



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 7OOE / pdb_00007ooe
Title : Plasmodium falciparum Hsp70-x chaperone nucleotide binding domain in complex with Z321318226
Authors : Mohamad, N.; O'Donoghue, A.; Kantsadi, A.L.; Vakonakis, I.
Deposited on : 2021-05-27
Resolution : 2.37 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

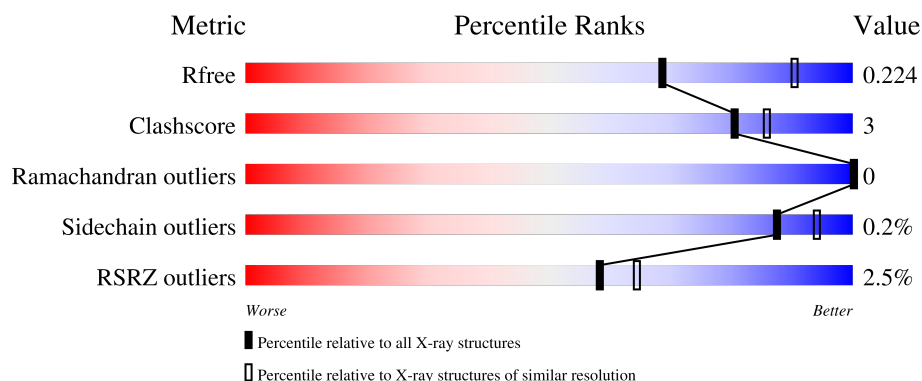
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	% 91% 7% .
1	B	393	4% 92% 5% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6228 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	3	0
			2976	1863	518	582	13			
1	B	380	Total	C	N	O	S	0	1	0
			2922	1832	504	574	12			

There are 4 discrepancies between the modelled and reference sequences:

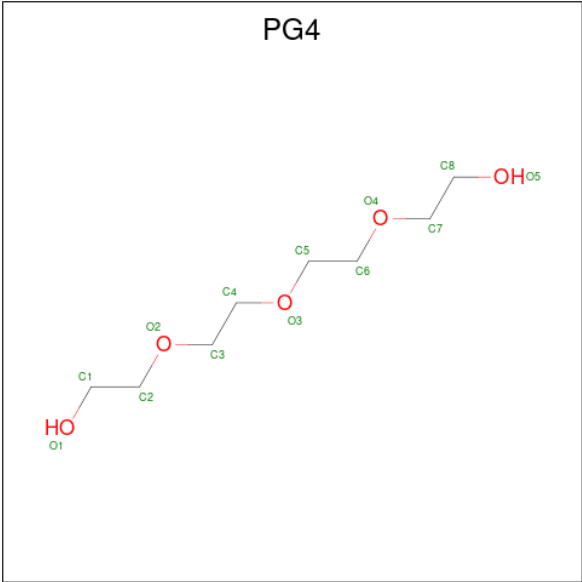
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP K7NTP5
A	28	PRO	-	expression tag	UNP K7NTP5
B	27	GLY	-	expression tag	UNP K7NTP5
B	28	PRO	-	expression tag	UNP K7NTP5

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



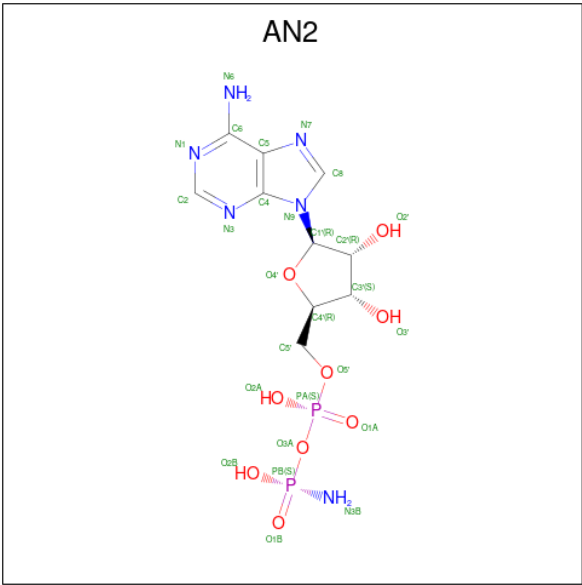
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).

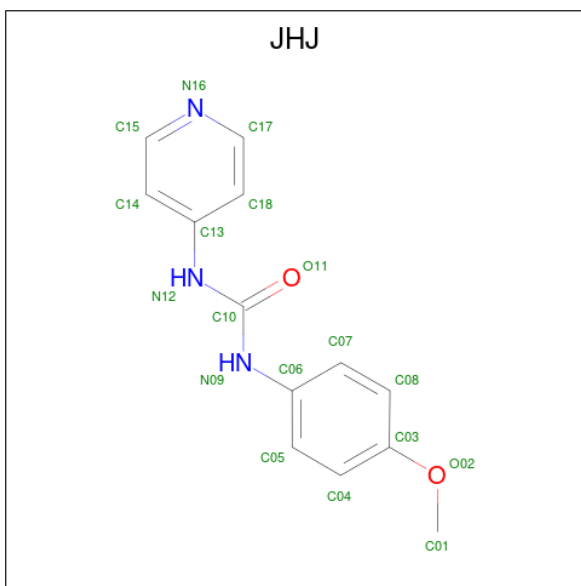


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	5	2		

- Molecule 4 is AMP PHOSPHORAMIDATE (CCD ID: AN2) (formula: C₁₀H₁₆N₆O₉P₂).

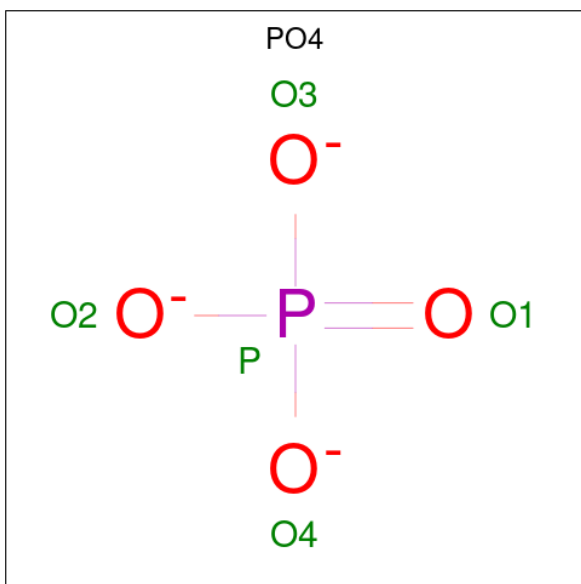


C₁₃H₁₃N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	13	3	2		
5	A	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	B	1	Total	Cl	0	0
			1	1		

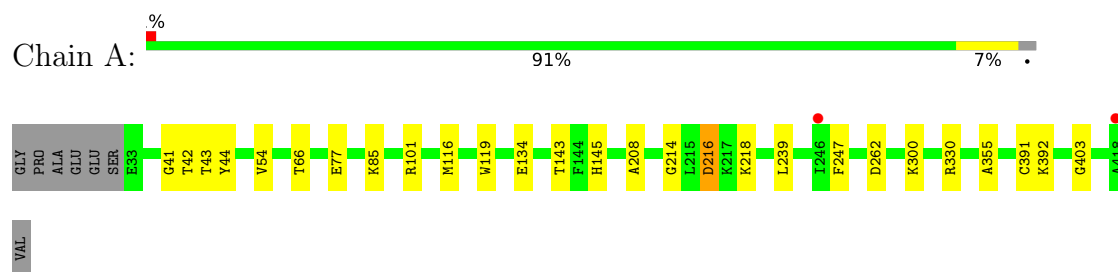
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	90	Total	O	0	0
			90	90		
8	B	28	Total	O	0	0
			28	28		

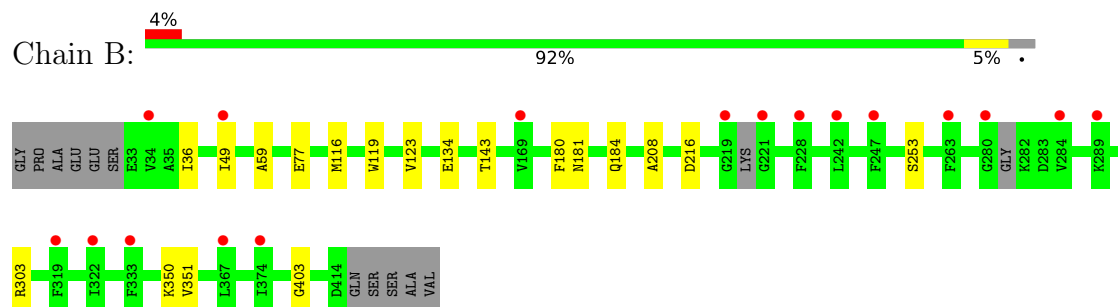
3 Residue-property plots [i](#)

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



- Molecule 1: Heat shock protein 70



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.22Å 102.68Å 103.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.01 – 2.37 73.01 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (73.01-2.37) 99.9 (73.01-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.37Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.204 , 0.236 0.199 , 0.224	Depositor DCC
R_{free} test set	1761 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6228	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: PO4, CSX, PG4, GOL, CL, AN2, JHJ

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	0.76	0/3012	1.00	3/4055 (0.1%)
1	B	0.68	0/2957	0.98	2/3981 (0.1%)
All	All	0.72	0/5969	0.99	5/8036 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASP	CA-CB-CG	6.87	119.47	112.60
1	B	216	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	77	GLU	N-CA-C	5.12	116.76	109.14
1	A	262	ASP	CA-CB-CG	-5.01	107.59	112.60
1	B	77	GLU	N-CA-C	5.01	116.60	109.14

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	2976	0	3008	19	0
1	B	2922	0	2940	12	0
2	A	66	0	88	9	0
2	B	36	0	48	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	6	0	0
4	A	27	0	14	2	0
4	B	27	0	14	0	0
5	A	36	0	0	1	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	A	90	0	0	1	0
8	B	28	0	0	0	0
All	All	6228	0	6118	32	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 (32) 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:43:THR:H	4:A:503:AN2:H3B1	1.18	0.90
1:A:44:TYR:H	4:A:503:AN2:H3B2	1.33	0.74
1:A:300:LYS:HG2	2:A:506:GOL:H2	1.69	0.74
1:A:145:HIS:ND1	5:A:509:JHJ:N16	2.36	0.73
1:B:181:ASN:HA	2:B:507:GOL:H31	1.73	0.69
2:A:504:GOL:H32	8:A:634:HOH:O	1.98	0.64
1:A:330:ARG:NH1	2:A:512:GOL:O1	2.29	0.64
1:B:59:ALA:H	2:B:506:GOL:H12	1.65	0.61
1:A:101:ARG:HA	2:A:504:GOL:H31	1.90	0.53
1:A:330:ARG:HH11	2:A:512:GOL:HO1	1.51	0.52
1:A:41:GLY:HA3	1:A:44:TYR:O	2.10	0.51
1:B:116:MET:HA	1:B:119:TRP:CE3	2.46	0.51
1:A:134:GLU:HG2	1:A:143:THR:HG22	1.94	0.50
1:A:85:LYS:NZ	2:A:508:GOL:H31	2.27	0.49
1:A:216:ASP:HB3	1:A:247:PHE:CE2	2.47	0.49
1:B:134:GLU:HG2	1:B:143:THR:HG22	1.95	0.49
1:A:239:LEU:HD23	1:A:355:ALA:CB	2.44	0.48
1:A:85:LYS:HZ1	2:A:508:GOL:H31	1.79	0.47
1:A:214:GLY:O	1:A:218:LYS:HG2	2.14	0.47
1:B:303:ARG:HH12	2:B:505:GOL:H31	1.78	0.47
1:B:253:SER:OG	1:B:351:VAL:HG13	2.15	0.46
1:A:66:THR:OG1	2:A:507:GOL:H31	2.16	0.46
1:A:208:ALA:O	1:A:403:GLY:HA3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LYS:O	2:A:513:GOL:H31	2.18	0.43
1:B:208:ALA:O	1:B:403:GLY:HA3	2.18	0.42
1:B:253:SER:HB2	1:B:350:LYS:NZ	2.35	0.42
1:B:36:ILE:HG22	1:B:49:ILE:CG2	2.50	0.41
1:B:116:MET:HE1	1:B:123:VAL:O	2.20	0.41
1:B:180:PHE:CD2	1:B:184:GLN:HB3	2.55	0.41
1:A:116:MET:HA	1:A:119:TRP:CE3	2.56	0.41
1:A:42:THR:OG1	6:A:516:PO4:O3	2.38	0.41
1:B:36:ILE:HG22	1:B:49:ILE:HG22	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	385/393 (98%)	382 (99%)	3 (1%)	0	100	100
1	B	374/393 (95%)	371 (99%)	3 (1%)	0	100	100
All	All	759/786 (97%)	753 (99%)	6 (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	323/326 (99%)	322 (100%)	1 (0%)	86	92
1	B	318/326 (98%)	318 (100%)	0	100	100
All	All	641/652 (98%)	640 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

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	223	GLN
1	A	325	ASN
1	B	325	ASN
1	B	340	GLN

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	A	391[B]	-	3,6,7	0.89	0	1,6,8	2.41	1 (100%)
1	CSX	A	391[A]	-	3,6,7	0.94	0	1,6,8	1.43	0
1	CSX	B	391	1	3,6,7	0.83	0	1,6,8	1.69	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
1	CSX	A	391[B]	-	-	0/2/5/7	-
1	CSX	A	391[A]	-	-	0/2/5/7	-
1	CSX	B	391	1	-	0/2/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391[B]	CSX	CA-CB-SG	2.41	118.85	113.17

There are no chirality outliers.

There are no torsion outliers.

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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	508	-	5,5,5	0.19	0	5,5,5	0.47	0
6	PO4	B	508	-	4,4,4	2.58	3 (75%)	6,6,6	0.45	0
2	GOL	A	501	-	5,5,5	0.07	0	5,5,5	0.28	0
3	PG4	A	502	-	6,6,12	0.26	0	5,5,11	0.15	0
2	GOL	A	514	-	5,5,5	0.07	0	5,5,5	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AN2	A	503	-	28,29,29	2.23	6 (21%)	40,45,45	1.93	10 (25%)
2	GOL	B	504	-	5,5,5	0.09	0	5,5,5	0.37	0
5	JHJ	A	509	-	19,19,19	0.34	0	24,24,24	0.69	0
2	GOL	A	512	-	5,5,5	0.05	0	5,5,5	0.16	0
2	GOL	A	507	-	5,5,5	0.36	0	5,5,5	0.53	0
2	GOL	B	501	-	5,5,5	0.19	0	5,5,5	0.14	0
2	GOL	A	513	-	5,5,5	0.18	0	5,5,5	0.55	0
2	GOL	A	510	-	5,5,5	0.10	0	5,5,5	0.32	0
2	GOL	A	504	-	5,5,5	0.55	0	5,5,5	0.70	0
5	JHJ	A	515	-	19,19,19	0.37	0	24,24,24	0.43	0
2	GOL	B	503	-	5,5,5	0.09	0	5,5,5	0.22	0
2	GOL	A	505	-	5,5,5	0.15	0	5,5,5	0.21	0
6	PO4	A	516	-	4,4,4	2.64	3 (75%)	6,6,6	0.82	0
4	AN2	B	502	-	28,29,29	2.48	8 (28%)	40,45,45	1.83	9 (22%)
2	GOL	B	507	-	5,5,5	0.05	0	5,5,5	0.28	0
2	GOL	A	506	-	5,5,5	0.16	0	5,5,5	0.24	0
2	GOL	B	505	-	5,5,5	0.20	0	5,5,5	0.36	0
2	GOL	B	506	-	5,5,5	0.09	0	5,5,5	0.37	0
2	GOL	A	511	-	5,5,5	0.12	0	5,5,5	0.38	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	508	-	-	0/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-
3	PG4	A	502	-	-	4/4/4/10	-
2	GOL	A	514	-	-	0/4/4/4	-
4	AN2	A	503	-	-	1/13/32/32	0/3/3/3
2	GOL	B	504	-	-	0/4/4/4	-
5	JHJ	A	509	-	-	0/10/10/10	0/2/2/2
2	GOL	A	512	-	-	0/4/4/4	-
2	GOL	A	507	-	-	4/4/4/4	-
2	GOL	B	501	-	-	1/4/4/4	-
2	GOL	A	513	-	-	2/4/4/4	-
2	GOL	A	510	-	-	1/4/4/4	-
2	GOL	A	504	-	-	2/4/4/4	-
5	JHJ	A	515	-	-	4/10/10/10	0/2/2/2
2	GOL	B	503	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	505	-	-	2/4/4/4	-
4	AN2	B	502	-	-	1/13/32/32	0/3/3/3
2	GOL	B	507	-	-	0/4/4/4	-
2	GOL	A	506	-	-	0/4/4/4	-
2	GOL	B	505	-	-	0/4/4/4	-
2	GOL	B	506	-	-	2/4/4/4	-
2	GOL	A	511	-	-	0/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	AN2	PB-O1B	9.59	1.60	1.46
4	A	503	AN2	PB-O1B	8.58	1.59	1.46
4	A	503	AN2	PB-O2B	-4.68	1.44	1.56
4	B	502	AN2	C5-C4	4.55	1.47	1.39
6	B	508	PO4	P-O1	4.25	1.60	1.50
6	A	516	PO4	P-O1	4.22	1.60	1.50
4	A	503	AN2	C5-C4	3.49	1.45	1.39
4	B	502	AN2	PA-O3A	3.35	1.63	1.59
4	B	502	AN2	PB-O2B	-3.24	1.48	1.56
4	B	502	AN2	C5-C6	3.04	1.49	1.41
4	B	502	AN2	C5-N7	-2.69	1.34	1.39
4	A	503	AN2	C5-C6	2.29	1.47	1.41
4	A	503	AN2	C4-N9	-2.22	1.33	1.37
4	A	503	AN2	PB-O3A	2.19	1.61	1.59
6	A	516	PO4	P-O2	2.12	1.60	1.54
4	B	502	AN2	PB-O3A	2.11	1.61	1.59
4	B	502	AN2	C8-N7	2.08	1.35	1.31
6	A	516	PO4	P-O4	2.06	1.60	1.54
6	B	508	PO4	P-O2	2.05	1.60	1.54
6	B	508	PO4	P-O4	2.02	1.60	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	AN2	C5-C4-N3	-5.88	118.62	126.72
4	A	503	AN2	C4-N9-C8	4.54	110.51	105.74
4	A	503	AN2	N3-C4-N9	4.53	134.87	127.17
4	B	502	AN2	N3-C4-N9	4.34	134.55	127.17
4	A	503	AN2	C5-C4-N3	-4.30	120.80	126.72
4	B	502	AN2	C4-C5-N7	-3.73	106.32	110.58
4	B	502	AN2	C2-N3-C4	3.70	120.87	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	AN2	N1-C2-N3	-3.43	123.39	128.58
4	A	503	AN2	C2-N3-C4	3.14	119.50	111.83
4	A	503	AN2	N9-C8-N7	-2.89	109.83	113.94
4	B	502	AN2	N1-C2-N3	-2.88	124.23	128.58
4	B	502	AN2	C5-N7-C8	2.66	107.62	103.45
4	A	503	AN2	O3'-C3'-C4'	-2.61	103.59	111.08
4	A	503	AN2	N6-C6-N1	2.29	123.48	118.38
4	A	503	AN2	C5-C6-N6	-2.24	117.74	123.29
4	A	503	AN2	C5-N7-C8	2.23	106.96	103.45
4	B	502	AN2	O4'-C1'-N9	2.23	112.37	108.09
4	B	502	AN2	C6-C5-N7	2.16	136.26	132.09
4	B	502	AN2	C4-N9-C8	2.01	107.84	105.74

There are no chirality outliers.

All (25) torsion outliers are listed below:

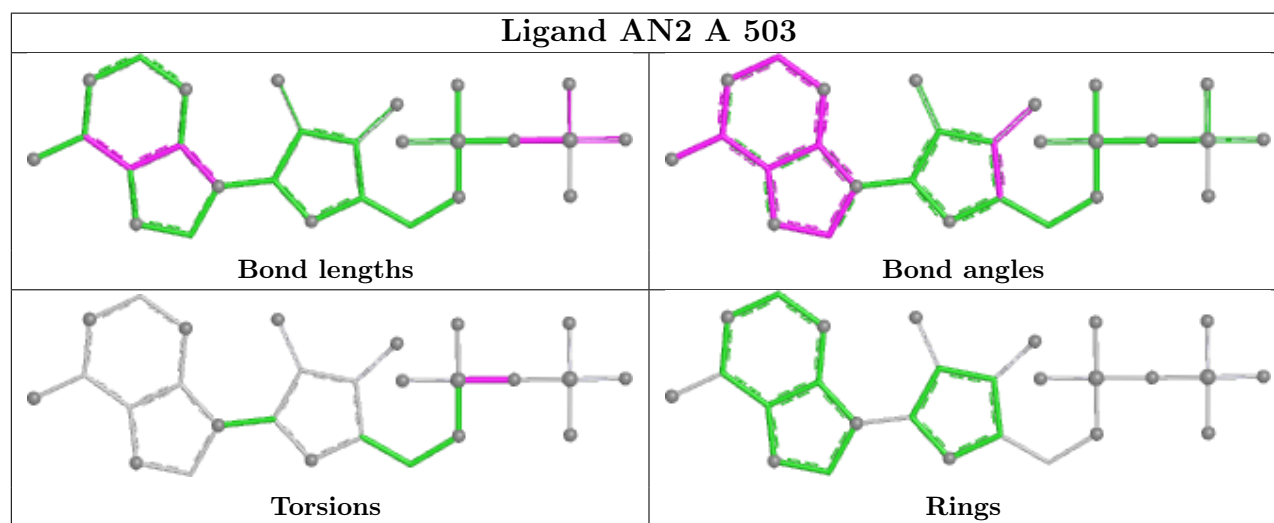
Mol	Chain	Res	Type	Atoms
2	A	507	GOL	O1-C1-C2-O2
2	A	507	GOL	O1-C1-C2-C3
2	A	507	GOL	C1-C2-C3-O3
2	A	507	GOL	O2-C2-C3-O3
2	A	513	GOL	O1-C1-C2-C3
2	B	506	GOL	O1-C1-C2-C3
2	B	506	GOL	O1-C1-C2-O2
3	A	502	PG4	O2-C3-C4-O3
2	A	505	GOL	O1-C1-C2-C3
2	B	503	GOL	C1-C2-C3-O3
2	A	513	GOL	O1-C1-C2-O2
5	A	515	JHJ	C08-C03-O02-C01
5	A	515	JHJ	N12-C10-N09-C06
2	A	510	GOL	C1-C2-C3-O3
3	A	502	PG4	C4-C3-O2-C2
2	B	501	GOL	O2-C2-C3-O3
5	A	515	JHJ	C04-C03-O02-C01
3	A	502	PG4	C6-C5-O3-C4
2	A	505	GOL	O1-C1-C2-O2
3	A	502	PG4	C3-C4-O3-C5
5	A	515	JHJ	O11-C10-N09-C06
2	A	504	GOL	C1-C2-C3-O3
2	A	504	GOL	O2-C2-C3-O3
4	A	503	AN2	PB-O3A-PA-O2A
4	B	502	AN2	PB-O3A-PA-O2A

There are no ring outliers.

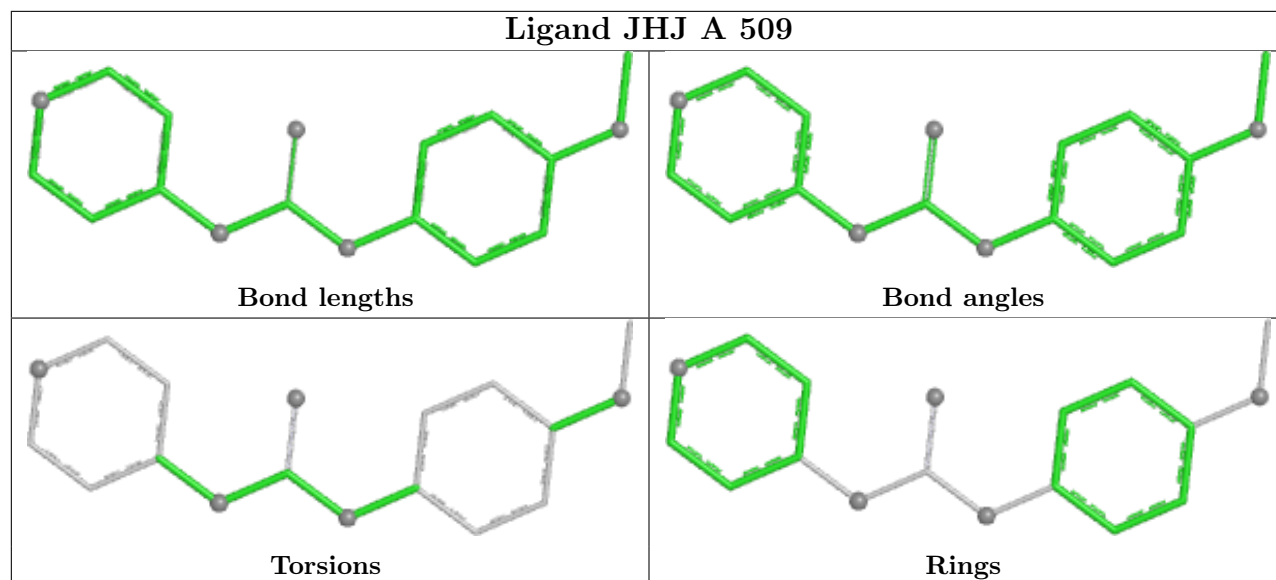
12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	508	GOL	2	0
4	A	503	AN2	2	0
5	A	509	JHJ	1	0
2	A	512	GOL	2	0
2	A	507	GOL	1	0
2	A	513	GOL	1	0
2	A	504	GOL	2	0
6	A	516	PO4	1	0
2	B	507	GOL	1	0
2	A	506	GOL	1	0
2	B	505	GOL	1	0
2	B	506	GOL	1	0

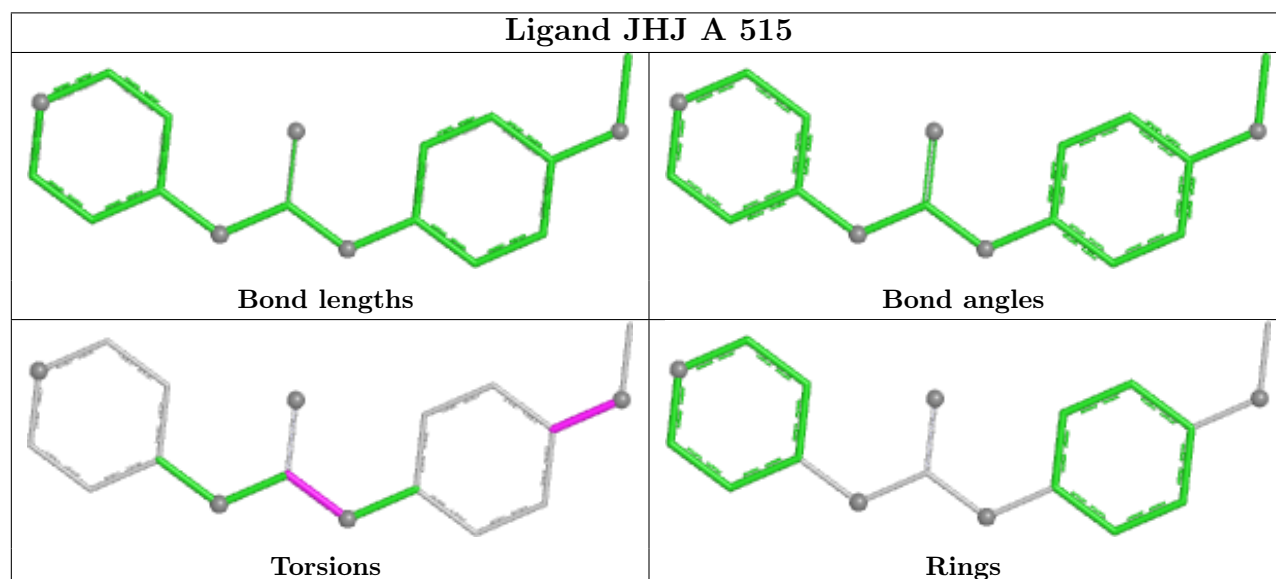
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



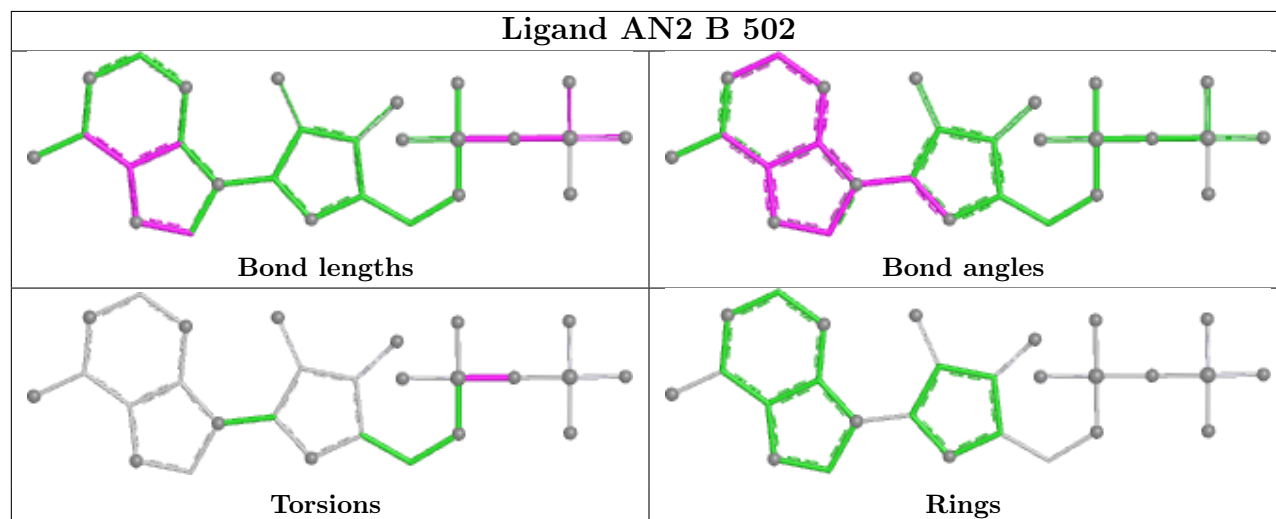
Ligand JHJ A 509



Ligand JHJ A 515



Ligand AN2 B 502



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	385/393 (97%)	0.02	2 (0%) 87 90	32, 70, 111, 123	2 (0%)
1	B	379/393 (96%)	0.50	17 (4%) 38 44	41, 103, 160, 193	1 (0%)
All	All	764/786 (97%)	0.26	19 (2%) 58 64	32, 82, 153, 193	3 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	ALA	4.3
1	B	333	PHE	4.0
1	B	169	VAL	3.1
1	B	280	GLY	2.8
1	B	284	VAL	2.7
1	B	219	GLY	2.7
1	B	319	PHE	2.6
1	B	374	ILE	2.6
1	B	289	LYS	2.4
1	B	34	VAL	2.4
1	B	49	ILE	2.3
1	A	246	ILE	2.3
1	B	322	ILE	2.3
1	B	263	PHE	2.3
1	B	242	LEU	2.2
1	B	367	LEU	2.1
1	B	247	PHE	2.1
1	B	221	GLY	2.1
1	B	228	PHE	2.0

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	0.87	0.10	63,66,71,72	4
1	CSX	A	391[B]	7/8	0.87	0.10	63,66,69,70	4
1	CSX	B	391	7/8	0.95	0.08	105,108,114,114	0

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(Å ²)	Q<0.9
2	GOL	B	507	6/6	0.67	0.16	141,141,142,142	0
2	GOL	A	507	6/6	0.71	0.19	93,94,95,95	0
2	GOL	A	506	6/6	0.75	0.15	104,105,105,105	0
2	GOL	B	504	6/6	0.76	0.16	108,108,108,108	0
6	PO4	B	508	5/5	0.78	0.13	182,182,182,182	0
2	GOL	A	512	6/6	0.79	0.13	106,106,106,107	0
2	GOL	B	505	6/6	0.79	0.15	106,106,106,106	0
2	GOL	A	501	6/6	0.80	0.13	92,92,92,93	0
2	GOL	A	513	6/6	0.80	0.20	89,90,90,90	0
2	GOL	A	510	6/6	0.81	0.10	129,129,129,129	0
6	PO4	A	516	5/5	0.81	0.16	100,101,102,102	0
2	GOL	A	511	6/6	0.81	0.15	102,103,104,104	0
2	GOL	A	514	6/6	0.82	0.11	119,119,119,120	0
2	GOL	A	505	6/6	0.82	0.15	101,102,102,102	0
7	CL	A	518	1/1	0.84	0.14	96,96,96,96	0
2	GOL	B	501	6/6	0.85	0.16	96,97,99,100	0
5	JHJ	A	515	18/18	0.87	0.18	67,68,69,69	18
2	GOL	A	508	6/6	0.87	0.13	80,84,85,86	0
7	CL	A	517	1/1	0.88	0.14	106,106,106,106	0
3	PG4	A	502	7/13	0.88	0.19	90,90,93,93	0
5	JHJ	A	509	18/18	0.90	0.11	76,79,85,86	18
2	GOL	B	503	6/6	0.91	0.12	110,110,110,110	0
2	GOL	B	506	6/6	0.91	0.11	87,87,88,89	0

Continued on next page...

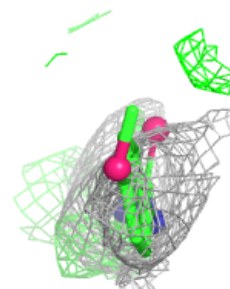
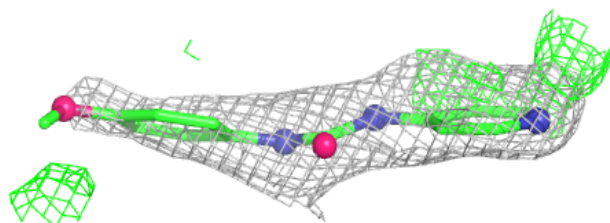
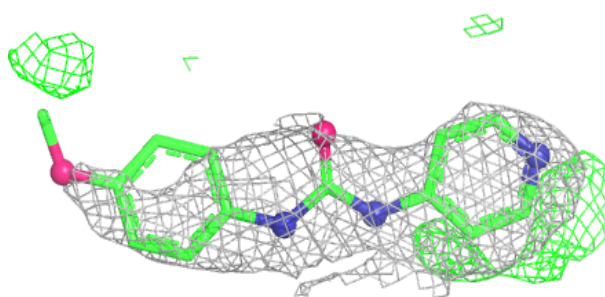
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	B	509	1/1	0.92	0.07	88,88,88,88	0
2	GOL	A	504	6/6	0.93	0.15	69,72,73,75	0
4	AN2	B	502	27/27	0.94	0.08	78,80,82,83	0
4	AN2	A	503	27/27	0.98	0.05	50,51,55,57	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.

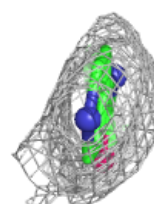
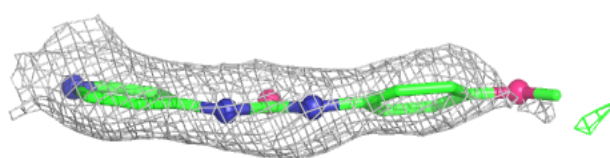
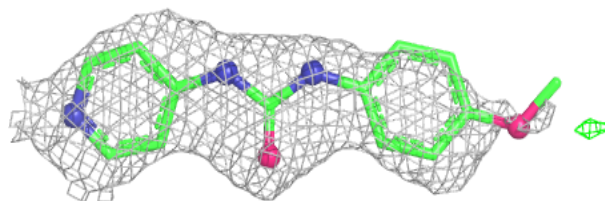
Electron density around JHJ A 515:

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

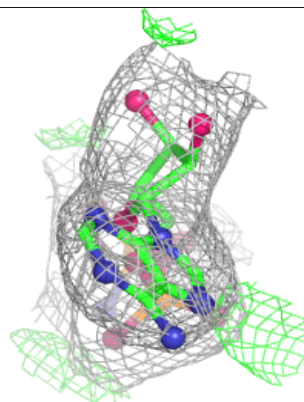
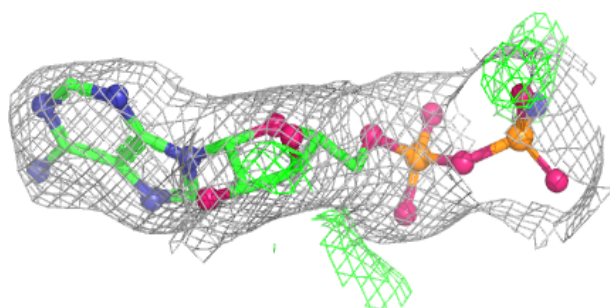
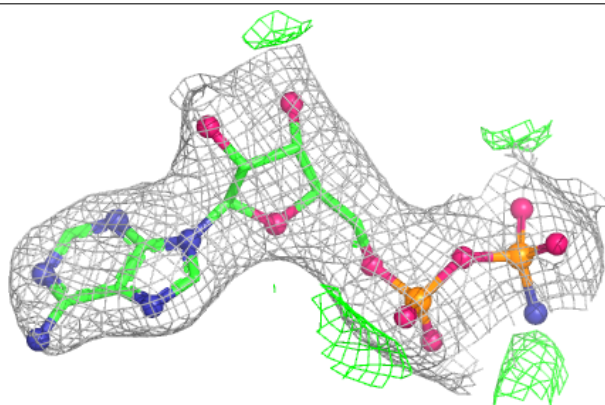


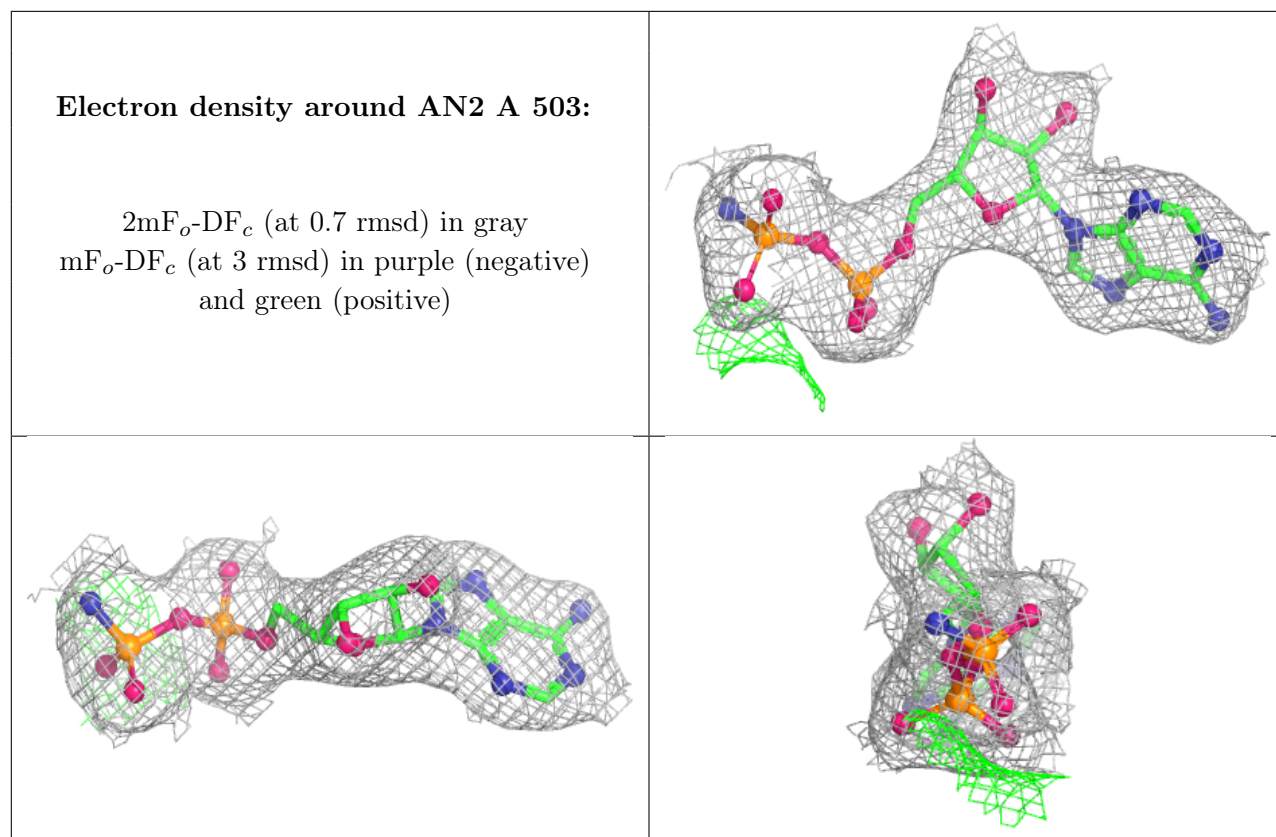
Electron density around JHJ A 509:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.