Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 05:43 PM EDT

PDB ID	:	4ZTM
Title	:	Irak4-inhibitor co-structure
Authors	:	Fischmann, T.O.
Deposited on	:	2015-05-14
Resolution	:	2.66 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 (i) 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 (i)) were used in the production of this report:

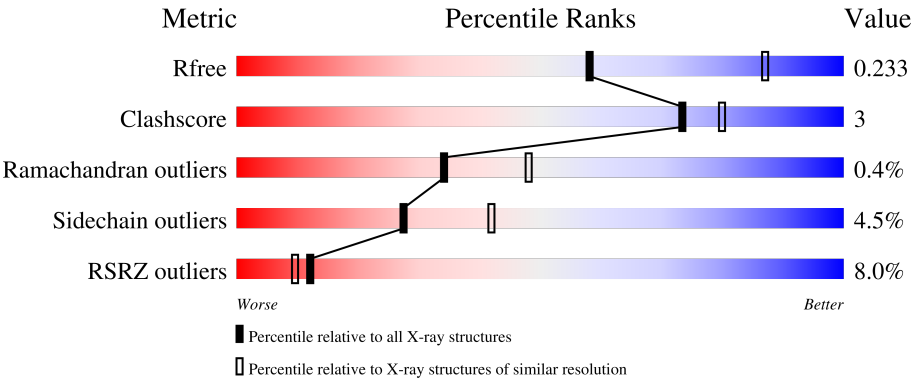
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	301	7% 85% 11% •
1	B	301	11% 80% 13% 6%
1	C	301	7% 84% 10% 5%
1	D	301	5% 82% 12% • 5%

2 Entry composition

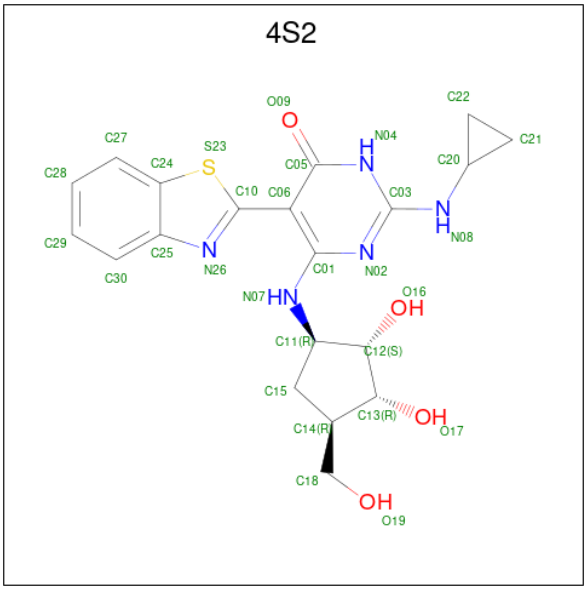
There are 3 unique types of molecules in this entry. The entry contains 9198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	P	S	0	0	3
			2273	1421	383	452	3	14			
1	B	283	Total	C	N	O	P	S	0	0	1
			2224	1394	375	438	3	14			
1	C	285	Total	C	N	O	P	S	0	0	2
			2231	1401	374	439	3	14			
1	D	285	Total	C	N	O	P	S	0	0	3
			2245	1407	379	442	3	14			

- Molecule 2 is 5-(1,3-benzothiazol-2-yl)-2-(cyclopropylamino)-6-{[(1R,2S,3R,4R)-2,3-dihydroxy-4-(hydroxymethyl)cyclopentyl]amino}pyrimidin-4(3H)-one (three-letter code: 4S2) (formula: $C_{20}H_{23}N_5O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	20	5	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			30	20	5	4	1		
2	C	1	Total	C	N	O	S	0	0
			30	20	5	4	1		
2	D	1	Total	C	N	O	S	0	0
			30	20	5	4	1		

- Molecule 3 is water.

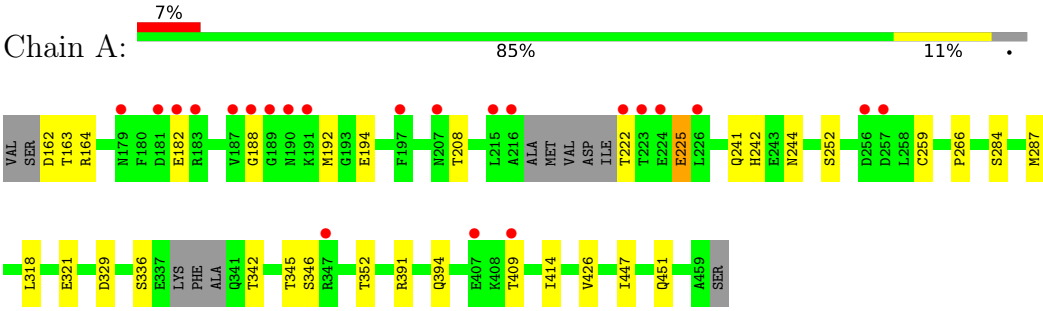
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	23	Total	O	0	0
			23	23		
3	C	29	Total	O	0	0
			29	29		
3	D	31	Total	O	0	0
			31	31		

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.

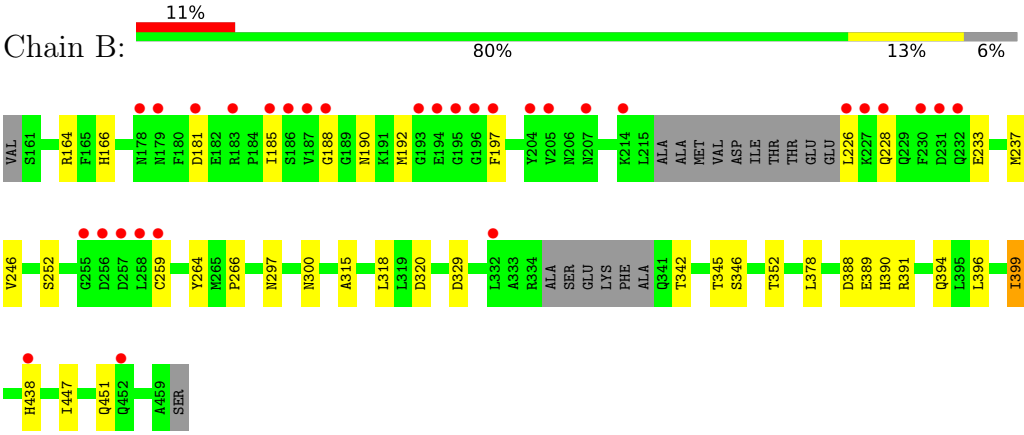
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



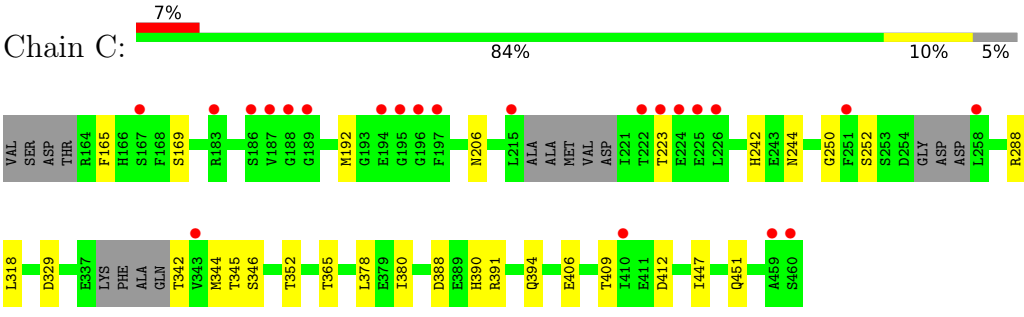
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



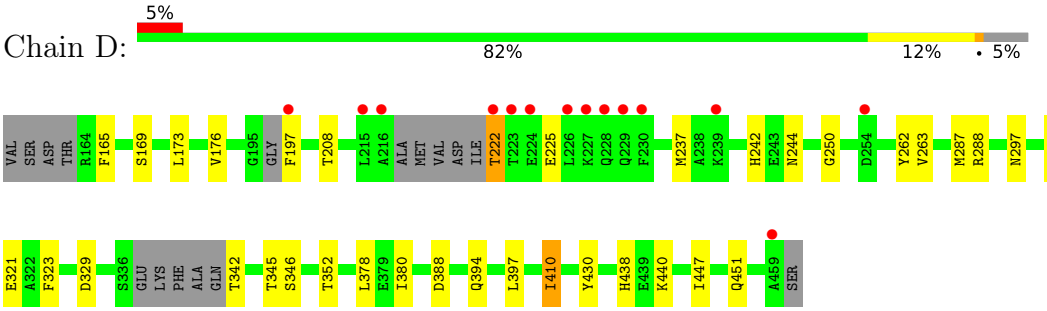
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C:



• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:


5%
82%
12%
• 5%
VAL SER ASP THR R164 F165 S169 L173 V176 G195 GLY F197 T208 L215 A216 ALA MET VAL ASP ILE T222 T223 E224 E225 L226 K227 Q228 Q229 F230 M237 A238 K239 H242 E243 N244 G250 D264 Y262 V263 M287 R288 N297 N300 L318
E321 A322 F323 D329 S336 GLU LYS PHE ALA GLN T342 T345 S346 T352 L378 E379 I380 D388 Q394 L397 I410 Y430 H438 E439 K440 I447 Q451 A459 SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.93Å 139.25Å 87.77Å 90.00° 124.26° 90.00°	Depositor
Resolution (Å)	47.32 – 2.66 47.32 – 2.66	Depositor EDS
% Data completeness (in resolution range)	92.3 (47.32-2.66) 92.5 (47.32-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.193 , 0.226 0.199 , 0.233	Depositor DCC
R_{free} test set	1892 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9198	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SEP, TPO, 4S2

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	0.51	0/2276	0.67	0/3065
1	B	0.50	0/2227	0.69	0/2998
1	C	0.50	0/2234	0.68	0/3009
1	D	0.51	0/2248	0.69	1/3028 (0.0%)
All	All	0.51	0/8985	0.68	1/12100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	397	LEU	N-CA-CB	-5.11	100.19	110.40

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	2273	0	2222	11	0
1	B	2224	0	2179	20	0
1	C	2231	0	2194	11	0
1	D	2245	0	2206	19	0
2	A	30	0	23	1	0
2	B	30	0	23	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	23	1	0
2	D	30	0	23	0	0
3	A	22	0	0	0	0
3	B	23	0	0	0	0
3	C	29	0	0	0	0
3	D	31	0	0	1	0
All	All	9198	0	8893	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:HIS:HB3	1:C:391:ARG:HA	1.48	0.96
1:B:391:ARG:HA	1:C:390:HIS:HB3	1.58	0.86
1:B:390:HIS:O	1:C:390:HIS:O	2.05	0.75
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.58	0.67
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.77	0.66
1:C:242:HIS:CD2	1:C:244:ASN:H	2.14	0.65
1:B:396:LEU:HD12	1:B:399:ILE:HD13	1.79	0.64
1:A:242:HIS:CD2	1:A:244:ASN:H	2.16	0.63
1:D:438:HIS:HD2	1:D:440:LYS:H	1.45	0.62
1:D:242:HIS:CD2	1:D:244:ASN:H	2.17	0.62
1:A:284:SER:H	1:A:287:MET:HE3	1.65	0.61
1:B:242:HIS:CD2	1:B:244:ASN:H	2.20	0.59
1:D:222:THR:HB	1:D:225:GLU:HB2	1.88	0.55
1:B:389:GLU:HA	1:B:394:GLN:OE1	2.07	0.54
1:B:181:ASP:HB3	1:B:190:ASN:HB2	1.90	0.52
1:D:242:HIS:HD2	1:D:244:ASN:H	1.58	0.51
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.93	0.50
1:C:242:HIS:HD2	1:C:244:ASN:H	1.55	0.49
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.95	0.49
1:B:185:ILE:HD11	1:B:192:MET:HG2	1.95	0.49
1:D:237:MET:HE3	1:D:262:TYR:CE2	2.45	0.48
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.94	0.48
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.95	0.48
1:A:222:THR:HB	1:A:225:GLU:HB2	1.95	0.48
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.96	0.47
1:D:288:ARG:HB3	1:D:380:ILE:HG23	1.97	0.47
1:A:266:PRO:O	2:A:501:4S2:H19	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:ILE:HG12	1:D:430:TYR:CD2	2.50	0.47
1:B:390:HIS:CB	1:C:391:ARG:HA	2.33	0.46
1:D:287:MET:CE	1:D:323:PHE:HB3	2.45	0.46
1:A:242:HIS:HD2	1:A:244:ASN:H	1.57	0.46
1:B:266:PRO:HD2	1:B:320:ASP:HA	1.97	0.46
1:B:396:LEU:O	1:B:399:ILE:HB	2.16	0.46
1:D:410:ILE:HG12	1:D:430:TYR:CG	2.50	0.46
1:A:391:ARG:O	1:A:394:GLN:HG3	2.15	0.46
1:A:163:THR:OG1	1:A:241:GLN:NE2	2.51	0.44
1:B:315:ALA:O	2:B:501:4S2:H12	2.17	0.44
1:C:297:ASN:HA	1:C:451:GLN:HE21	1.83	0.43
1:B:297:ASN:HA	1:B:451:GLN:HE21	1.83	0.43
1:D:388:ASP:O	1:D:394:GLN:HG2	2.19	0.43
1:D:287:MET:HE1	1:D:323:PHE:CB	2.49	0.43
1:D:165:PHE:HB3	1:D:250:GLY:HA2	2.01	0.42
1:A:297:ASN:HA	1:A:451:GLN:HE21	1.83	0.42
1:B:399:ILE:HG12	1:B:413:TYR:CZ	2.54	0.42
1:B:164:ARG:HH11	1:B:166:HIS:HA	1.84	0.42
2:C:501:4S2:H1	2:C:501:4S2:H15	1.77	0.42
1:C:388:ASP:O	1:C:394:GLN:HG2	2.20	0.42
1:D:297:ASN:HA	1:D:451:GLN:HE21	1.85	0.41
1:D:321:GLU:H	1:D:321:GLU:CD	2.23	0.41
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.01	0.41
1:D:173:LEU:HA	1:D:176:VAL:HG22	2.03	0.41
1:D:263:VAL:HG13	3:D:605:HOH:O	2.20	0.41
1:B:237:MET:HE1	1:B:246:VAL:HG23	2.03	0.41
1:C:288:ARG:HB3	1:C:380:ILE:HG23	2.03	0.41
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.02	0.41
1:B:264:TYR:O	1:B:266:PRO:HD3	2.21	0.41
1:B:388:ASP:O	1:B:394:GLN:HG2	2.21	0.40
2:B:501:4S2:O09	2:B:501:4S2:S23	2.79	0.40
1:D:287:MET:HE1	1:D:323:PHE:HB3	2.04	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	281/301 (93%)	271 (96%)	9 (3%)	1 (0%)	34	48
1	B	274/301 (91%)	258 (94%)	15 (6%)	1 (0%)	34	48
1	C	275/301 (91%)	263 (96%)	10 (4%)	2 (1%)	22	33
1	D	275/301 (91%)	263 (96%)	12 (4%)	0	100	100
All	All	1105/1204 (92%)	1055 (96%)	46 (4%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	206	ASN
1	B	188	GLY
1	C	406	GLU
1	A	188	GLY

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	248/259 (96%)	235 (95%)	13 (5%)	23	36
1	B	242/259 (93%)	232 (96%)	10 (4%)	30	46
1	C	243/259 (94%)	231 (95%)	12 (5%)	25	38
1	D	245/259 (95%)	236 (96%)	9 (4%)	34	50
All	All	978/1036 (94%)	934 (96%)	44 (4%)	27	42

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	164	ARG

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Mol	Chain	Res	Type
1	A	182	GLU
1	A	192	MET
1	A	194	GLU
1	A	208	THR
1	A	225	GLU
1	A	318	LEU
1	A	321	GLU
1	A	329	ASP
1	A	336	SER
1	A	352	THR
1	A	409	THR
1	B	197	PHE
1	B	226	LEU
1	B	228	GLN
1	B	233	GLU
1	B	318	LEU
1	B	329	ASP
1	B	352	THR
1	B	378	LEU
1	B	399	ILE
1	B	438	HIS
1	C	169	SER
1	C	192	MET
1	C	223	THR
1	C	252	SER
1	C	318	LEU
1	C	329	ASP
1	C	344	MET
1	C	352	THR
1	C	365	THR
1	C	378	LEU
1	C	409	THR
1	C	412	ASP
1	D	169	SER
1	D	197	PHE
1	D	208	THR
1	D	222	THR
1	D	318	LEU
1	D	329	ASP
1	D	352	THR
1	D	378	LEU
1	D	410	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	242	HIS
1	A	451	GLN
1	B	232	GLN
1	B	242	HIS
1	B	451	GLN
1	C	166	HIS
1	C	232	GLN
1	C	242	HIS
1	C	394	GLN
1	C	438	HIS
1	C	451	GLN
1	D	166	HIS
1	D	242	HIS
1	D	394	GLN
1	D	438	HIS
1	D	451	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	TPO	A	345	1	8,10,11	1.11	0	10,14,16	1.56	1 (10%)
1	TPO	A	342	1	8,10,11	1.04	1 (12%)	10,14,16	1.43	1 (10%)
1	SEP	B	346	1	8,9,10	0.91	0	8,12,14	1.61	1 (12%)
1	TPO	C	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	TPO	D	345	1	8,10,11	1.08	0	10,14,16	1.18	2 (20%)
1	TPO	B	345	1	8,10,11	0.98	0	10,14,16	1.18	1 (10%)
1	TPO	C	342	1	8,10,11	1.07	1 (12%)	10,14,16	1.31	1 (10%)
1	TPO	D	342	1	8,10,11	1.08	1 (12%)	10,14,16	1.31	1 (10%)
1	SEP	D	346	1	8,9,10	1.05	0	8,12,14	1.07	1 (12%)
1	TPO	B	342	1	8,10,11	1.02	0	10,14,16	1.36	1 (10%)
1	SEP	A	346	1	8,9,10	0.93	0	8,12,14	1.48	1 (12%)
1	SEP	C	346	1	8,9,10	0.93	0	8,12,14	1.21	1 (12%)

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	TPO	A	345	1	-	3/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	0/5/8/10	-
1	SEP	C	346	1	-	0/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-2.35	1.54	1.59
1	C	342	TPO	P-OG1	-2.24	1.55	1.59
1	A	342	TPO	P-OG1	-2.16	1.55	1.59
1	C	345	TPO	P-OG1	-2.00	1.55	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	SEP	P-OG-CB	-3.73	108.01	118.30
1	A	346	SEP	P-OG-CB	-3.35	109.06	118.30
1	A	342	TPO	P-OG1-CB	-3.17	113.62	123.21
1	B	342	TPO	P-OG1-CB	-3.00	114.14	123.21
1	C	342	TPO	P-OG1-CB	-2.99	114.18	123.21
1	D	342	TPO	P-OG1-CB	-2.99	114.18	123.21
1	C	346	SEP	P-OG-CB	-2.88	110.37	118.30
1	A	345	TPO	P-OG1-CB	-2.69	115.08	123.21
1	D	346	SEP	P-OG-CB	-2.55	111.27	118.30
1	D	345	TPO	O3P-P-OG1	2.44	116.90	105.99
1	B	345	TPO	O3P-P-OG1	2.23	115.98	105.99
1	D	345	TPO	P-OG1-CB	-2.07	116.96	123.21

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-P-O1P
1	A	342	TPO	C-CA-CB-CG2
1	B	342	TPO	C-CA-CB-CG2
1	C	342	TPO	C-CA-CB-CG2
1	D	342	TPO	C-CA-CB-CG2
1	A	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	4S2	A	501	-	32,34,34	1.69	6 (18%)	35,50,50	1.83	7 (20%)
2	4S2	D	501	-	32,34,34	2.12	9 (28%)	35,50,50	2.00	11 (31%)
2	4S2	C	501	-	32,34,34	2.02	10 (31%)	35,50,50	1.71	6 (17%)
2	4S2	B	501	-	32,34,34	2.06	9 (28%)	35,50,50	1.84	10 (28%)

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	4S2	A	501	-	-	4/10/32/32	0/5/5/5
2	4S2	D	501	-	-	5/10/32/32	0/5/5/5
2	4S2	C	501	-	-	5/10/32/32	0/5/5/5
2	4S2	B	501	-	-	2/10/32/32	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4S2	C10-N26	5.95	1.40	1.31
2	C	501	4S2	C01-N02	5.33	1.44	1.36
2	D	501	4S2	C01-N02	4.87	1.43	1.36
2	D	501	4S2	C10-S23	4.72	1.80	1.73
2	D	501	4S2	C10-N26	4.72	1.38	1.31
2	C	501	4S2	C10-S23	4.58	1.80	1.73
2	B	501	4S2	C10-S23	4.33	1.79	1.73
2	B	501	4S2	C01-N02	3.89	1.41	1.36
2	D	501	4S2	C28-C27	3.88	1.45	1.36
2	A	501	4S2	C28-C27	3.78	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4S2	C06-C05	3.70	1.52	1.43
2	A	501	4S2	C03-N04	3.59	1.42	1.36
2	C	501	4S2	C06-C05	3.24	1.51	1.43
2	B	501	4S2	C01-N07	3.22	1.42	1.35
2	A	501	4S2	C29-C30	3.19	1.44	1.36
2	C	501	4S2	C29-C30	3.10	1.43	1.36
2	D	501	4S2	C29-C30	3.08	1.43	1.36
2	C	501	4S2	C10-N26	3.04	1.35	1.31
2	C	501	4S2	C03-N04	3.01	1.41	1.36
2	B	501	4S2	C29-C30	3.00	1.43	1.36
2	A	501	4S2	C10-N26	3.00	1.35	1.31
2	C	501	4S2	C18-C14	2.95	1.58	1.52
2	D	501	4S2	C03-N04	2.91	1.41	1.36
2	B	501	4S2	C06-C05	2.77	1.50	1.43
2	D	501	4S2	C06-C05	2.76	1.50	1.43
2	A	501	4S2	C01-N07	2.74	1.41	1.35
2	B	501	4S2	C28-C27	2.69	1.42	1.36
2	C	501	4S2	C28-C27	2.55	1.42	1.36
2	B	501	4S2	O17-C13	2.45	1.48	1.43
2	C	501	4S2	C01-N07	2.44	1.40	1.35
2	B	501	4S2	C03-N04	2.40	1.40	1.36
2	D	501	4S2	C22-C20	2.38	1.53	1.48
2	D	501	4S2	O17-C13	2.16	1.48	1.43
2	C	501	4S2	C21-C20	2.07	1.53	1.48

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	4S2	C03-N02-C01	5.35	123.25	112.64
2	A	501	4S2	C03-N02-C01	5.26	123.05	112.64
2	D	501	4S2	C13-C12-C11	5.22	110.81	102.55
2	C	501	4S2	C03-N02-C01	4.58	121.71	112.64
2	A	501	4S2	C10-N26-C25	4.08	111.86	103.78
2	C	501	4S2	C10-N26-C25	4.03	111.78	103.78
2	D	501	4S2	C03-N02-C01	3.97	120.52	112.64
2	D	501	4S2	O09-C05-C06	-3.55	121.46	124.89
2	D	501	4S2	C24-C25-N26	3.47	116.12	108.04
2	B	501	4S2	C10-N26-C25	3.43	110.59	103.78
2	A	501	4S2	C20-N08-C03	3.43	133.61	124.95
2	D	501	4S2	C15-C14-C13	3.07	110.18	102.66
2	C	501	4S2	C21-C20-N08	3.03	122.95	118.61
2	C	501	4S2	N04-C03-N02	-3.00	119.31	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	4S2	C15-C11-C12	-2.98	98.44	103.17
2	A	501	4S2	C22-C20-N08	-2.98	114.33	118.61
2	C	501	4S2	C24-C25-N26	2.97	114.95	108.04
2	B	501	4S2	C15-C14-C13	2.92	109.81	102.66
2	D	501	4S2	C10-N26-C25	2.80	109.33	103.78
2	B	501	4S2	C24-C25-N26	2.69	114.30	108.04
2	A	501	4S2	C24-C25-N26	2.65	114.22	108.04
2	B	501	4S2	O09-C05-C06	-2.64	122.34	124.89
2	C	501	4S2	C14-C15-C11	2.55	106.37	103.32
2	B	501	4S2	N04-C03-N02	-2.52	120.06	123.95
2	A	501	4S2	N04-C03-N02	-2.51	120.06	123.95
2	B	501	4S2	C03-N04-C05	-2.51	121.60	124.48
2	D	501	4S2	N04-C03-N02	-2.49	120.10	123.95
2	D	501	4S2	C20-N08-C03	2.31	130.79	124.95
2	D	501	4S2	C15-C11-C12	2.25	106.74	103.17
2	B	501	4S2	C14-C15-C11	-2.23	100.66	103.32
2	D	501	4S2	C22-C20-N08	2.18	121.73	118.61
2	B	501	4S2	C13-C12-C11	2.11	105.88	102.55
2	D	501	4S2	C12-C11-N07	-2.07	108.19	112.32
2	B	501	4S2	C28-C29-C30	-2.05	117.56	120.44

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	4S2	C12-C11-N07-C01
2	A	501	4S2	C13-C14-C18-O19
2	A	501	4S2	C15-C14-C18-O19
2	B	501	4S2	N02-C03-N08-C20
2	B	501	4S2	C12-C11-N07-C01
2	C	501	4S2	C12-C11-N07-C01
2	C	501	4S2	C13-C14-C18-O19
2	C	501	4S2	C15-C14-C18-O19
2	D	501	4S2	C15-C14-C18-O19
2	D	501	4S2	C12-C11-N07-C01
2	A	501	4S2	N02-C03-N08-C20
2	C	501	4S2	N02-C03-N08-C20
2	D	501	4S2	N02-C03-N08-C20
2	D	501	4S2	C15-C11-N07-C01
2	D	501	4S2	C13-C14-C18-O19
2	C	501	4S2	C15-C11-N07-C01

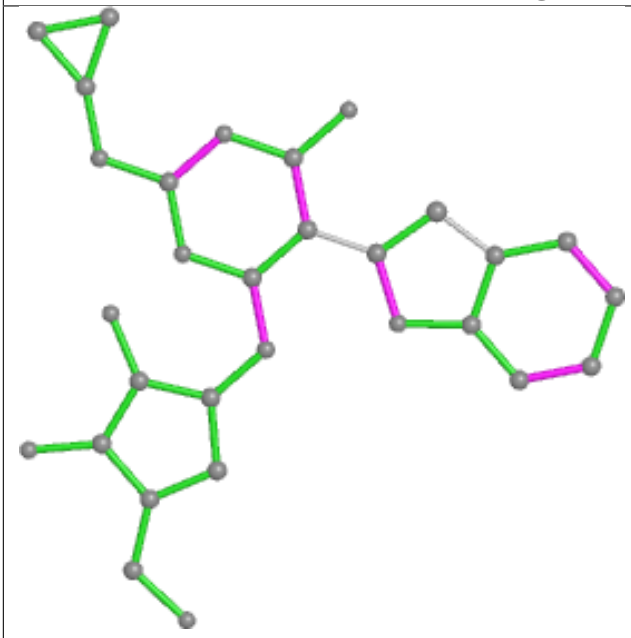
There are no ring outliers.

3 monomers are involved in 4 short contacts:

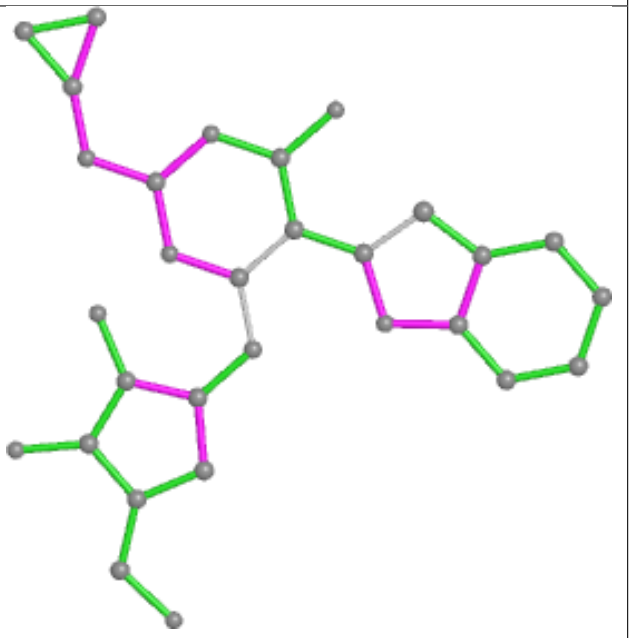
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4S2	1	0
2	C	501	4S2	1	0
2	B	501	4S2	2	0

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.

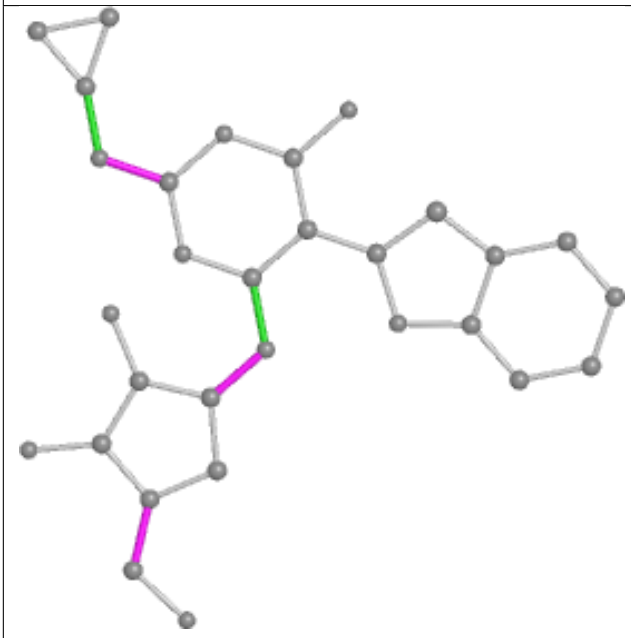
Ligand 4S2 A 501



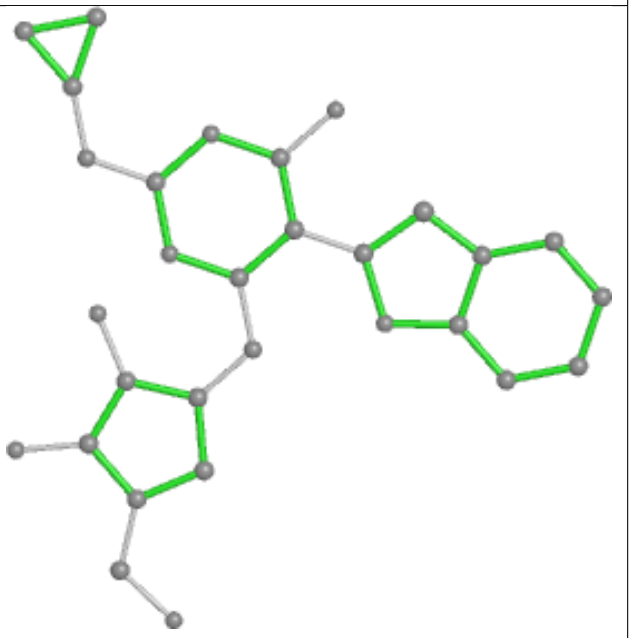
Bond lengths



Bond angles

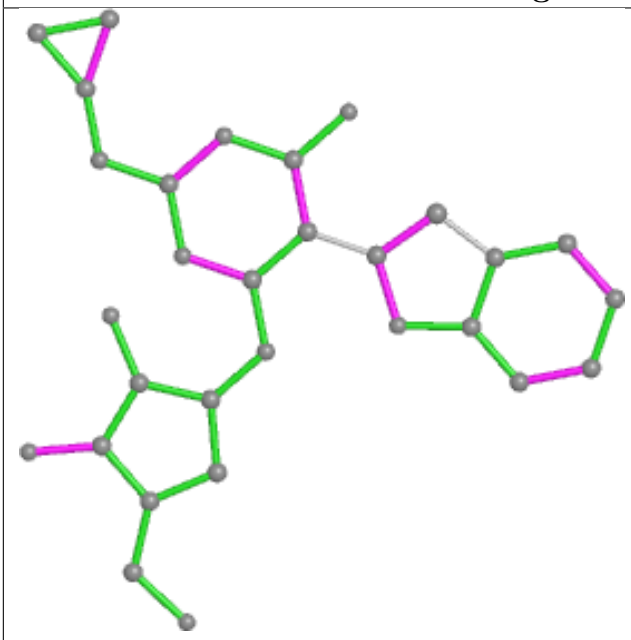


Torsions



Rings

Ligand 4S2 D 501



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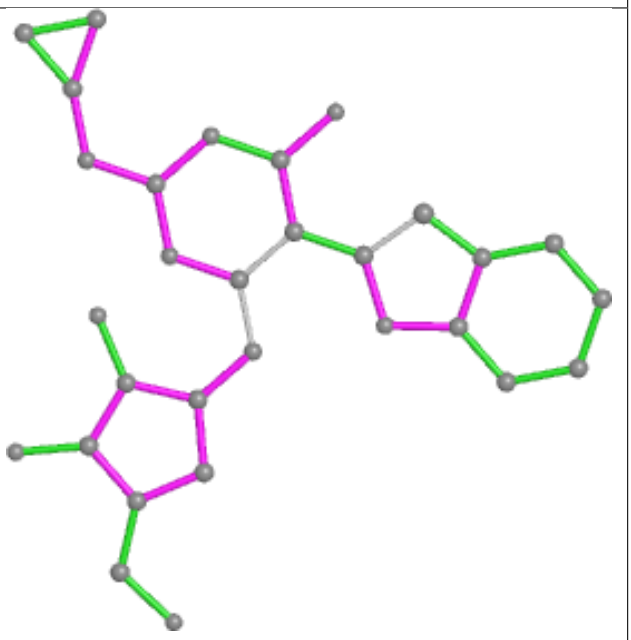
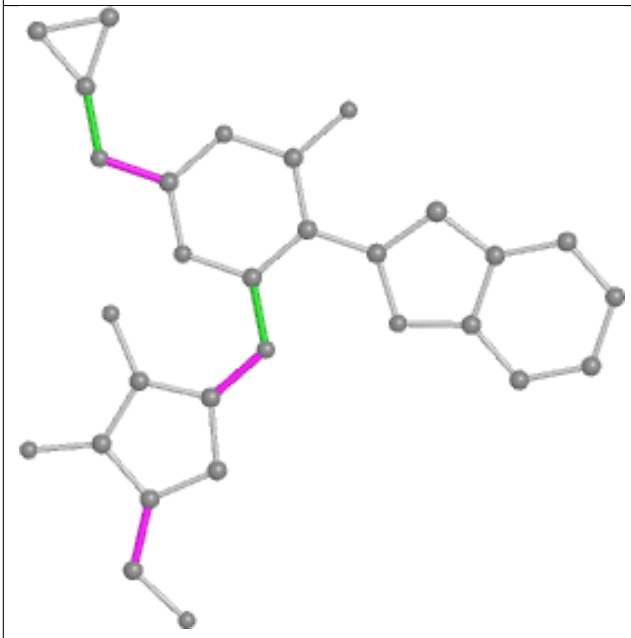
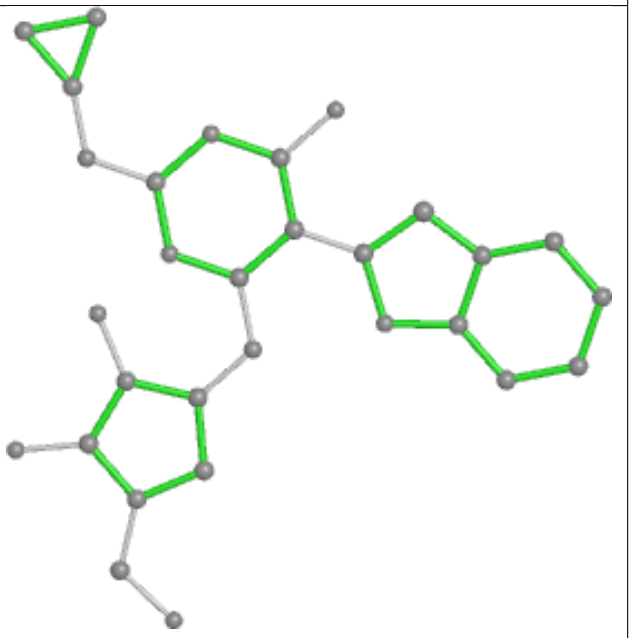


Bond angles

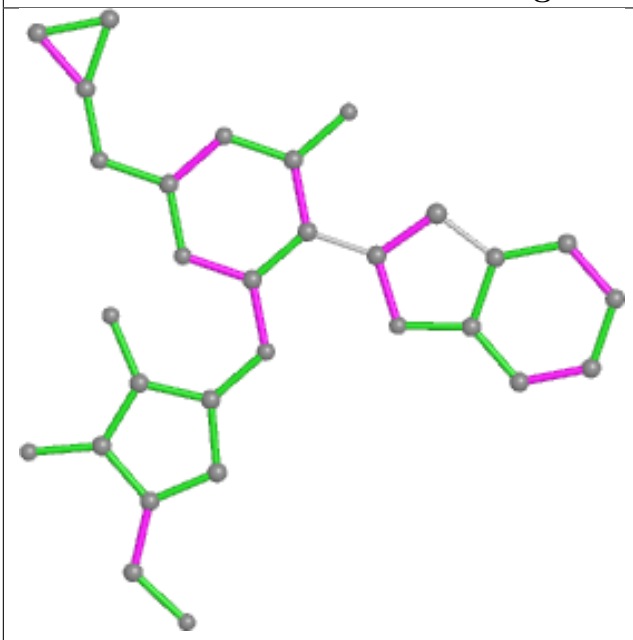


Torsions

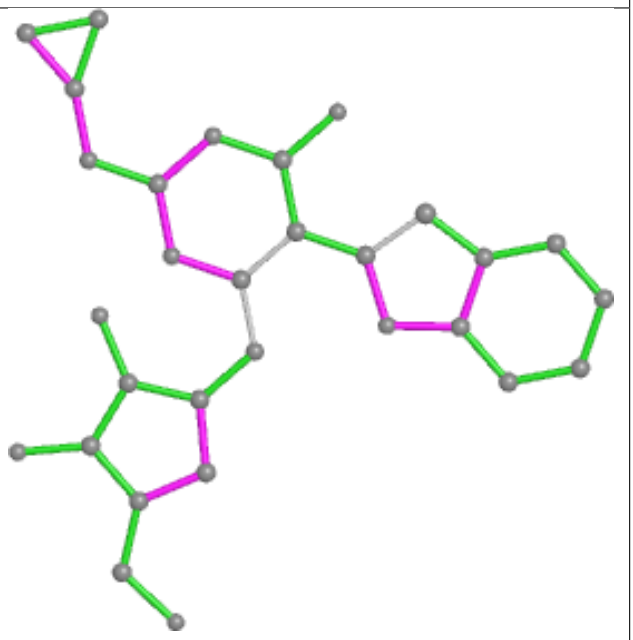


Rings

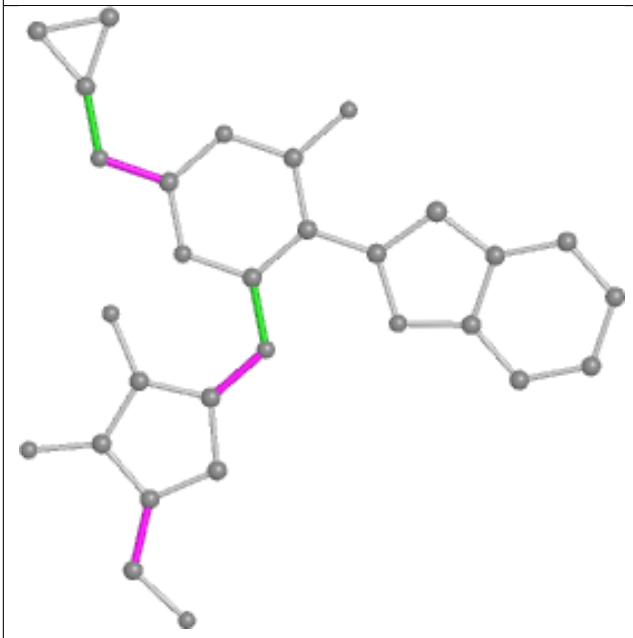
Ligand 4S2 C 501



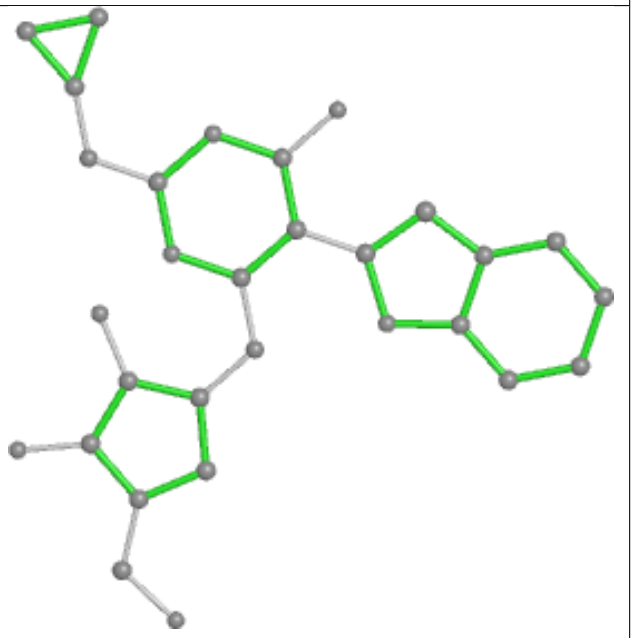
Bond lengths



Bond angles

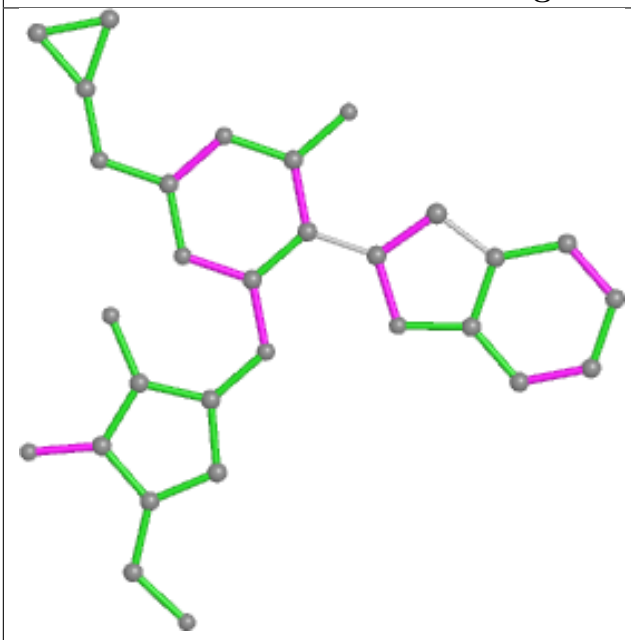


Torsions

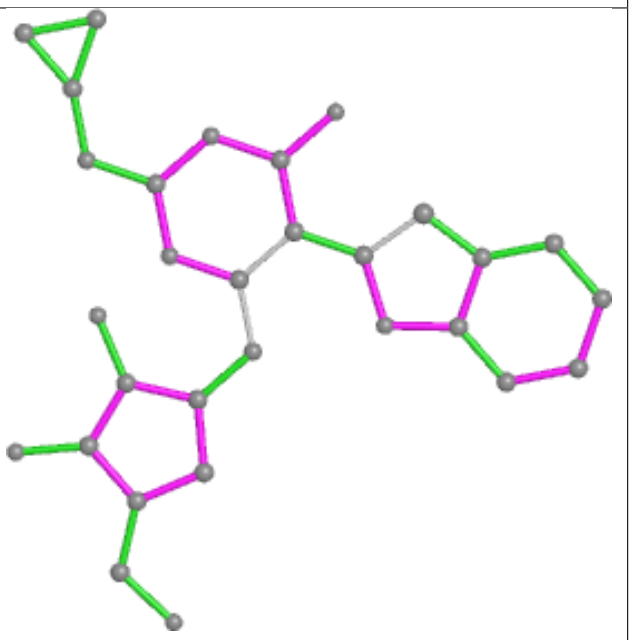


Rings

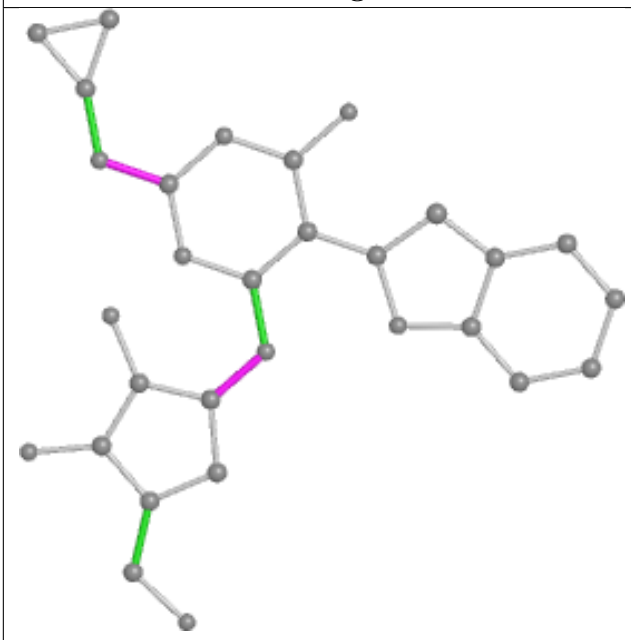
Ligand 4S2 B 501



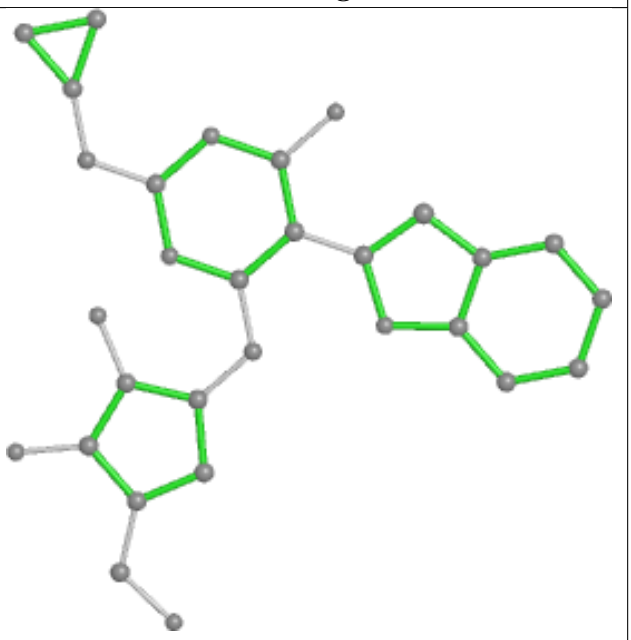
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	287/301 (95%)	0.27	22 (7%)	13	10	28, 49, 93, 113	0
1	B	280/301 (93%)	0.57	33 (11%)	4	3	24, 50, 111, 127	0
1	C	282/301 (93%)	0.34	22 (7%)	13	10	25, 47, 98, 118	0
1	D	282/301 (93%)	0.19	14 (4%)	28	25	23, 45, 82, 119	0
All	All	1131/1204 (93%)	0.34	91 (8%)	12	9	23, 48, 99, 127	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	460	SER	7.9
1	B	196	GLY	6.8
1	D	197	PHE	6.4
1	D	223	THR	6.3
1	C	222	THR	5.9
1	A	188	GLY	5.1
1	C	197	PHE	5.0
1	C	195	GLY	4.9
1	B	187	VAL	4.7
1	B	258	LEU	4.7
1	B	197	PHE	4.7
1	B	204	TYR	4.6
1	A	224	GLU	4.5
1	B	226	LEU	4.4
1	B	185	ILE	4.4
1	C	459	ALA	4.3
1	A	187	VAL	4.2
1	B	259	CYS	4.2
1	B	179	ASN	4.2
1	B	188	GLY	4.2
1	A	226	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	228	GLN	4.1
1	C	196	GLY	4.1
1	A	216	ALA	3.8
1	A	179	ASN	3.7
1	A	183	ARG	3.6
1	D	226	LEU	3.6
1	A	222	THR	3.6
1	B	227	LYS	3.5
1	A	223	THR	3.5
1	B	195	GLY	3.5
1	C	251	PHE	3.5
1	B	214	LYS	3.4
1	C	343	VAL	3.4
1	B	194	GLU	3.3
1	B	230	PHE	3.3
1	C	258	LEU	3.2
1	D	230	PHE	3.2
1	A	197	PHE	3.1
1	C	223	THR	3.1
1	C	226	LEU	3.1
1	D	216	ALA	3.1
1	B	438	HIS	3.0
1	C	225	GLU	3.0
1	C	187	VAL	3.0
1	A	257	ASP	2.9
1	D	459	ALA	2.9
1	D	222	THR	2.9
1	B	257	ASP	2.9
1	B	183	ARG	2.9
1	A	181	ASP	2.8
1	A	190	ASN	2.8
1	C	224	GLU	2.7
1	D	227	LYS	2.7
1	B	232	GLN	2.6
1	D	228	GLN	2.6
1	C	194	GLU	2.6
1	D	215	LEU	2.6
1	A	409	THR	2.6
1	C	189	GLY	2.6
1	B	207	ASN	2.5
1	A	182	GLU	2.5
1	C	188	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	407	GLU	2.4
1	A	207	ASN	2.4
1	B	181	ASP	2.4
1	A	215	LEU	2.4
1	B	452	GLN	2.3
1	B	231	ASP	2.3
1	D	254	ASP	2.3
1	A	189	GLY	2.3
1	B	332	LEU	2.3
1	C	186	SER	2.2
1	B	256	ASP	2.2
1	C	183	ARG	2.2
1	B	205	VAL	2.2
1	B	186	SER	2.2
1	C	215	LEU	2.2
1	B	193	GLY	2.2
1	C	410	ILE	2.1
1	A	347	ARG	2.1
1	A	407	GLU	2.1
1	B	255	GLY	2.1
1	D	224	GLU	2.1
1	D	229	GLN	2.1
1	A	191	LYS	2.0
1	B	178	ASN	2.0
1	A	256	ASP	2.0
1	C	167	SER	2.0
1	B	406	GLU	2.0
1	D	239	LYS	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, 95^{th} 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	SEP	B	346	10/11	0.78	0.24	83,89,97,97	0
1	TPO	D	342	11/12	0.78	0.23	87,91,98,99	0
1	SEP	D	346	10/11	0.79	0.18	77,83,91,91	0
1	TPO	A	342	11/12	0.81	0.28	89,91,96,97	0
1	SEP	A	346	10/11	0.83	0.17	75,81,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	C	342	11/12	0.85	0.20	81,83,90,90	0
1	SEP	C	346	10/11	0.87	0.18	72,79,88,89	0
1	TPO	B	342	11/12	0.90	0.17	81,83,86,86	0
1	TPO	B	345	11/12	0.94	0.12	77,78,83,84	0
1	TPO	A	345	11/12	0.94	0.13	73,73,77,78	0
1	TPO	D	345	11/12	0.96	0.15	71,72,76,77	0
1	TPO	C	345	11/12	0.96	0.14	64,65,70,72	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

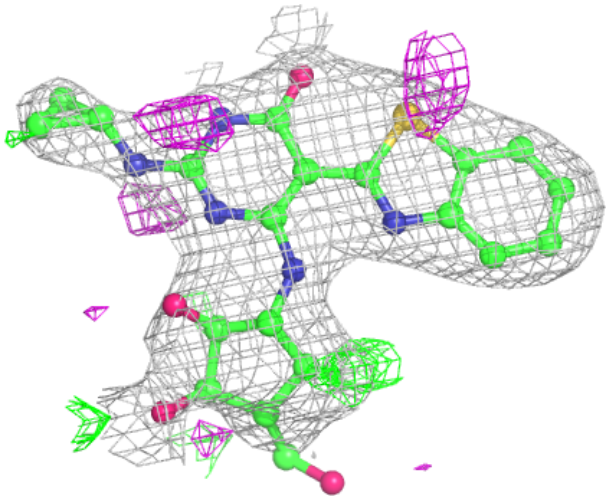
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

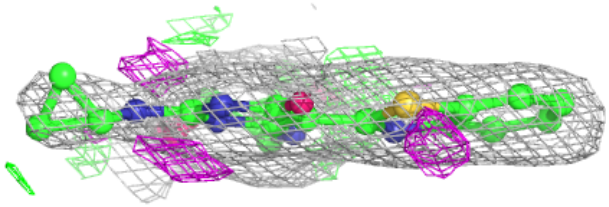
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4S2	B	501	30/30	0.89	0.19	47,57,83,89	0
2	4S2	A	501	30/30	0.92	0.18	56,65,87,89	0
2	4S2	C	501	30/30	0.92	0.16	47,61,86,86	0
2	4S2	D	501	30/30	0.93	0.17	40,51,68,73	0

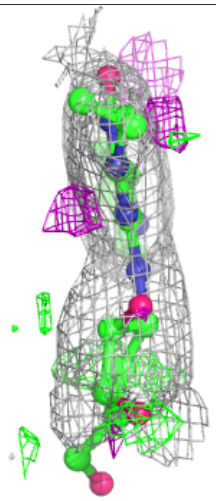
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4S2 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)

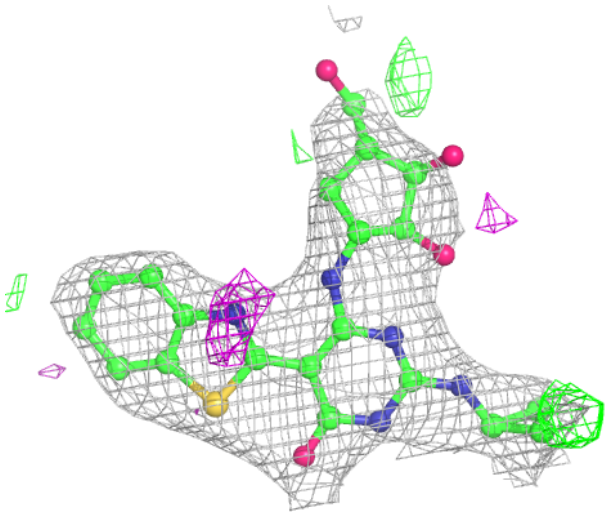


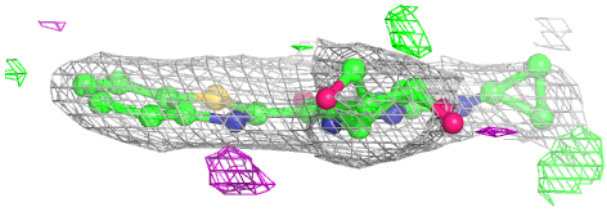


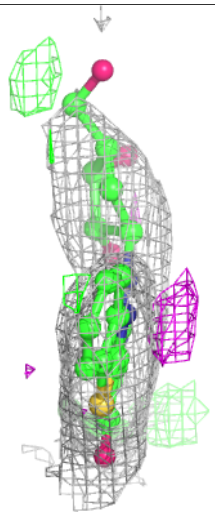


Electron density around 4S2 A 501:

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

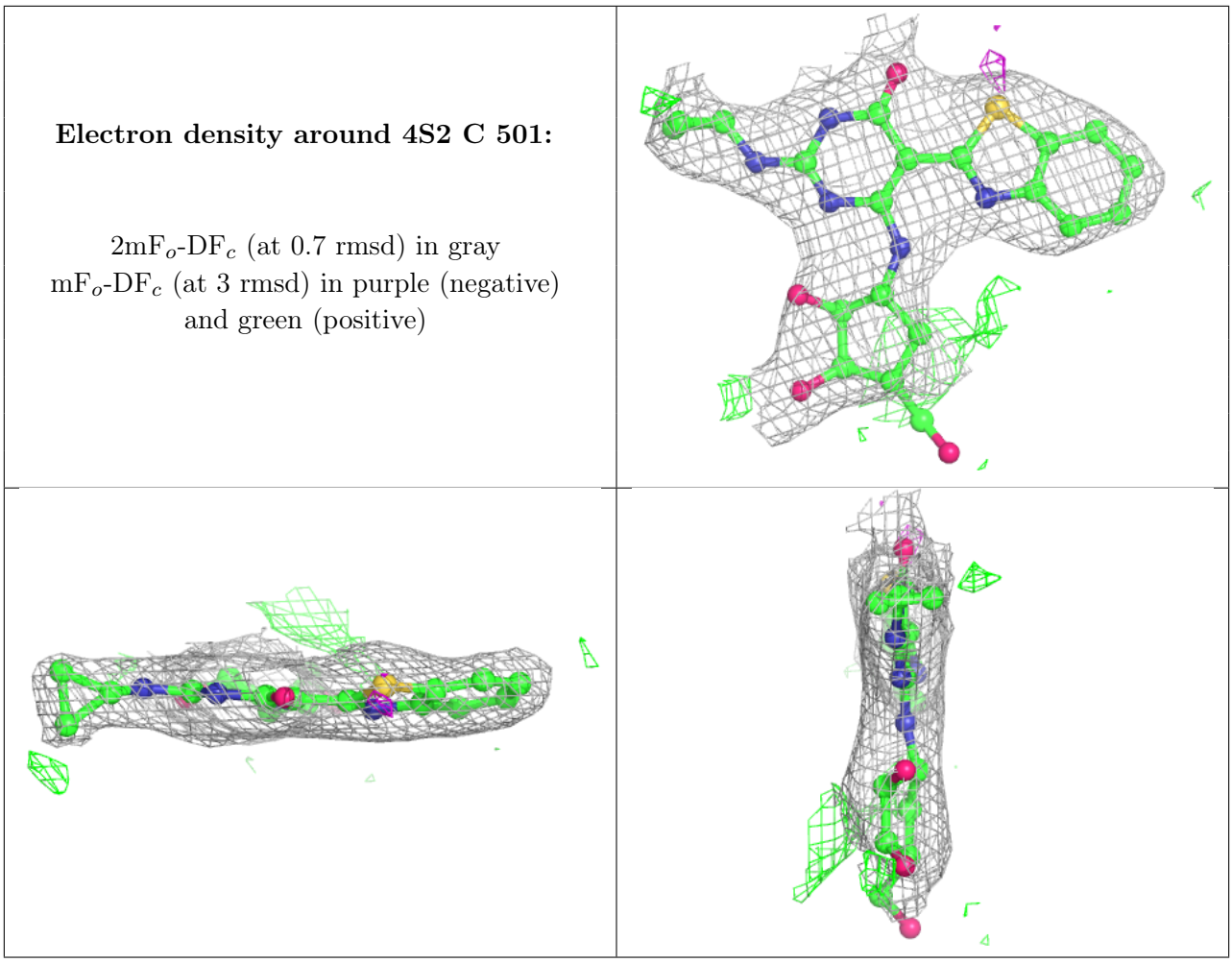






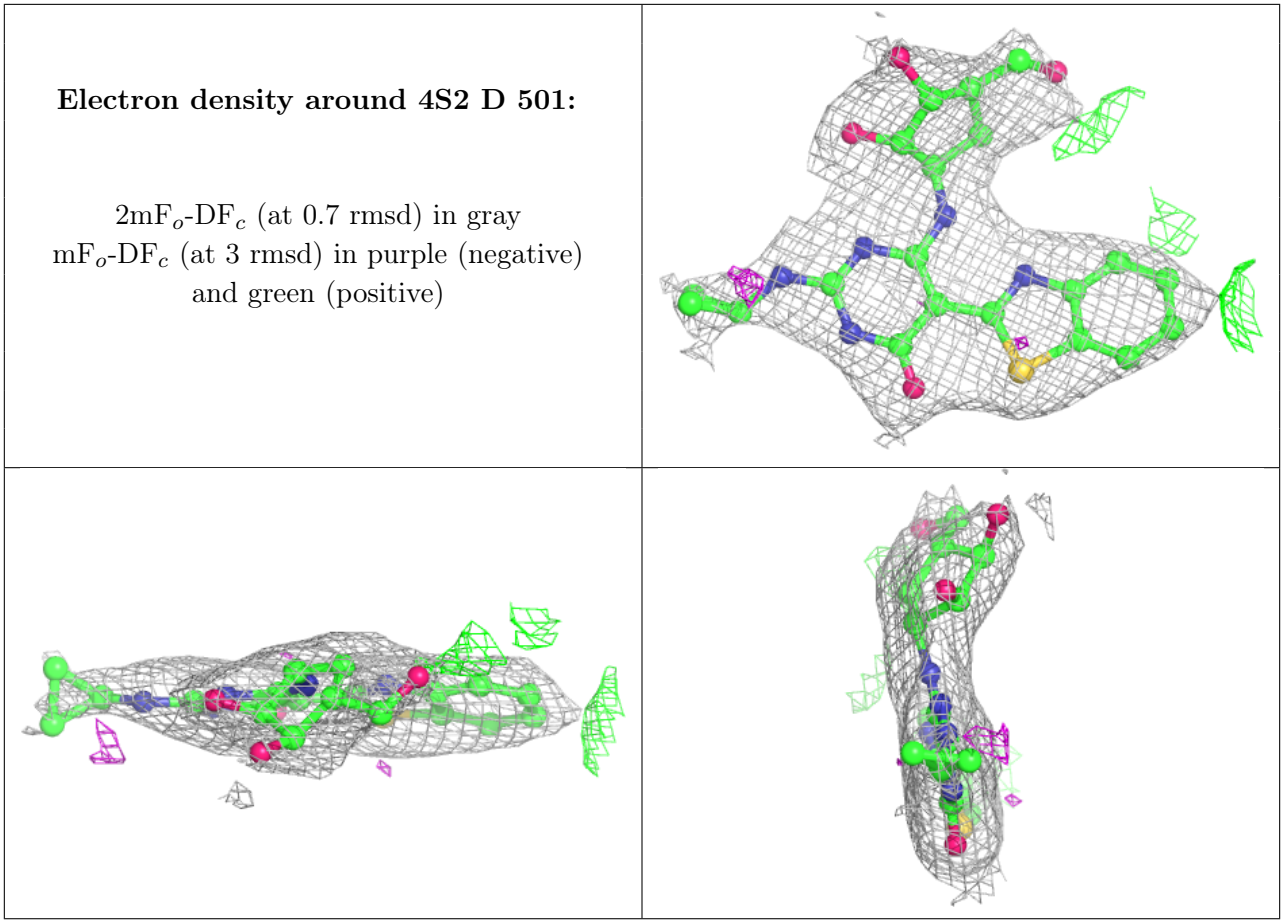
Electron density around 4S2 C 501:

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



Electron density around 4S2 D 501:

$2mF_o$-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.