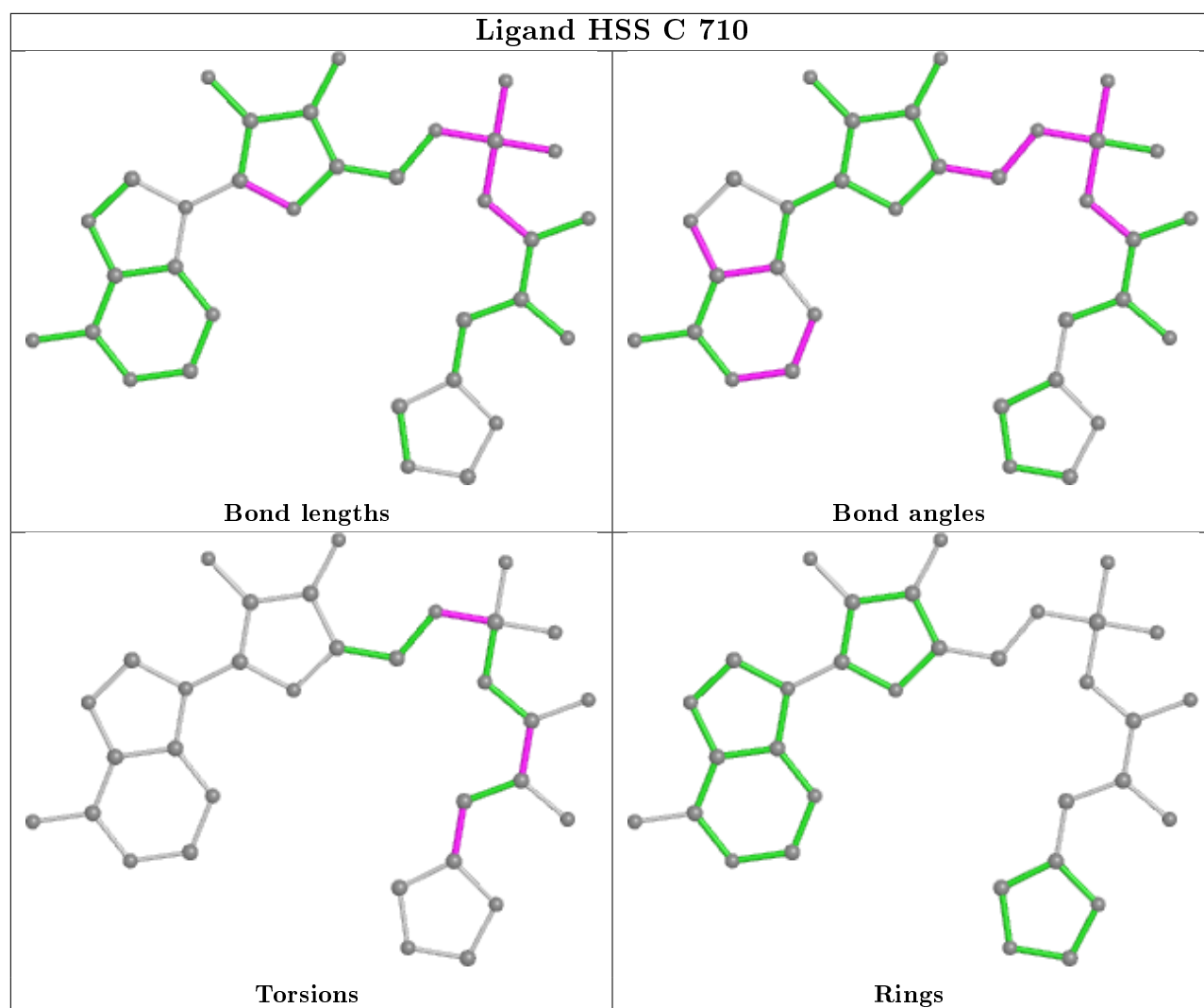
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	510	HSS	4	0
2	B	610	HSS	2	0
2	C	710	HSS	9	0
2	D	810	HSS	5	0

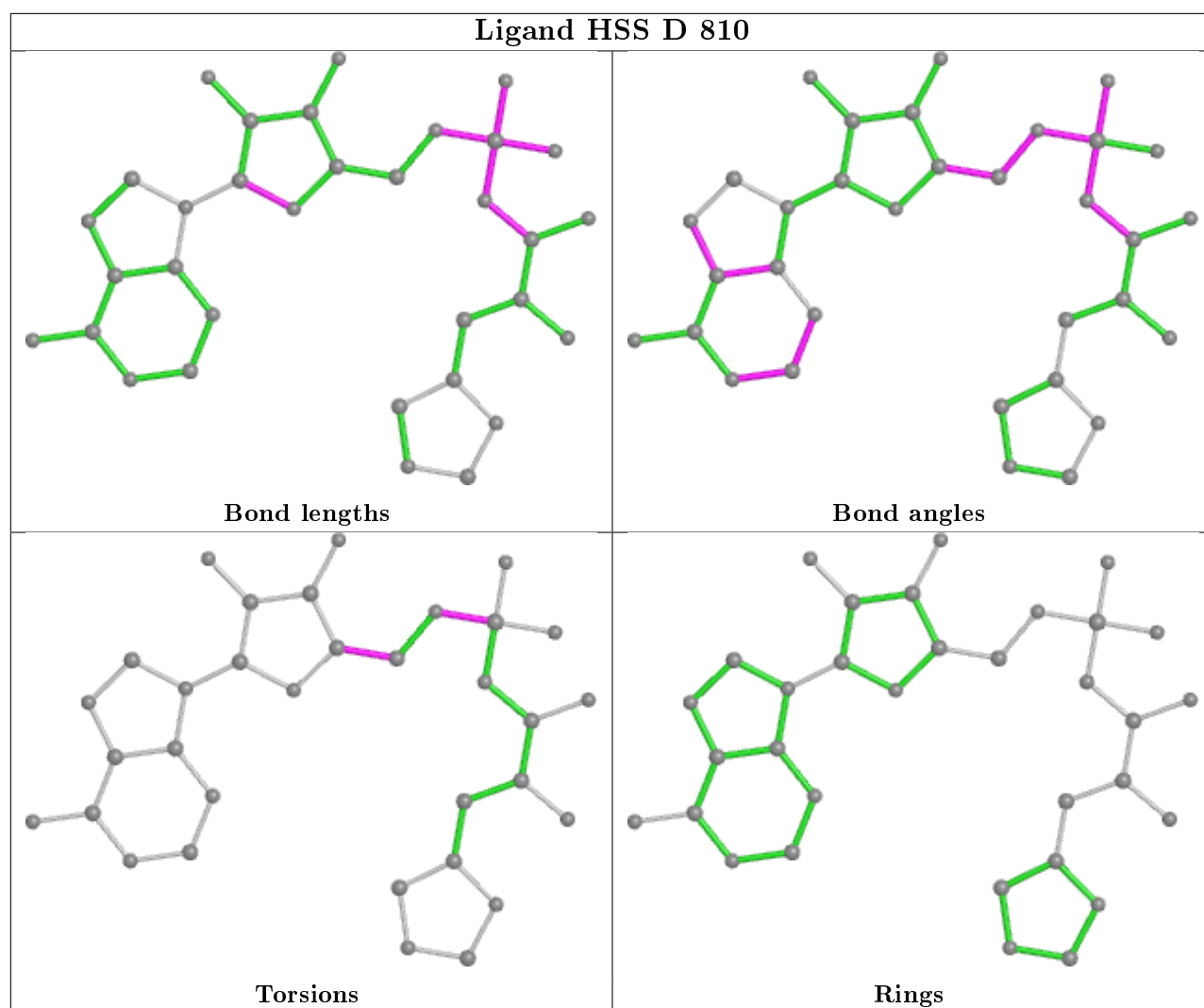
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HSS B 610







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	372/431 (86%)	0.15	22 (5%) 22 21	27, 57, 113, 140	0
1	B	376/431 (87%)	-0.14	1 (0%) 94 95	21, 50, 90, 109	0
1	C	372/431 (86%)	0.12	18 (4%) 30 28	27, 56, 111, 129	0
1	D	385/431 (89%)	-0.09	1 (0%) 94 95	19, 51, 97, 136	0
All	All	1505/1724 (87%)	0.01	42 (2%) 53 54	19, 54, 104, 140	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	LEU	6.1
1	A	225	LEU	5.4
1	A	175	ALA	5.2
1	A	228	TYR	4.7
1	C	173	ALA	4.6

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

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

6.3 Carbohydrates [i](#)

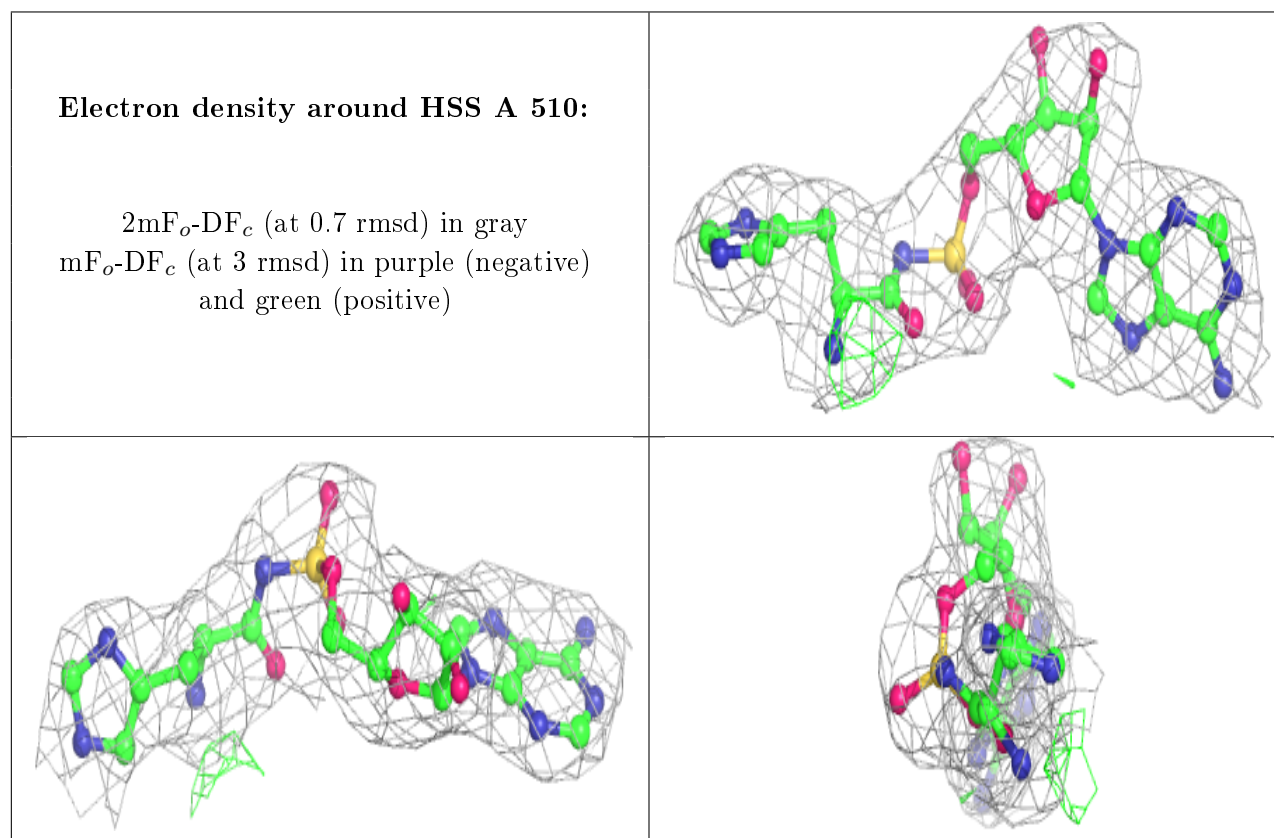
There are no carbohydrates in this entry.

6.4 Ligands [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.

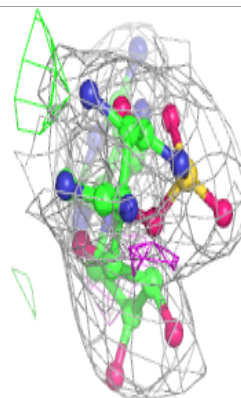
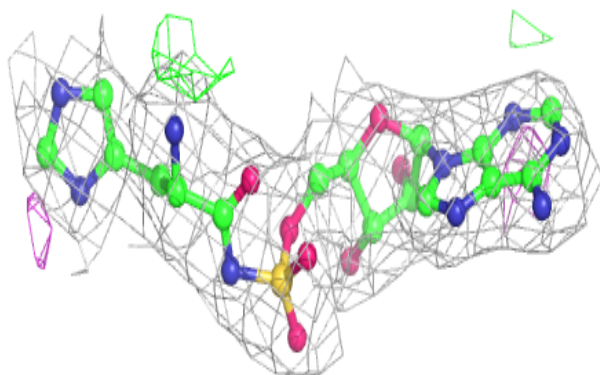
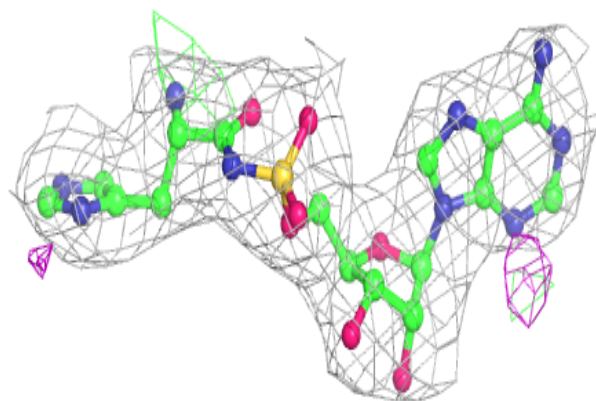
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HSS	A	510	33/33	0.97	0.15	23,48,71,77	0
2	HSS	C	710	33/33	0.97	0.16	39,49,66,71	0
2	HSS	B	610	33/33	0.98	0.17	17,31,38,49	0
2	HSS	D	810	33/33	0.98	0.15	15,30,37,44	0

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.

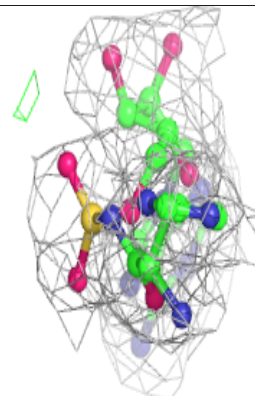
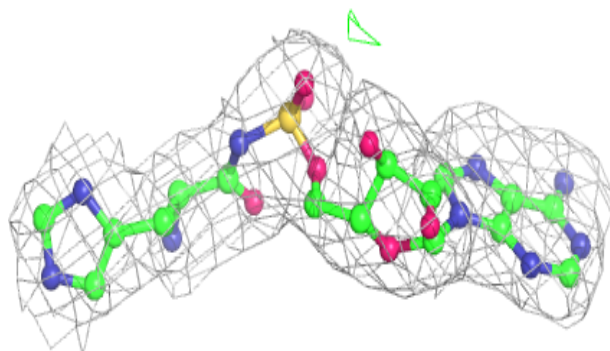
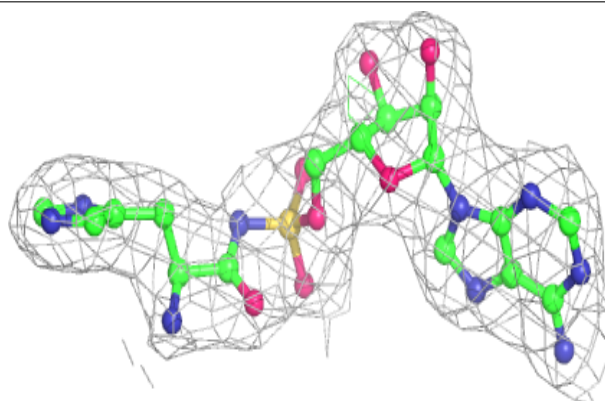


Electron density around HSS C 710:

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

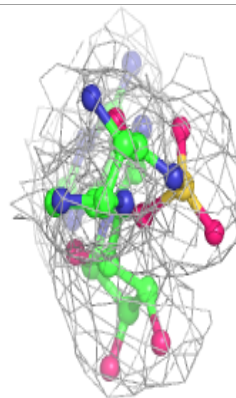
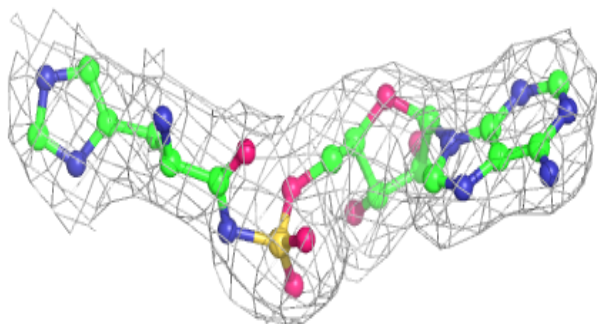
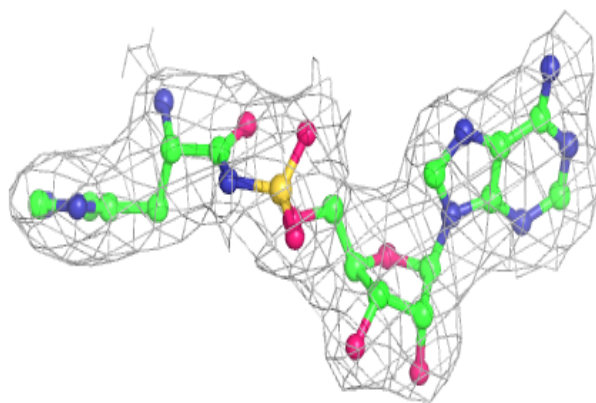
**Electron density around HSS B 610:**

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



Electron density around HSS D 810:

$2mF_o-DF_c$ (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.