



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2024 – 04:50 pm BST

PDB ID : 7OOG
Title : Plasmodium falciparum Hsp70-x chaperone nucleotide binding domain in complex with NCL-00023823
Authors : Mohamad, N.; O'Donoghue, A.; Kantsadi, A.L.; Vakonakis, I.
Deposited on : 2021-05-27
Resolution : 2.42 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

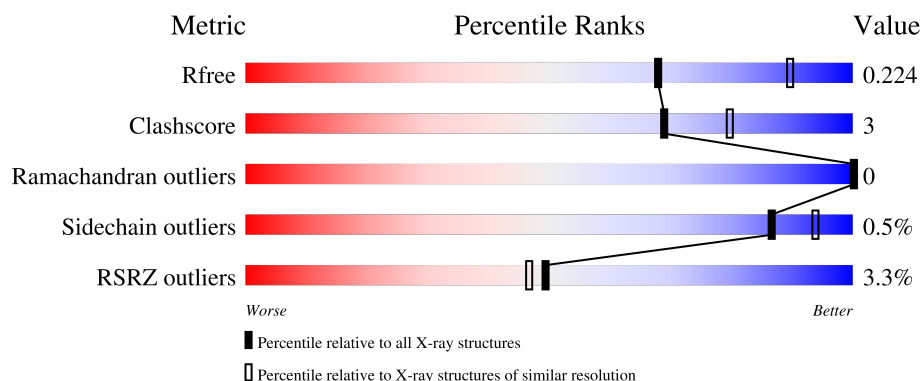
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

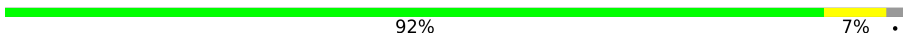

The reported resolution of this entry is 2.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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 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	393	
1	B	393	

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
2	GOL	B	505	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6195 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.

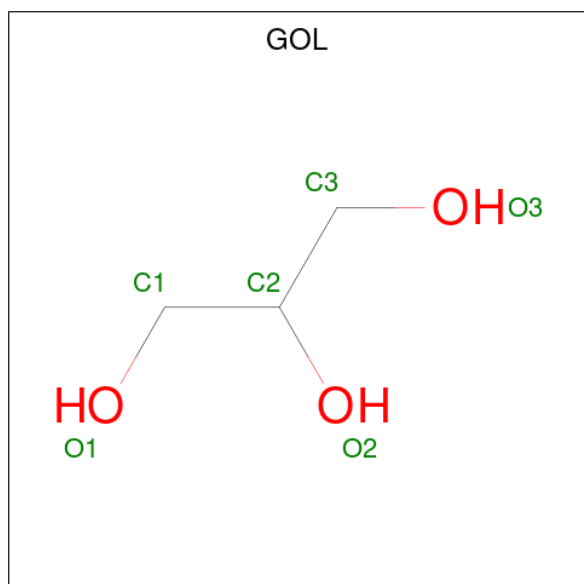
- Molecule 1 is a protein called Heat shock protein 70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	2	0
			2968	1858	515	582	13			
1	B	380	Total	C	N	O	S	0	0	0
			2917	1829	504	572	12			

There are 4 discrepancies between the modelled and reference sequences:

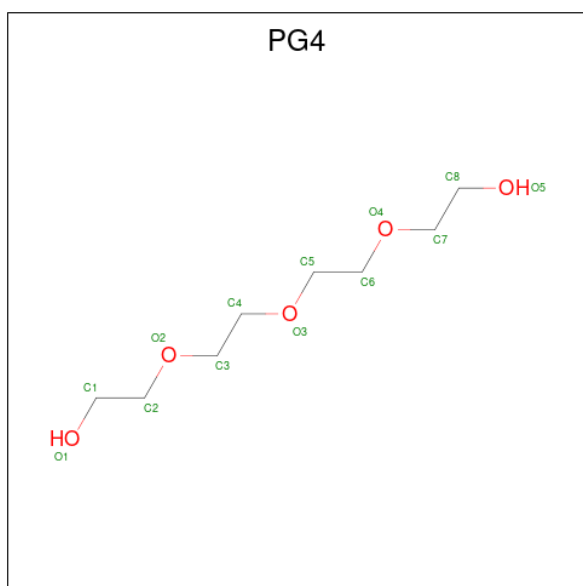
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP K7NTP5
A	28	PRO	-	expression tag	UNP K7NTP5
B	27	GLY	-	expression tag	UNP K7NTP5
B	28	PRO	-	expression tag	UNP K7NTP5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



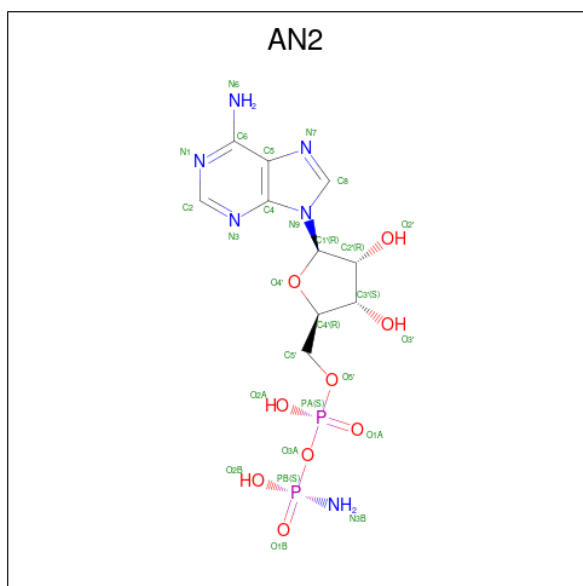
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0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

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



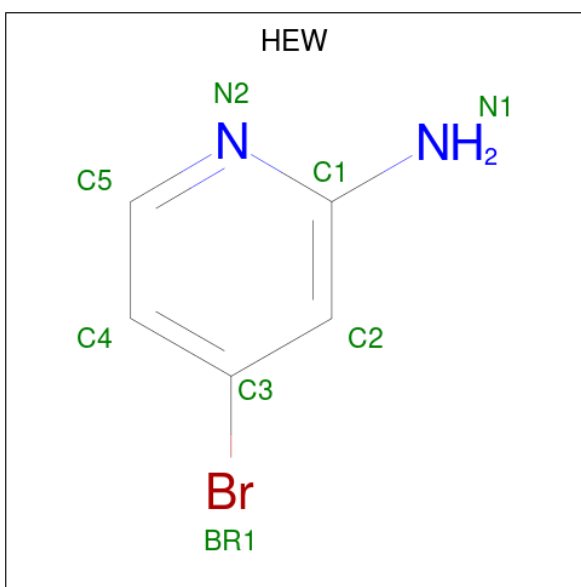
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	5	2		

- Molecule 4 is AMP PHOSPHORAMIDATE (three-letter code: AN2) (formula: $C_{10}H_{16}N_6O_9P_2$).



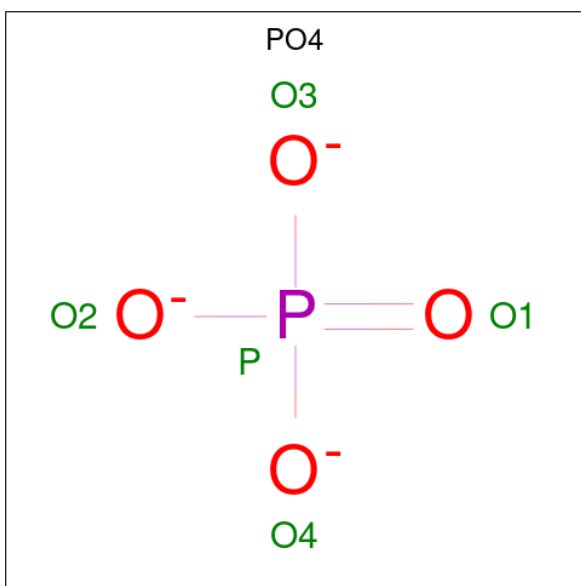
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

- Molecule 5 is 4-bromanlypyridin-2-amine (three-letter code: HEW) (formula: $C_5H_5BrN_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	95	Total	O	0	0
			95	95		
9	B	46	Total	O	0	0
			46	46		

3 Residue-property plots [i](#)

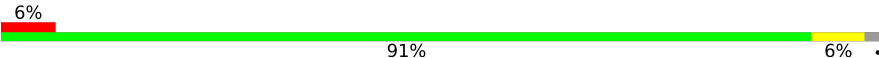
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

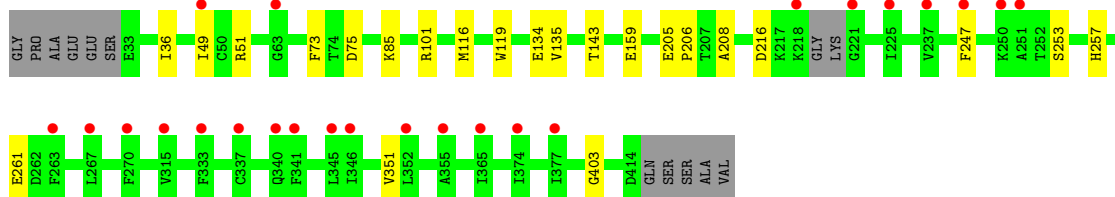
- Molecule 1: Heat shock protein 70

Chain A:  92% 7% .



- Molecule 1: Heat shock protein 70

Chain B:  6% 91% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 101.03Å 103.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.19 – 2.42 72.19 – 2.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.19-2.42) 100.0 (72.19-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.209 , 0.234 0.202 , 0.224	Depositor DCC
R_{free} test set	1609 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: PG4, GOL, PO4, HEW, CL, CSX, MG, AN2

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	0.45	0/3001	0.57	0/4041
1	B	0.38	0/2950	0.54	0/3973
All	All	0.42	0/5951	0.56	0/8014

There are no bond length outliers.

There are no bond angle outliers.

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	2968	0	2995	20	0
1	B	2917	0	2937	20	0
2	A	48	0	64	7	0
2	B	30	0	40	10	0
3	A	7	0	6	1	0
4	A	27	0	14	2	0
4	B	27	0	14	0	0
5	A	8	0	0	1	0
5	B	8	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	2	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	95	0	0	1	0
9	B	46	0	0	0	0
All	All	6195	0	6070	41	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 3.

All (41) 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:216:ASP:HA	1:A:242:LEU:HD21	1.43	0.98
1:A:303:ARG:HH12	2:A:507:GOL:H12	1.29	0.96
1:A:44:TYR:H	4:A:503:AN2:H3B2	1.17	0.93
1:A:101:ARG:HA	2:A:504:GOL:H31	1.60	0.82
1:A:43:THR:H	4:A:503:AN2:H3B1	1.29	0.79
1:B:85:LYS:HZ1	2:B:505:GOL:H12	1.57	0.70
2:A:505:GOL:H32	9:A:665:HOH:O	1.91	0.70
1:B:85:LYS:NZ	2:B:505:GOL:H11	2.08	0.69
1:B:85:LYS:HZ1	2:B:505:GOL:C1	2.08	0.67
1:B:85:LYS:HZ2	2:B:505:GOL:H11	1.62	0.65
1:A:134:GLU:HG2	1:A:143:THR:HG22	1.80	0.63
1:B:85:LYS:NZ	2:B:505:GOL:C1	2.62	0.63
1:A:216:ASP:HA	1:A:242:LEU:CD2	2.25	0.62
1:B:134:GLU:HG2	1:B:143:THR:HG22	1.83	0.61
1:B:51:ARG:NH2	2:B:501:GOL:O1	2.35	0.59
1:A:261:GLU:OE2	5:A:511:HEW:C1	2.53	0.57
1:A:59:ALA:HB3	3:A:502:PG4:H51	1.88	0.56
1:A:105:ARG:HH21	2:A:504:GOL:H32	1.71	0.56
1:A:303:ARG:HH12	2:A:507:GOL:C1	2.12	0.55
1:B:101:ARG:HG2	2:B:503:GOL:H11	1.88	0.54
1:B:116:MET:HA	1:B:119:TRP:CE3	2.45	0.52
1:B:36:ILE:HG22	1:B:49:ILE:HG22	1.92	0.52
1:A:303:ARG:NH1	2:A:507:GOL:H12	2.13	0.50
1:A:239:LEU:HD23	1:A:355:ALA:CB	2.43	0.48
1:B:36:ILE:HG22	1:B:49:ILE:CG2	2.43	0.48
1:B:159:GLU:HB3	2:B:504:GOL:H11	1.95	0.48
1:B:257:HIS:HD2	5:B:511:HEW:C3	2.26	0.48
1:A:261:GLU:HB3	2:A:508:GOL:H31	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLU:HB3	2:B:505:GOL:H31	1.98	0.46
1:A:208:ALA:O	1:A:403:GLY:HA3	2.17	0.44
1:B:208:ALA:O	1:B:403:GLY:HA3	2.18	0.43
1:B:253:SER:OG	1:B:351:VAL:HG13	2.19	0.42
1:A:41:GLY:HA3	1:A:44:TYR:O	2.19	0.42
1:A:216:ASP:HB3	1:A:247:PHE:CE2	2.54	0.42
1:B:205:GLU:N	1:B:206:PRO:HD2	2.34	0.42
1:B:216:ASP:HB3	1:B:247:PHE:CE2	2.54	0.42
1:B:73:PHE:CD1	1:B:135:VAL:HG21	2.55	0.42
1:B:159:GLU:CB	2:B:504:GOL:H11	2.49	0.41
1:A:73:PHE:CD1	1:A:135:VAL:HG21	2.55	0.41
1:A:205:GLU:N	1:A:206:PRO:HD2	2.36	0.40
1:A:230:LEU:HG	1:A:371:SER:HB2	2.03	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	384/393 (98%)	379 (99%)	5 (1%)	0	100	100
1	B	375/393 (95%)	372 (99%)	3 (1%)	0	100	100
All	All	759/786 (97%)	751 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	322/326 (99%)	320 (99%)	2 (1%)	84	92
1	B	317/326 (97%)	316 (100%)	1 (0%)	91	96
All	All	639/652 (98%)	636 (100%)	3 (0%)	86	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	A	111	THR
1	B	75	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	CSX	B	391	1	3,6,7	0.79	0	1,6,8	0.76	0
1	CSX	A	391[A]	-	3,6,7	0.68	0	1,6,8	2.42	1 (100%)
1	CSX	A	391[B]	-	3,6,7	0.96	0	1,6,8	2.10	1 (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
1	CSX	B	391	1	-	1/1/5/7	-
1	CSX	A	391[A]	-	-	0/1/5/7	-
1	CSX	A	391[B]	-	-	0/1/5/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	391[A]	CSX	CA-CB-SG	-2.42	108.06	113.36
1	A	391[B]	CSX	CA-CB-SG	2.10	117.94	113.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	391	CSX	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.11	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	501	-	5,5,5	0.21	0	5,5,5	0.24	0
3	PG4	A	502	-	6,6,12	0.17	0	5,5,11	0.09	0
6	PO4	B	508	8	4,4,4	2.49	2 (50%)	6,6,6	0.53	0
2	GOL	B	505	-	5,5,5	0.11	0	5,5,5	0.32	0
4	AN2	B	502	-	24,29,29	2.15	5 (20%)	25,45,45	1.34	3 (12%)
2	GOL	A	508	-	5,5,5	0.20	0	5,5,5	0.49	0
4	AN2	A	503	8	24,29,29	2.02	2 (8%)	25,45,45	1.53	3 (12%)
2	GOL	A	510	-	5,5,5	0.20	0	5,5,5	0.22	0
2	GOL	A	506	-	5,5,5	0.11	0	5,5,5	0.21	0
2	GOL	B	506	-	5,5,5	0.12	0	5,5,5	0.31	0
2	GOL	B	504	-	5,5,5	0.11	0	5,5,5	0.24	0
5	HEW	B	511	-	8,8,8	0.37	0	9,10,10	0.70	0
2	GOL	A	509	-	5,5,5	0.11	0	5,5,5	0.16	0
2	GOL	B	503	-	5,5,5	0.13	0	5,5,5	0.33	0
2	GOL	A	504	-	5,5,5	0.35	0	5,5,5	0.78	0
5	HEW	A	511	-	8,8,8	0.50	0	9,10,10	0.86	0
2	GOL	A	505	-	5,5,5	0.12	0	5,5,5	0.38	0
2	GOL	A	507	-	5,5,5	0.27	0	5,5,5	0.39	0
6	PO4	A	512	-	4,4,4	2.49	1 (25%)	6,6,6	0.37	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
2	GOL	A	501	-	-	0/4/4/4	-
2	GOL	B	501	-	-	2/4/4/4	-
2	GOL	A	509	-	-	2/4/4/4	-
2	GOL	B	503	-	-	2/4/4/4	-
2	GOL	A	504	-	-	1/4/4/4	-
2	GOL	A	508	-	-	4/4/4/4	-
3	PG4	A	502	-	-	2/4/4/10	-
4	AN2	A	503	8	-	0/9/32/32	0/3/3/3
2	GOL	A	505	-	-	2/4/4/4	-
2	GOL	A	507	-	-	0/4/4/4	-
2	GOL	A	510	-	-	2/4/4/4	-
2	GOL	A	506	-	-	0/4/4/4	-
2	GOL	B	506	-	-	1/4/4/4	-
5	HEW	A	511	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	504	-	-	4/4/4/4	-
5	HEW	B	511	-	-	-	0/1/1/1
4	AN2	B	502	-	-	1/9/32/32	0/3/3/3
2	GOL	B	505	-	-	0/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	AN2	PB-O1B	8.71	1.60	1.46
4	A	503	AN2	PB-O1B	8.57	1.59	1.46
6	A	512	PO4	P-O1	4.11	1.60	1.50
6	B	508	PO4	P-O1	4.10	1.60	1.50
4	A	503	AN2	PB-O2B	-3.09	1.48	1.56
4	B	502	AN2	PB-O2B	-2.92	1.48	1.56
4	B	502	AN2	PB-O3A	2.34	1.62	1.59
4	B	502	AN2	C5-C4	2.32	1.47	1.40
4	B	502	AN2	C2-N3	2.08	1.35	1.32
6	B	508	PO4	P-O2	2.01	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	AN2	O4'-C1'-C2'	-4.17	100.83	106.93
4	B	502	AN2	N3-C2-N1	-3.68	122.92	128.68
4	A	503	AN2	N3-C2-N1	-3.64	122.98	128.68
4	B	502	AN2	O4'-C1'-C2'	-2.77	102.88	106.93
4	B	502	AN2	C4-C5-N7	-2.25	107.06	109.40
4	A	503	AN2	N6-C6-N1	2.13	123.00	118.57

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	509	GOL	C1-C2-C3-O3
2	A	504	GOL	C1-C2-C3-O3
2	A	508	GOL	C1-C2-C3-O3
2	A	510	GOL	C1-C2-C3-O3
2	B	501	GOL	C1-C2-C3-O3
2	B	503	GOL	C1-C2-C3-O3
2	B	504	GOL	O1-C1-C2-C3
2	A	509	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	504	GOL	O1-C1-C2-O2
2	A	508	GOL	O1-C1-C2-O2
3	A	502	PG4	C6-C5-O3-C4
2	A	508	GOL	O2-C2-C3-O3
2	A	510	GOL	O2-C2-C3-O3
2	B	501	GOL	O2-C2-C3-O3
3	A	502	PG4	C3-C4-O3-C5
2	A	508	GOL	O1-C1-C2-C3
2	B	504	GOL	C1-C2-C3-O3
4	B	502	AN2	PB-O3A-PA-O2A
2	A	505	GOL	C1-C2-C3-O3
2	B	506	GOL	O1-C1-C2-C3
2	A	505	GOL	O2-C2-C3-O3
2	B	503	GOL	O2-C2-C3-O3
2	B	504	GOL	O2-C2-C3-O3

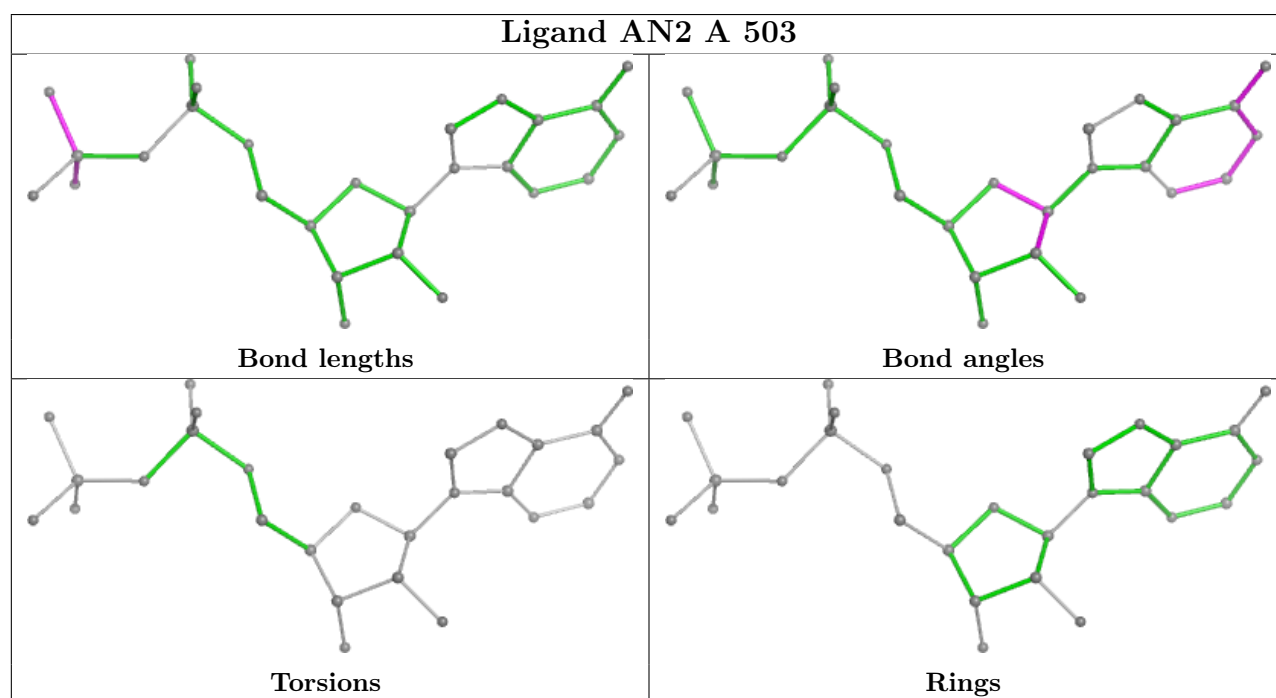
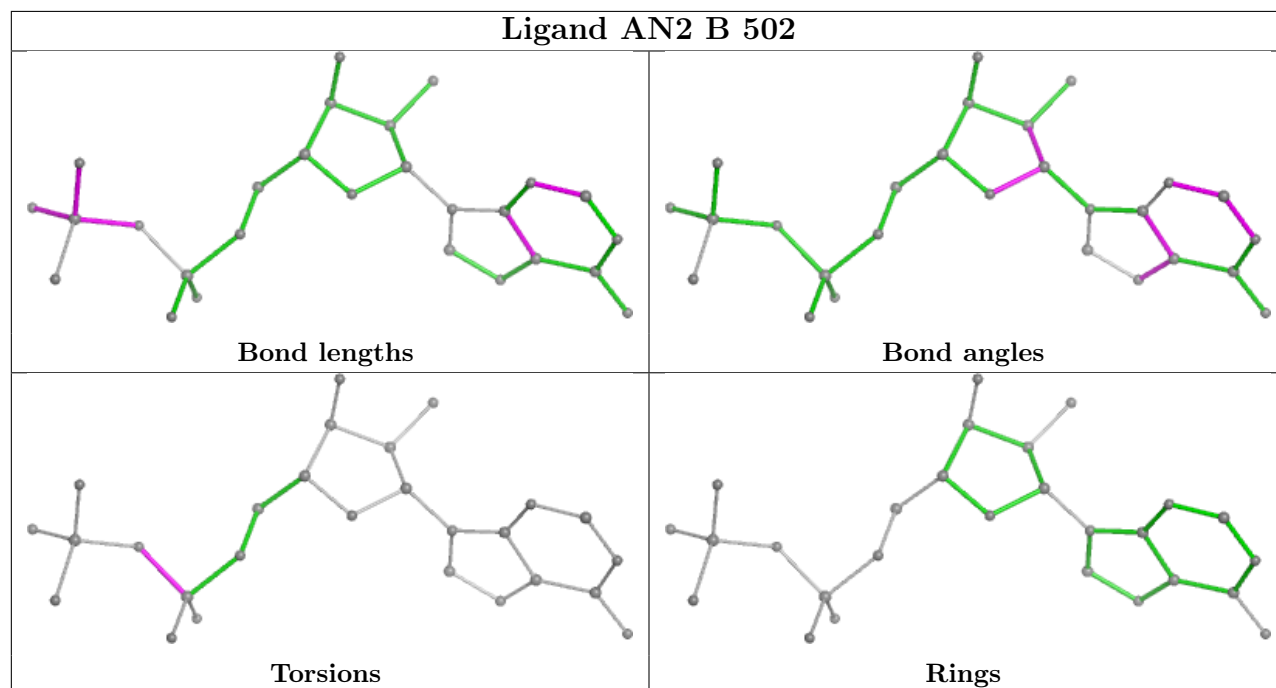
There are no ring outliers.

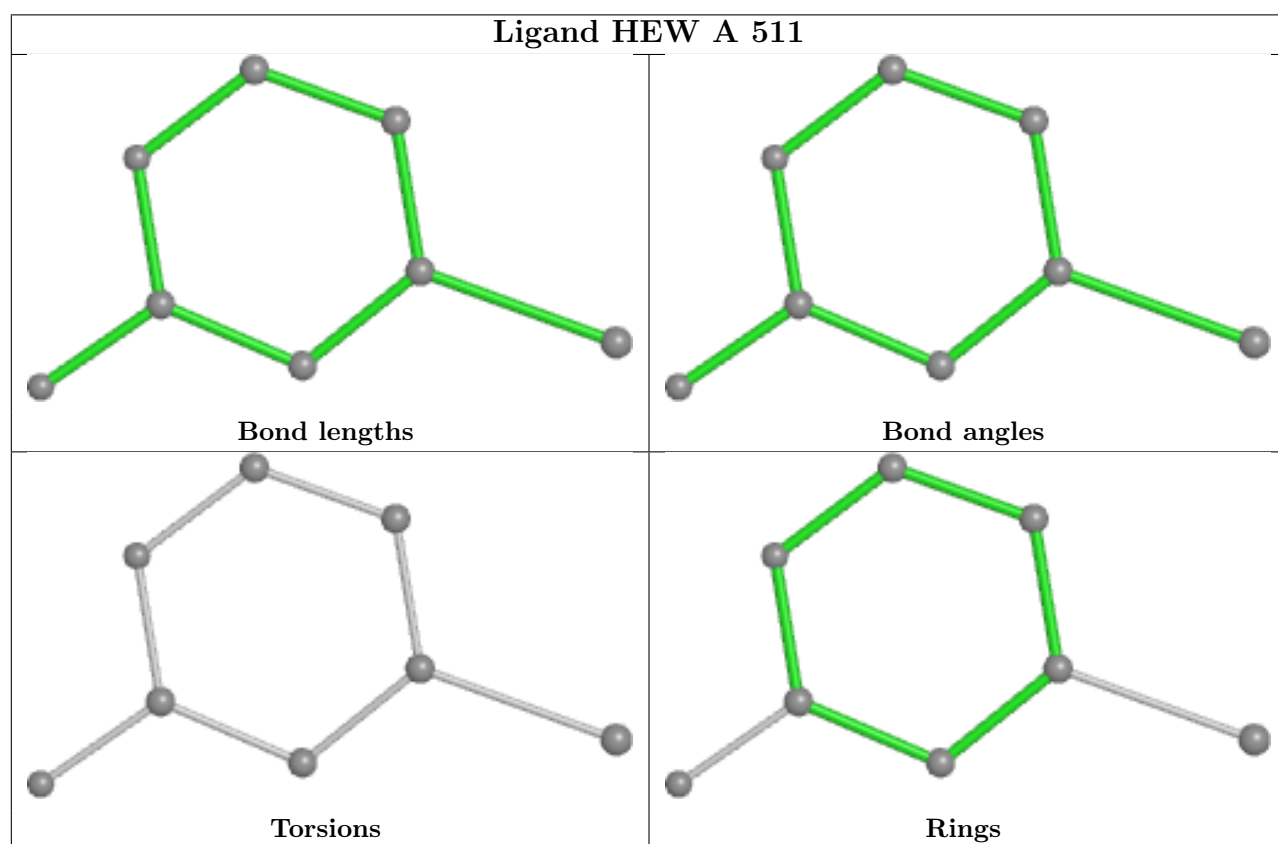
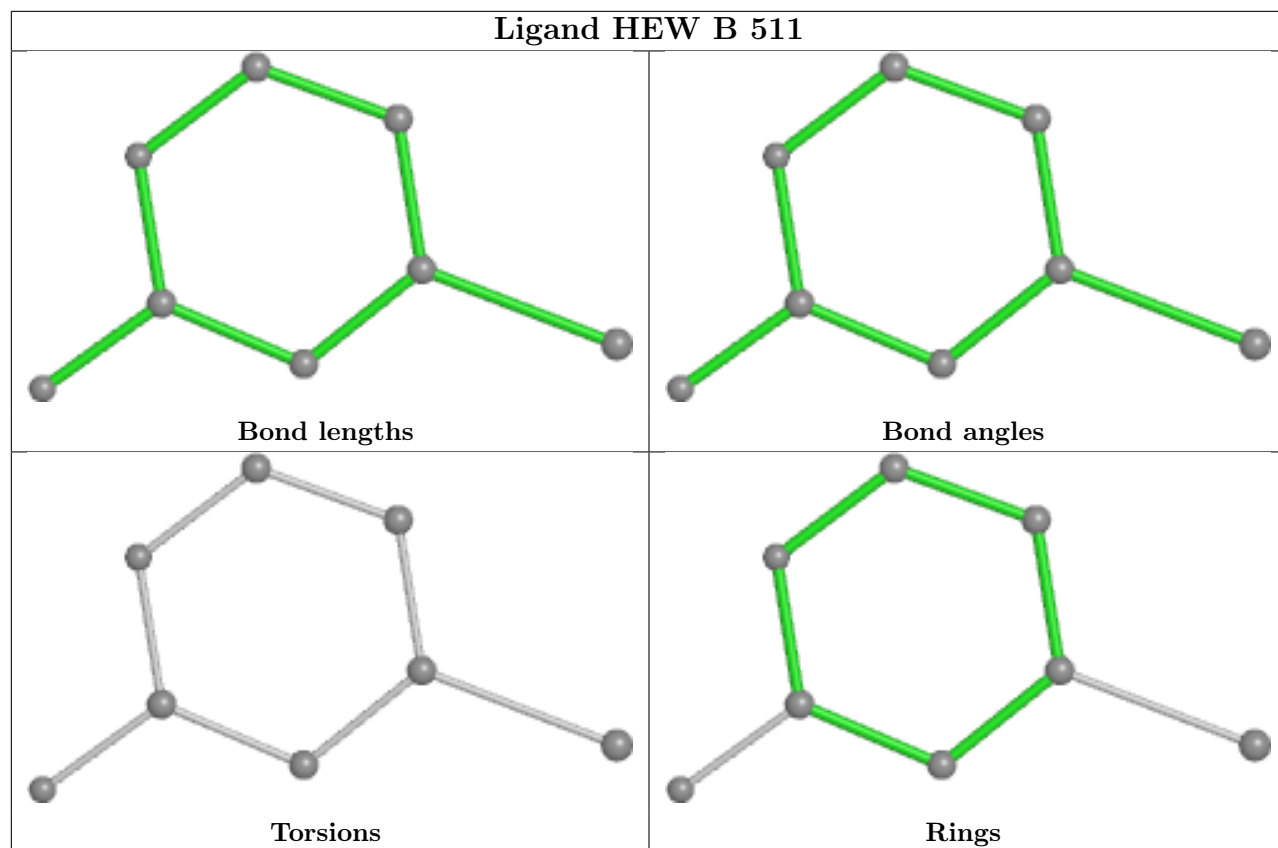
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	GOL	1	0
3	A	502	PG4	1	0
2	B	505	GOL	6	0
2	A	508	GOL	1	0
4	A	503	AN2	2	0
2	B	504	GOL	2	0
5	B	511	HEW	1	0
2	B	503	GOL	1	0
2	A	504	GOL	2	0
5	A	511	HEW	1	0
2	A	505	GOL	1	0
2	A	507	GOL	3	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

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	385/393 (97%)	0.03	1 (0%) 90 89	30, 67, 102, 119	1 (0%)
1	B	379/393 (96%)	0.68	24 (6%) 27 25	53, 91, 148, 170	0
All	All	764/786 (97%)	0.35	25 (3%) 49 47	30, 77, 138, 170	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	333	PHE	5.7
1	A	418	ALA	3.3
1	B	377	ILE	3.1
1	B	225	ILE	2.7
1	B	263	PHE	2.7
1	B	270	PHE	2.7
1	B	237	VAL	2.6
1	B	346	ILE	2.6
1	B	340	GLN	2.6
1	B	250	LYS	2.5
1	B	345	LEU	2.5
1	B	355	ALA	2.4
1	B	251	ALA	2.4
1	B	374	ILE	2.4
1	B	221	GLY	2.4
1	B	315	VAL	2.2
1	B	267	LEU	2.2
1	B	365	ILE	2.2
1	B	218	LYS	2.2
1	B	337	CYS	2.1
1	B	352	LEU	2.1
1	B	247	PHE	2.1
1	B	341	PHE	2.1
1	B	63	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	A	391[A]	7/8	0.89	0.11	64,66,72,72	4
1	CSX	A	391[B]	7/8	0.89	0.11	64,65,70,70	4
1	CSX	B	391	7/8	0.91	0.12	100,103,108,108	0

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
2	GOL	A	506	6/6	0.61	0.18	98,98,99,99	0
2	GOL	B	506	6/6	0.65	0.24	106,107,107,107	0
2	GOL	A	505	6/6	0.69	0.17	103,103,104,105	0
6	PO4	B	508	5/5	0.73	0.14	131,131,131,131	0
2	GOL	A	510	6/6	0.78	0.14	92,92,92,92	0
8	MG	B	509	1/1	0.78	0.14	91,91,91,91	0
2	GOL	A	501	6/6	0.80	0.14	103,103,103,103	0
2	GOL	A	507	6/6	0.80	0.15	81,83,83,83	0
8	MG	A	515	1/1	0.81	0.19	84,84,84,84	0
2	GOL	B	505	6/6	0.81	0.14	95,95,95,96	0
6	PO4	A	512	5/5	0.83	0.14	112,112,113,113	0
2	GOL	A	509	6/6	0.86	0.20	99,99,100,100	0
5	HEW	B	511	8/8	0.87	0.15	124,124,125,125	8
2	GOL	B	501	6/6	0.87	0.17	90,90,91,92	0

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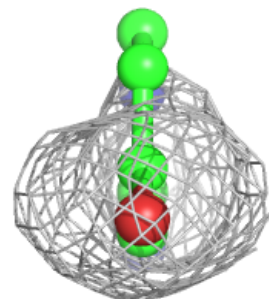
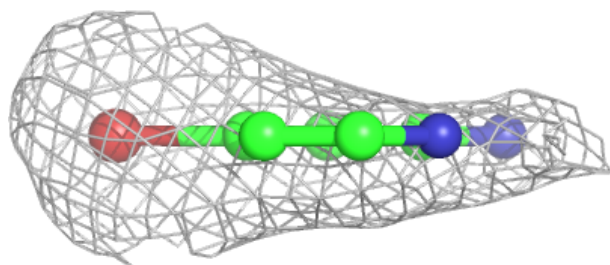
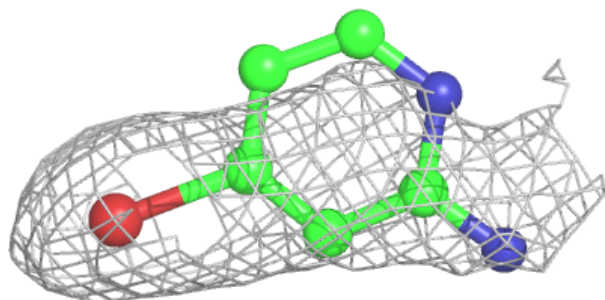
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	A	504	6/6	0.87	0.23	75,76,76,77	0
2	GOL	A	508	6/6	0.87	0.14	71,73,74,75	0
3	PG4	A	502	7/13	0.87	0.19	89,89,90,90	0
2	GOL	B	503	6/6	0.88	0.16	95,96,96,96	0
7	CL	A	514	1/1	0.89	0.14	86,86,86,86	0
2	GOL	B	504	6/6	0.90	0.10	97,98,98,98	0
7	CL	A	513	1/1	0.91	0.07	93,93,93,93	0
4	AN2	B	502	27/27	0.93	0.09	68,71,74,75	0
5	HEW	A	511	8/8	0.95	0.14	67,69,71,74	8
4	AN2	A	503	27/27	0.97	0.06	50,51,53,54	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.

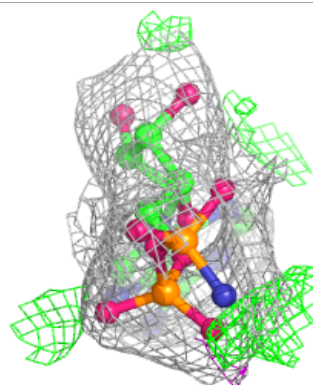
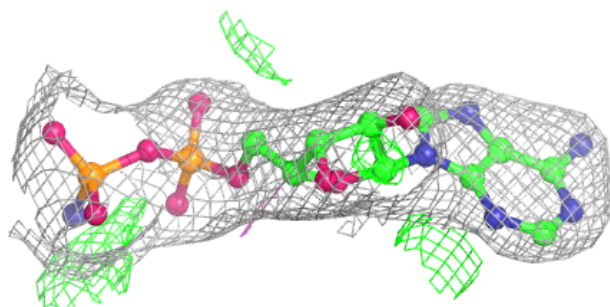
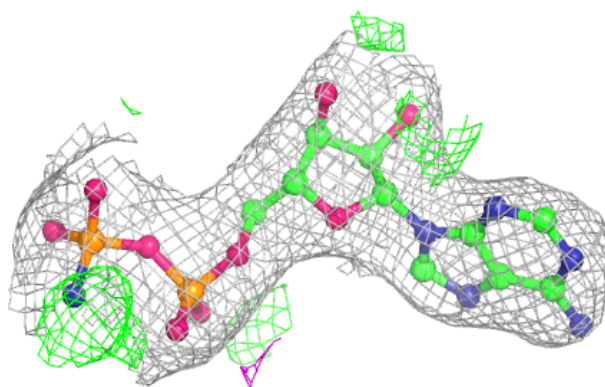
Electron density around HEW B 511:

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

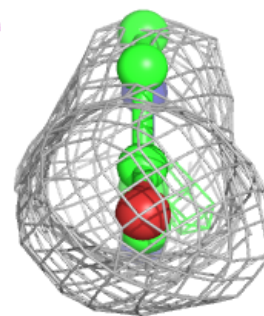
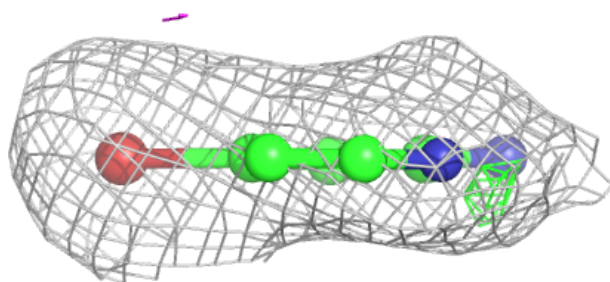
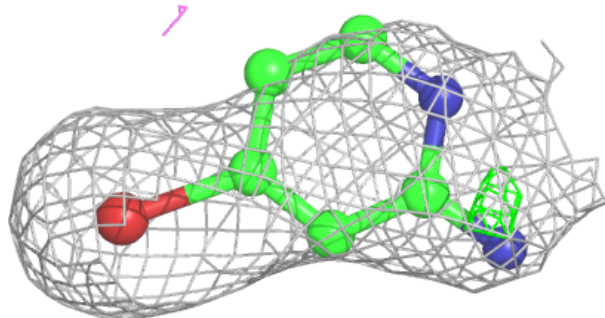


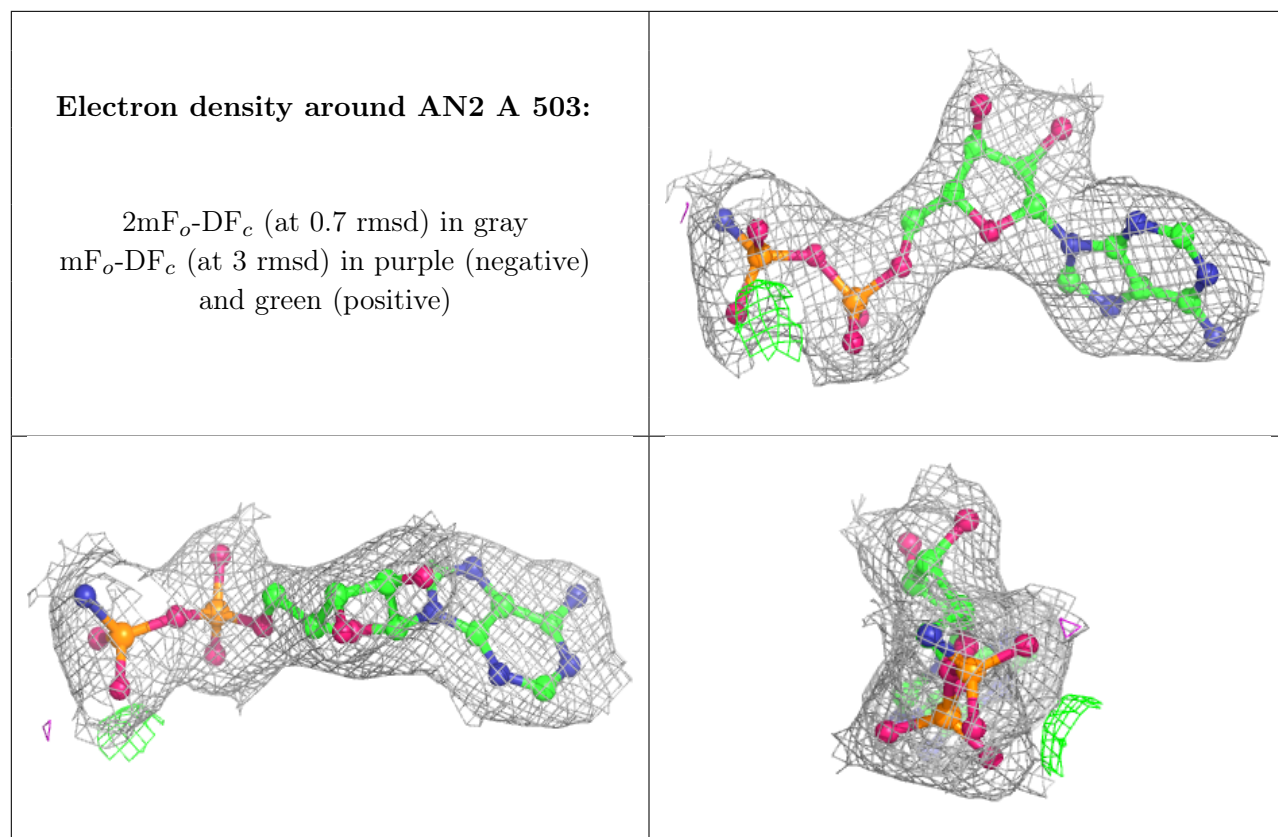
Electron density around AN2 B 502:

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

**Electron density around HEW A 511:**

$2mF_o-DF_c$ (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.