



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:46 AM UTC

PDB ID : 4ZTM / pdb_00004ztm
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 ⓘ 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

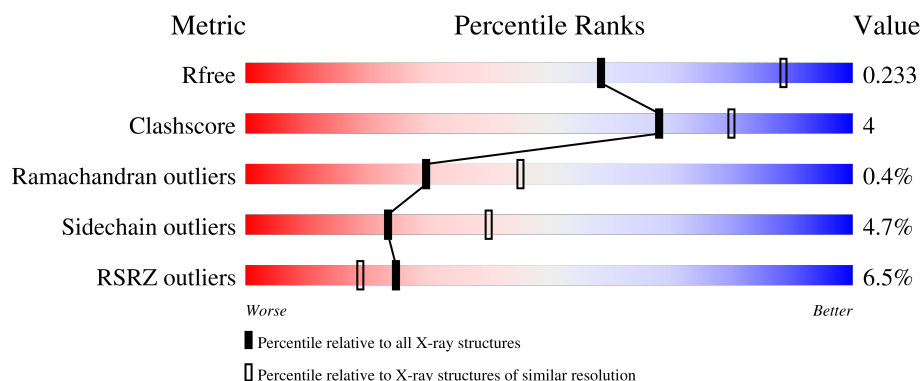
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	301	5% 84% 12% • •
1	B	301	10% 79% 14% • 6%
1	C	301	6% 82% 12% • 5%
1	D	301	3% 81% 13% • 5%

2 Entry composition [i](#)

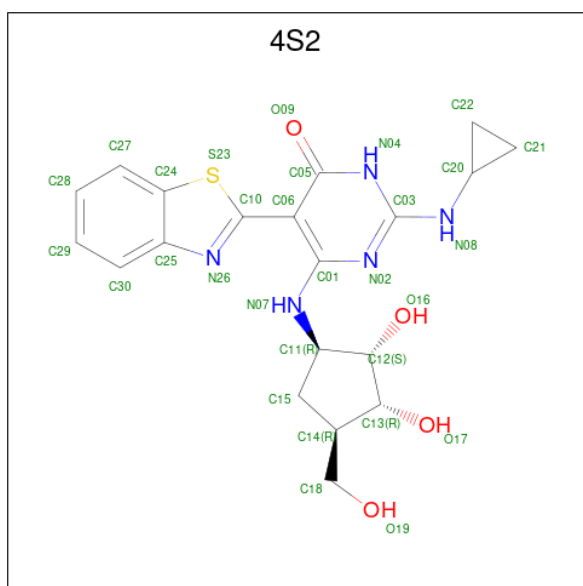
There are 3 unique types of molecules in this entry. The entry contains 9198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 4S2) (formula: C₂₀H₂₃N₅O₄S).



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		

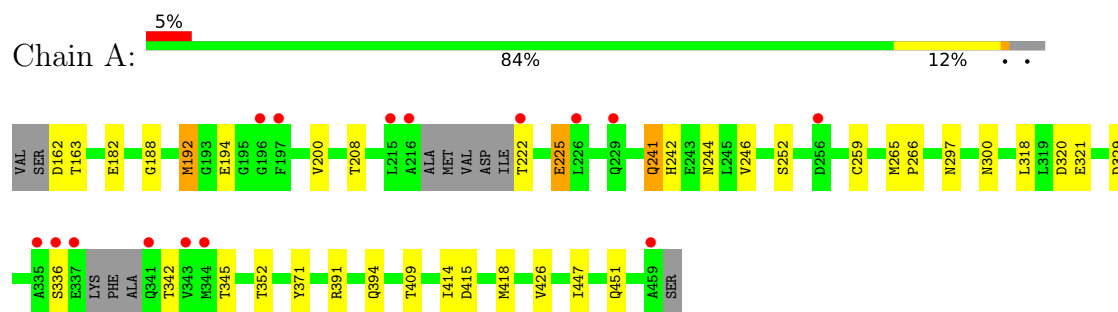
- Molecule 3 is water.

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		

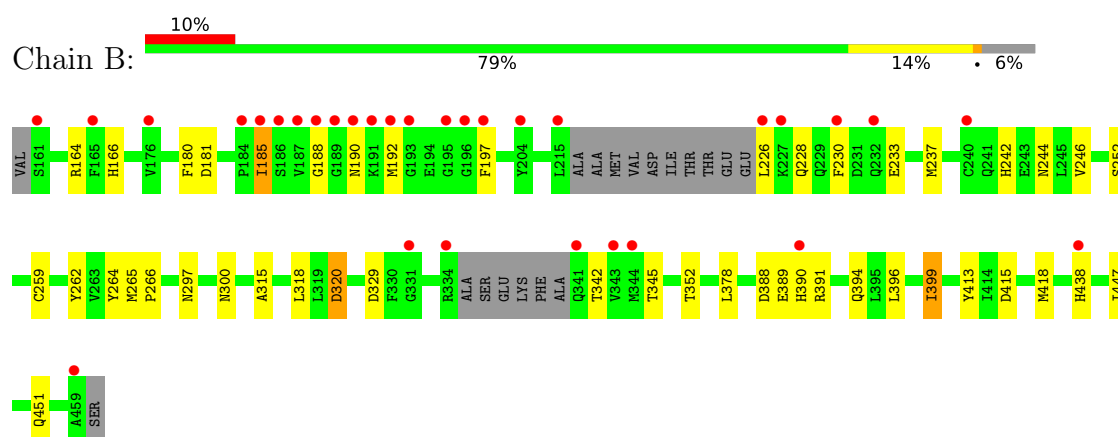
3 Residue-property plots [i](#)

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.

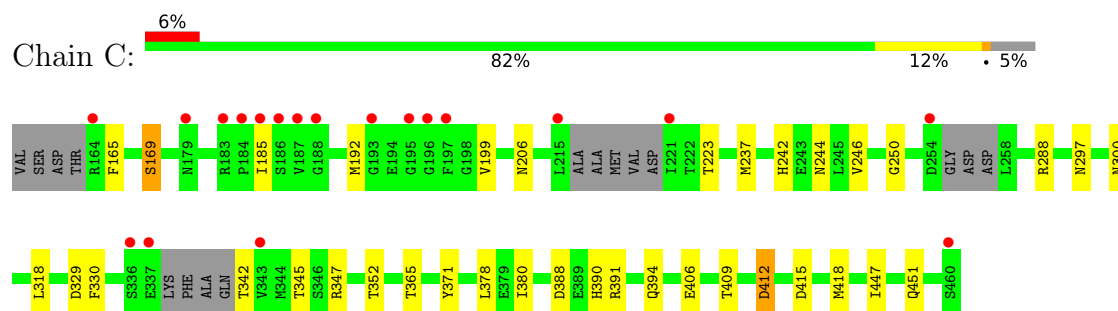
- Molecule 1: Interleukin-1 receptor-associated kinase 4



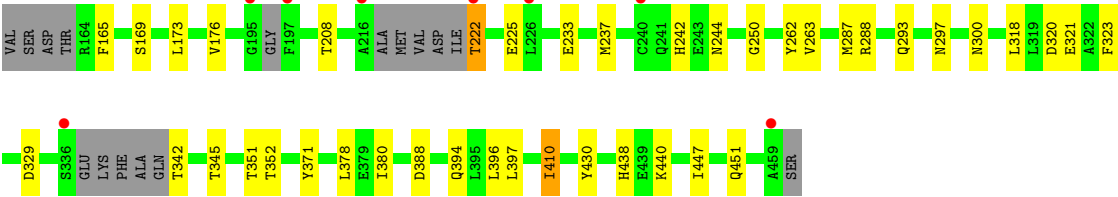
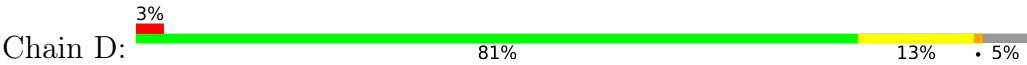
- Molecule 1: Interleukin-1 receptor-associated kinase 4



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



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



4 Data and refinement statistics

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) 92.4 (47.32-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.68%)	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 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: 4S2, SEP, TPO

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	0.84	0/2276	1.34	4/3065 (0.1%)
1	B	0.84	0/2227	1.39	5/2998 (0.2%)
1	C	0.85	0/2234	1.37	6/3009 (0.2%)
1	D	0.85	0/2248	1.37	12/3028 (0.4%)
All	All	0.85	0/8985	1.37	27/12100 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	PHE	CA-CB-CG	7.03	120.83	113.80
1	C	412	ASP	CA-CB-CG	6.68	119.28	112.60
1	C	169	SER	N-CA-C	-6.38	101.08	110.52
1	D	320	ASP	CA-CB-CG	6.23	118.83	112.60
1	D	397	LEU	N-CA-CB	-6.10	100.19	110.49
1	B	265	MET	CA-C-N	6.07	126.50	119.47
1	B	265	MET	C-N-CA	6.07	126.50	119.47
1	B	320	ASP	CA-CB-CG	5.82	118.42	112.60
1	D	396	LEU	CA-C-N	5.79	132.60	121.54
1	D	396	LEU	C-N-CA	5.79	132.60	121.54
1	A	320	ASP	CA-C-N	5.73	128.74	120.38
1	A	320	ASP	C-N-CA	5.73	128.74	120.38
1	D	293	GLN	CA-C-N	5.63	126.19	119.94
1	D	293	GLN	C-N-CA	5.63	126.19	119.94
1	D	351	THR	CA-C-N	5.22	128.66	120.82
1	D	351	THR	C-N-CA	5.22	128.66	120.82
1	C	371	TYR	CA-C-N	5.20	127.50	120.38
1	C	371	TYR	C-N-CA	5.20	127.50	120.38
1	A	371	TYR	CA-C-N	5.17	127.46	120.38
1	A	371	TYR	C-N-CA	5.17	127.46	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	PHE	CA-C-N	5.17	125.71	119.98
1	C	330	PHE	C-N-CA	5.17	125.71	119.98
1	B	180	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	371	TYR	CA-C-N	5.06	127.31	120.38
1	D	371	TYR	C-N-CA	5.06	127.31	120.38
1	D	320	ASP	CA-C-N	5.03	127.02	120.28
1	D	320	ASP	C-N-CA	5.03	127.02	120.28

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	2223	13	0
1	B	2224	0	2180	22	0
1	C	2231	0	2194	13	0
1	D	2245	0	2206	18	0
2	A	30	0	23	1	0
2	B	30	0	23	2	0
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	8895	64	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 4.

All (64) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:HA	1:C:390:HIS:HB3	1.58	0.86
1:D:287:MET:HE2	1:D:323:PHE:HB3	1.62	0.80
1:B:390:HIS:O	1:C:390:HIS:O	2.05	0.75
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.56	0.71
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:C:237:MET:HE1	1:C:246:VAL:HG23	1.80	0.62
1:D:438:HIS:HD2	1:D:440:LYS:H	1.45	0.62
1:D:287:MET:HE2	1:D:323:PHE:CB	2.30	0.62
1:D:242:HIS:CD2	1:D:244:ASN:H	2.17	0.62
1:B:242:HIS:CD2	1:B:244:ASN:H	2.20	0.59
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.87	0.56
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: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:415:ASP:HB3	1:B:418:MET:HE2	1.95	0.47
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
1:D:410:ILE:HG12	1:D:430:TYR:CD2	2.50	0.47
1:A:192:MET:HE2	1:A:200:VAL:HG12	1.96	0.46
1:B:390:HIS:CB	1:C:391:ARG:HA	2.33	0.46
1:D:321:GLU:H	1:D:321:GLU:CD	2.23	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:246:VAL:HG12	1:A:265:MET:HE3	1.97	0.45
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.99	0.45
1:B:237:MET:HE2	1:B:262:TYR:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.98	0.45
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: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:D:237:MET:HE3	1:D:262:TYR:CE2	2.45	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: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: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

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%)	30	45
1	B	274/301 (91%)	258 (94%)	15 (6%)	1 (0%)	30	45
1	C	275/301 (91%)	263 (96%)	10 (4%)	2 (1%)	18	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	275/301 (91%)	263 (96%)	12 (4%)	0	100	100
All	All	1105/1204 (92%)	1055 (96%)	46 (4%)	4 (0%)	30	45

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 ⓘ

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%)	21	36
1	B	242/259 (93%)	231 (96%)	11 (4%)	24	42
1	C	243/259 (94%)	230 (95%)	13 (5%)	20	35
1	D	245/259 (95%)	236 (96%)	9 (4%)	30	50
All	All	978/1036 (94%)	932 (95%)	46 (5%)	23	40

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	182	GLU
1	A	192	MET
1	A	194	GLU
1	A	208	THR
1	A	225	GLU
1	A	241	GLN
1	A	318	LEU
1	A	321	GLU
1	A	329	ASP

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Mol	Chain	Res	Type
1	A	336	SER
1	A	352	THR
1	A	409	THR
1	B	185	ILE
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	185	ILE
1	C	192	MET
1	C	199	VAL
1	C	223	THR
1	C	318	LEU
1	C	329	ASP
1	C	347	ARG
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	208	THR
1	D	222	THR
1	D	233	GLU
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	242	HIS
1	A	297	ASN
1	A	451	GLN
1	B	242	HIS
1	B	297	ASN
1	B	438	HIS
1	B	451	GLN
1	C	242	HIS
1	C	297	ASN
1	C	307	HIS
1	C	394	GLN
1	C	438	HIS
1	C	451	GLN
1	D	206	ASN
1	D	242	HIS
1	D	297	ASN
1	D	394	GLN
1	D	438	HIS
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	B	345	1	8,10,11	1.05	0	10,14,16	1.31	2 (20%)
1	TPO	C	345	1	8,10,11	1.35	1 (12%)	10,14,16	1.23	2 (20%)
1	TPO	C	342	1	8,10,11	1.17	1 (12%)	10,14,16	1.43	1 (10%)
1	TPO	B	342	1	8,10,11	1.11	1 (12%)	10,14,16	1.51	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	342	1	8,10,11	1.13	1 (12%)	10,14,16	1.56	1 (10%)
1	TPO	A	345	1	8,10,11	1.18	0	10,14,16	1.68	1 (10%)
1	SEP	C	346	1	8,9,10	0.97	0	7,12,14	0.72	0
1	SEP	B	346	1	8,9,10	0.95	0	7,12,14	1.00	0
1	SEP	A	346	1	8,9,10	0.97	0	7,12,14	0.97	0
1	TPO	D	342	1	8,10,11	1.18	1 (12%)	10,14,16	1.46	1 (10%)
1	TPO	D	345	1	8,10,11	1.17	1 (12%)	10,14,16	1.33	2 (20%)
1	SEP	D	346	1	8,9,10	1.09	0	7,12,14	0.61	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	TPO	B	345	1	-	3/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-2.66	1.54	1.59
1	C	342	TPO	P-OG1	-2.54	1.55	1.59
1	A	342	TPO	P-OG1	-2.46	1.55	1.59
1	C	345	TPO	P-OG1	-2.28	1.55	1.59
1	B	342	TPO	P-OG1	-2.17	1.55	1.59
1	D	345	TPO	P-OG1	-2.15	1.55	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	TPO	P-OG1-CB	-3.57	113.62	123.33
1	B	342	TPO	P-OG1-CB	-3.38	114.14	123.33
1	C	342	TPO	P-OG1-CB	-3.37	114.18	123.33
1	D	342	TPO	P-OG1-CB	-3.37	114.18	123.33
1	A	345	TPO	P-OG1-CB	-3.04	115.08	123.33
1	D	345	TPO	O3P-P-OG1	2.84	116.90	105.85
1	B	345	TPO	O3P-P-OG1	2.60	115.98	105.85
1	D	345	TPO	P-OG1-CB	-2.34	116.96	123.33
1	C	345	TPO	P-OG1-CB	-2.20	117.34	123.33
1	B	345	TPO	P-OG1-CB	-2.15	117.49	123.33
1	C	345	TPO	OG1-P-O1P	2.02	116.55	109.33

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	C	345	TPO	N-CA-CB-OG1
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
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	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	501	-	34,34,34	2.05	13 (38%)	43,50,50	1.70	10 (23%)
2	4S2	B	501	-	34,34,34	1.98	13 (38%)	43,50,50	1.59	10 (23%)
2	4S2	C	501	-	34,34,34	1.91	10 (29%)	43,50,50	1.51	7 (16%)
2	4S2	A	501	-	34,34,34	1.66	6 (17%)	43,50,50	1.56	7 (16%)

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	D	501	-	-	5/13/32/32	0/5/5/5
2	4S2	B	501	-	-	3/13/32/32	0/5/5/5
2	4S2	C	501	-	-	4/13/32/32	0/5/5/5
2	4S2	A	501	-	-	5/13/32/32	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4S2	C01-N02	5.08	1.44	1.36
2	D	501	4S2	C01-N02	4.65	1.43	1.36
2	D	501	4S2	C28-C27	3.88	1.45	1.38
2	B	501	4S2	C24-S23	3.75	1.81	1.74
2	A	501	4S2	C28-C27	3.75	1.45	1.38
2	B	501	4S2	C01-N02	3.72	1.41	1.36
2	A	501	4S2	C06-C05	3.67	1.52	1.44
2	B	501	4S2	C10-N26	3.64	1.40	1.30
2	A	501	4S2	C03-N04	3.62	1.42	1.36
2	D	501	4S2	C10-S23	3.43	1.80	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4S2	C25-C24	3.38	1.45	1.40
2	C	501	4S2	C10-S23	3.29	1.80	1.75
2	D	501	4S2	C30-C25	3.27	1.45	1.40
2	B	501	4S2	C01-N07	3.22	1.42	1.35
2	D	501	4S2	C06-C10	3.21	1.53	1.45
2	C	501	4S2	C06-C05	3.17	1.51	1.44
2	B	501	4S2	C30-C25	3.08	1.44	1.40
2	C	501	4S2	C03-N04	3.04	1.41	1.36
2	C	501	4S2	C18-C14	3.03	1.58	1.52
2	B	501	4S2	C10-S23	3.03	1.79	1.75
2	A	501	4S2	C29-C30	2.95	1.44	1.38
2	D	501	4S2	C03-N04	2.94	1.41	1.36
2	D	501	4S2	C10-N26	2.93	1.38	1.30
2	C	501	4S2	C29-C30	2.84	1.43	1.38
2	D	501	4S2	C29-C30	2.82	1.43	1.38
2	A	501	4S2	C01-N07	2.74	1.41	1.35
2	B	501	4S2	C29-C30	2.71	1.43	1.38
2	B	501	4S2	C06-C05	2.65	1.50	1.44
2	D	501	4S2	C06-C05	2.64	1.50	1.44
2	C	501	4S2	C25-C24	2.54	1.44	1.40
2	D	501	4S2	C25-C24	2.44	1.44	1.40
2	C	501	4S2	C01-N07	2.44	1.40	1.35
2	B	501	4S2	C03-N04	2.42	1.40	1.36
2	C	501	4S2	C06-C10	2.40	1.51	1.45
2	B	501	4S2	O17-C13	2.34	1.48	1.43
2	B	501	4S2	C28-C27	2.29	1.42	1.38
2	D	501	4S2	C22-C20	2.22	1.53	1.48
2	A	501	4S2	C30-C25	2.19	1.43	1.40
2	C	501	4S2	C28-C27	2.11	1.42	1.38
2	D	501	4S2	O17-C13	2.07	1.48	1.43
2	B	501	4S2	C06-C10	2.02	1.50	1.45
2	D	501	4S2	C24-S23	2.02	1.78	1.74

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4S2	C13-C12-C11	5.45	110.81	102.55
2	B	501	4S2	C03-N02-C01	5.36	123.25	112.60
2	A	501	4S2	C03-N02-C01	5.26	123.05	112.60
2	C	501	4S2	C03-N02-C01	4.59	121.71	112.60
2	D	501	4S2	C03-N02-C01	3.98	120.52	112.60
2	A	501	4S2	C20-N08-C03	3.45	133.61	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4S2	C21-C20-N08	3.38	122.95	118.52
2	A	501	4S2	C22-C20-N08	-3.19	114.33	118.52
2	A	501	4S2	N04-C03-N08	3.06	119.89	116.67
2	C	501	4S2	C14-C13-C12	3.00	107.40	103.87
2	A	501	4S2	C15-C11-C12	-2.98	98.44	103.17
2	D	501	4S2	C15-C14-C13	2.87	110.18	102.89
2	B	501	4S2	C15-C14-C13	2.73	109.81	102.89
2	C	501	4S2	C06-C10-S23	2.61	125.38	121.06
2	C	501	4S2	N04-C03-N02	-2.60	119.31	123.68
2	D	501	4S2	C14-C13-C12	-2.52	100.90	103.87
2	D	501	4S2	C22-C20-N08	2.45	121.73	118.52
2	B	501	4S2	C03-N04-C05	-2.44	121.60	124.55
2	B	501	4S2	C24-S23-C10	-2.43	87.31	88.92
2	A	501	4S2	C24-S23-C10	2.39	90.50	88.92
2	D	501	4S2	C20-N08-C03	2.32	130.79	124.95
2	D	501	4S2	C06-C10-N26	-2.26	120.21	123.82
2	D	501	4S2	C15-C11-C12	2.25	106.74	103.17
2	B	501	4S2	C21-C20-N08	2.20	121.41	118.52
2	B	501	4S2	C13-C12-C11	2.20	105.88	102.55
2	B	501	4S2	C28-C29-C30	-2.17	117.56	120.24
2	B	501	4S2	N04-C03-N02	-2.15	120.06	123.68
2	A	501	4S2	N04-C03-N02	-2.15	120.06	123.68
2	D	501	4S2	N04-C03-N02	-2.12	120.10	123.68
2	C	501	4S2	C06-C10-N26	-2.10	120.46	123.82
2	B	501	4S2	N04-C03-N08	2.07	118.85	116.67
2	B	501	4S2	C14-C15-C11	-2.07	100.66	103.55
2	C	501	4S2	C14-C15-C11	2.02	106.37	103.55
2	D	501	4S2	C12-C11-N07	-2.02	108.19	112.24

There are no chirality outliers.

All (17) 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

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Mol	Chain	Res	Type	Atoms
2	D	501	4S2	N02-C03-N08-C20
2	D	501	4S2	C12-C11-N07-C01
2	B	501	4S2	N04-C03-N08-C20
2	A	501	4S2	N02-C03-N08-C20
2	C	501	4S2	N02-C03-N08-C20
2	D	501	4S2	C13-C14-C18-O19
2	D	501	4S2	C15-C11-N07-C01
2	A	501	4S2	N04-C03-N08-C20

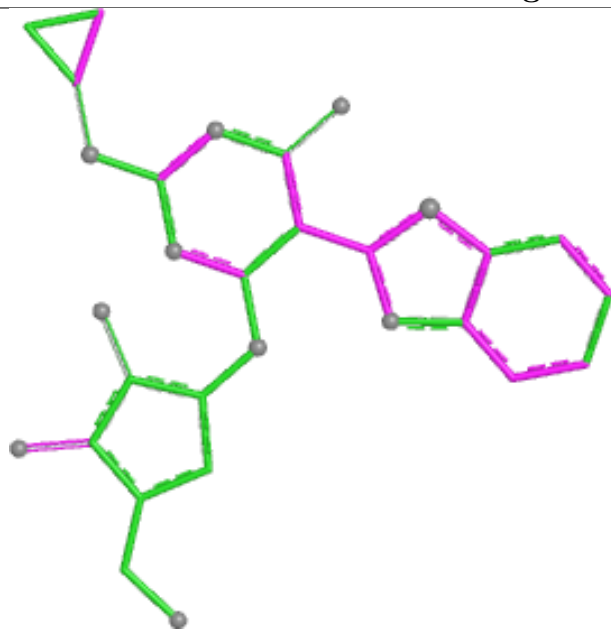
There are no ring outliers.

3 monomers are involved in 4 short contacts:

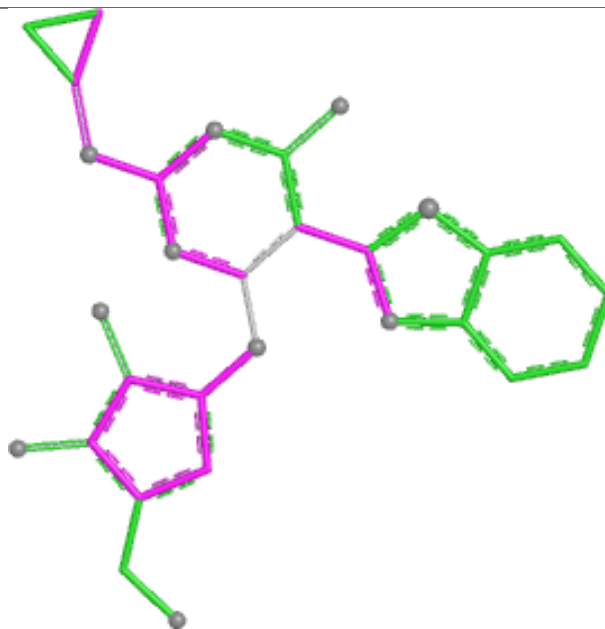
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	4S2	2	0
2	C	501	4S2	1	0
2	A	501	4S2	1	0

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.

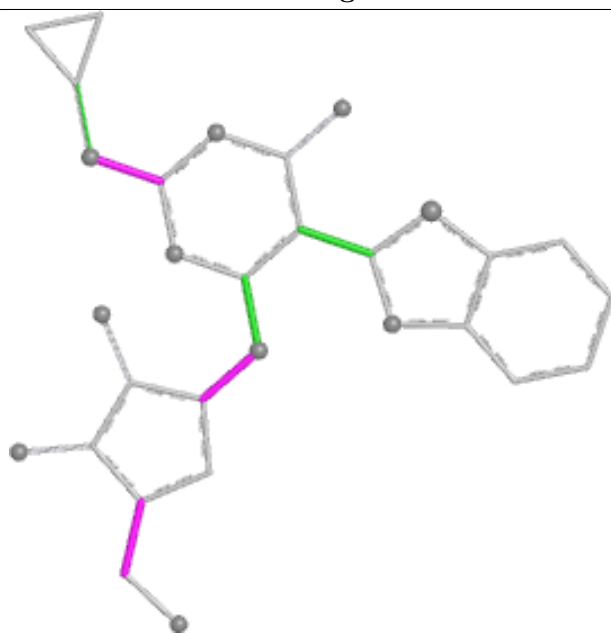
Ligand 4S2 D 501



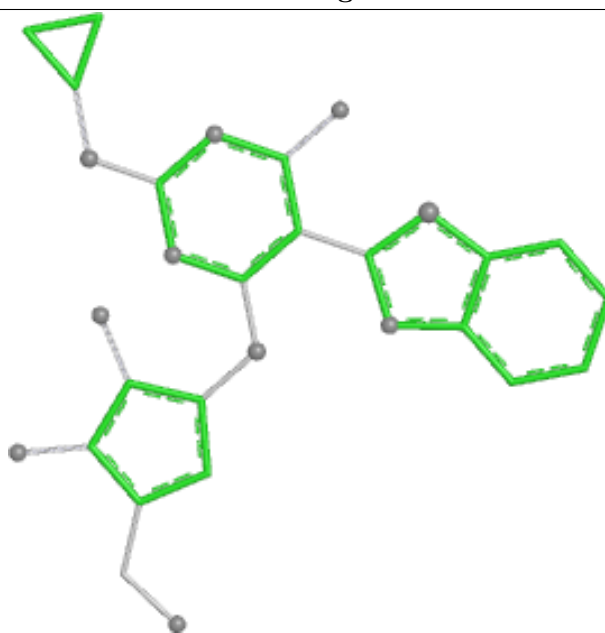
Bond lengths



Bond angles

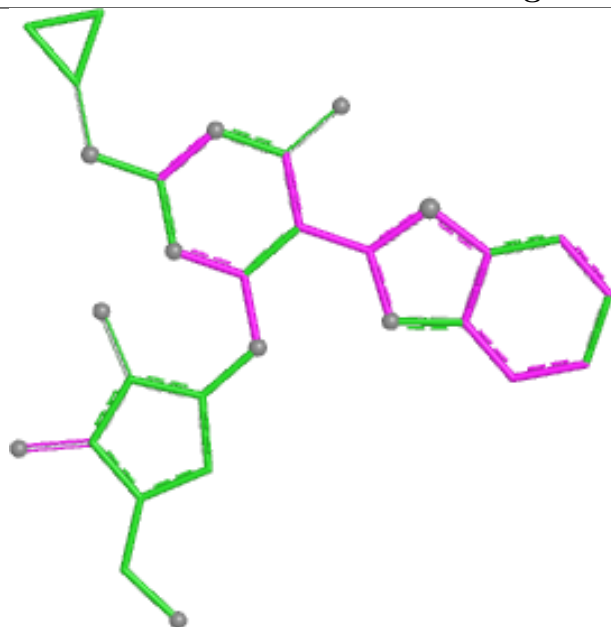


Torsions

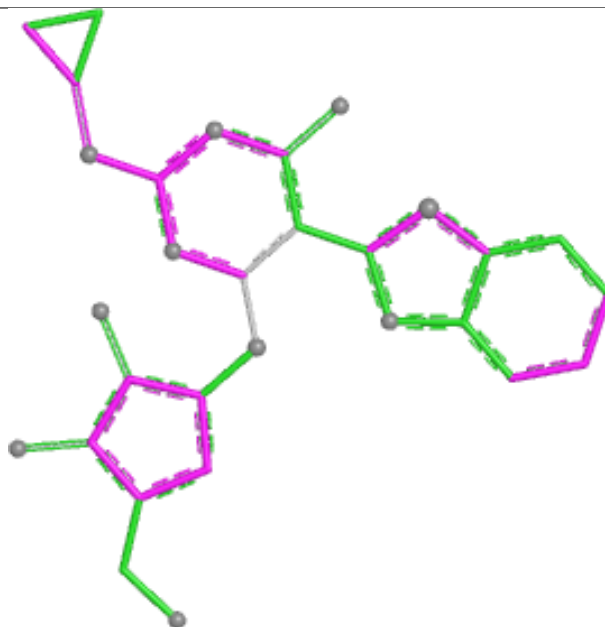


Rings

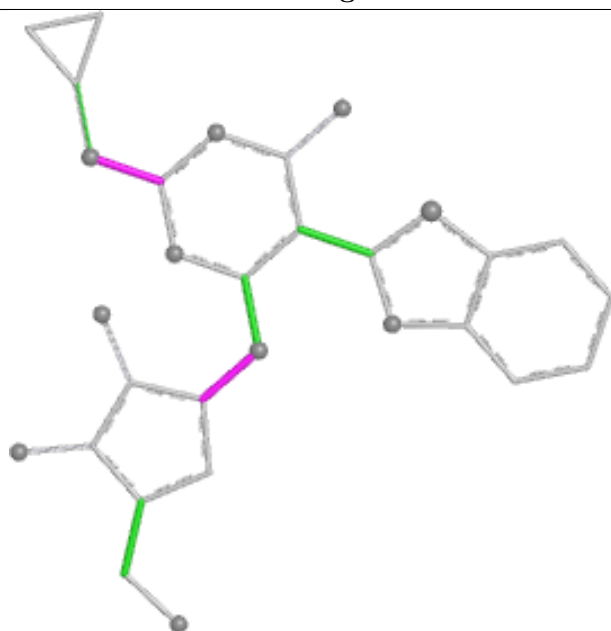
Ligand 4S2 B 501



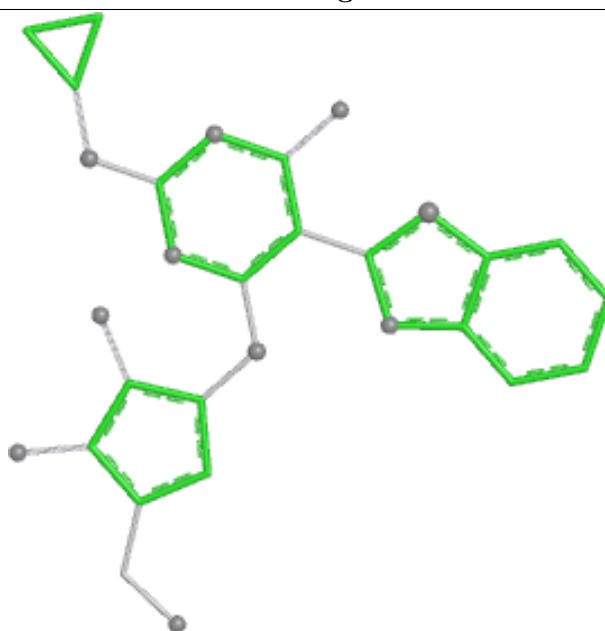
Bond lengths



Bond angles

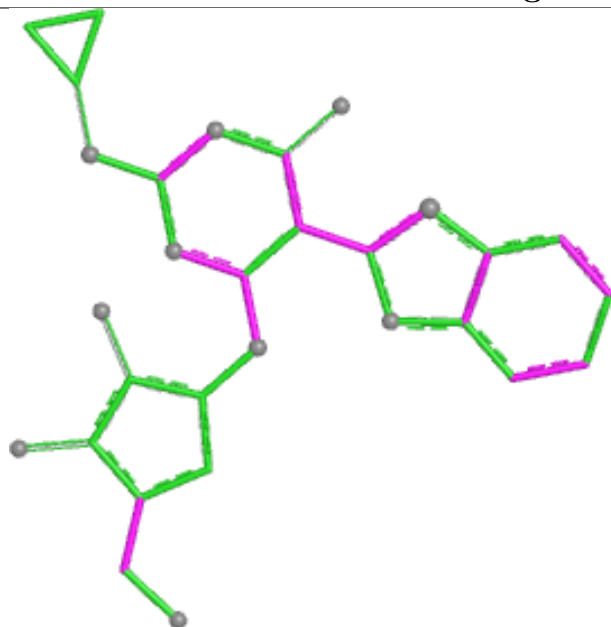


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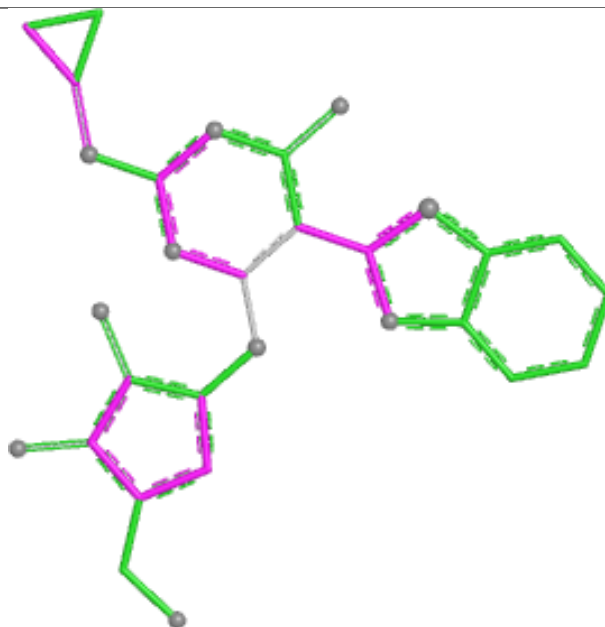


Rings

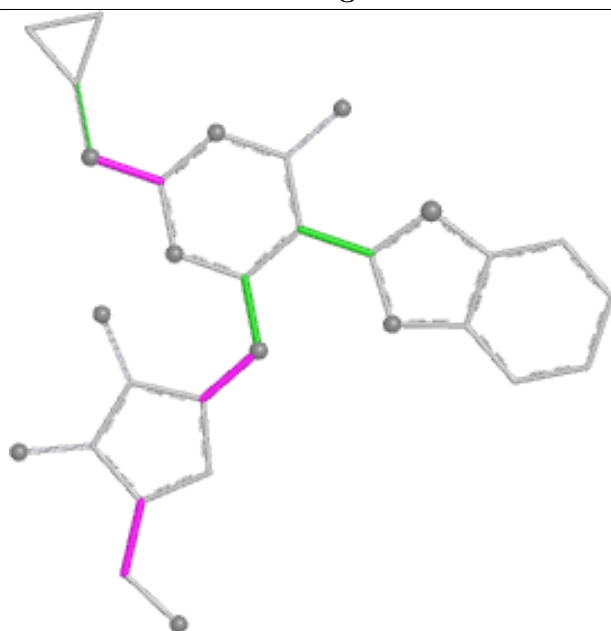
Ligand 4S2 C 501



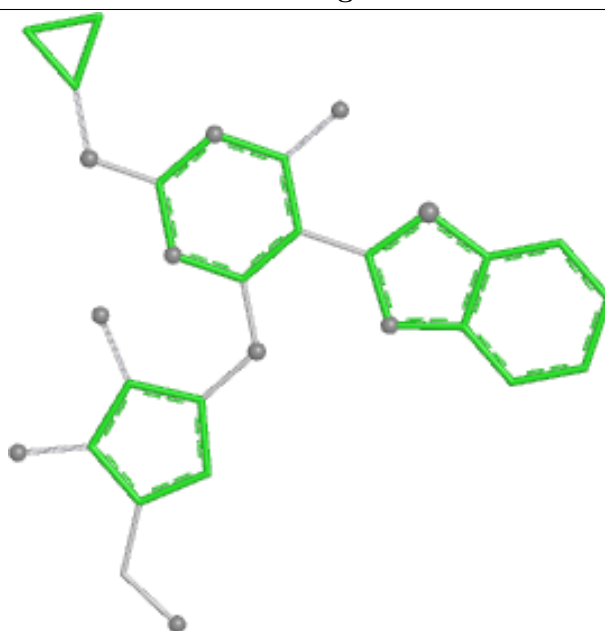
Bond lengths



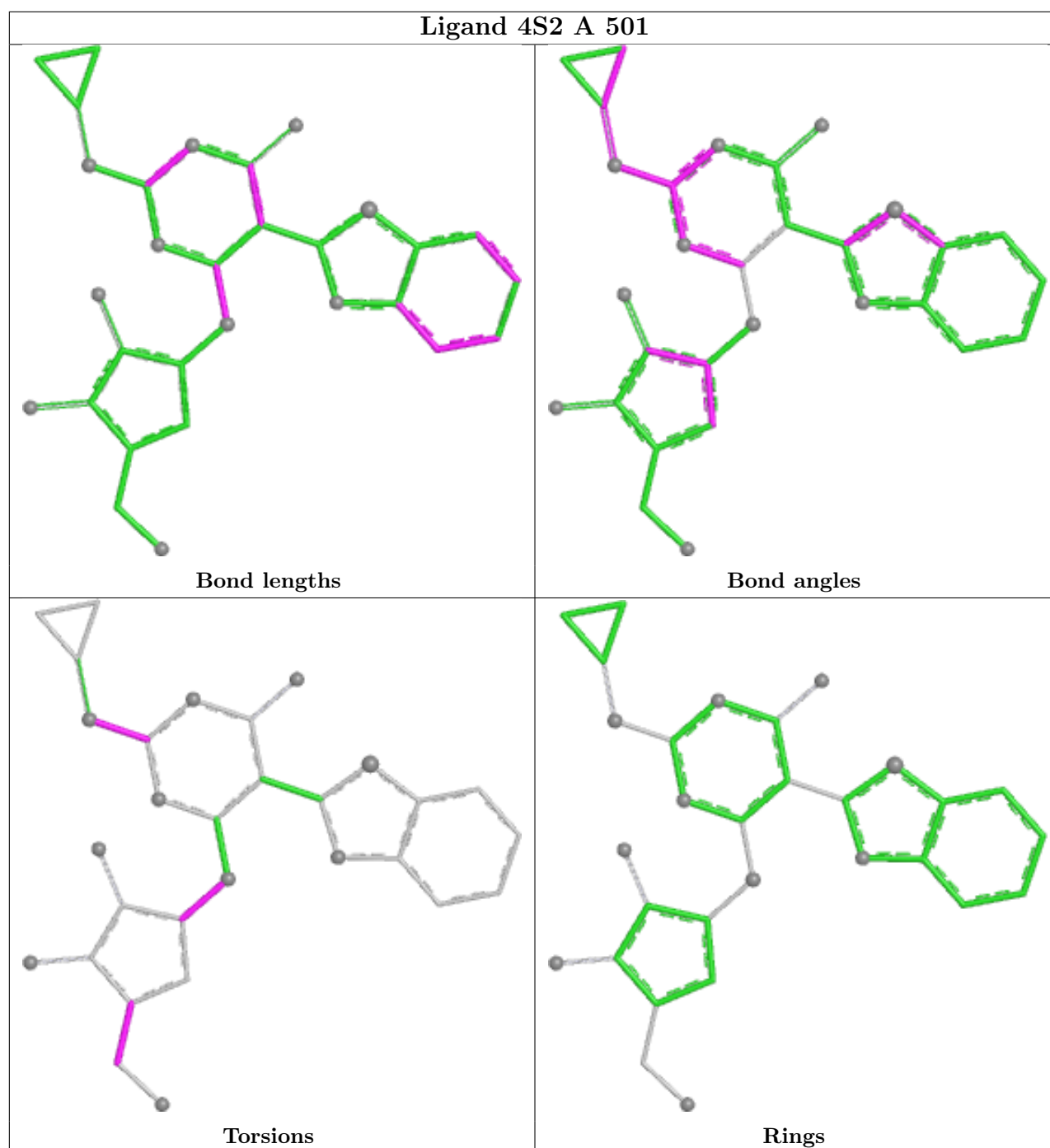
Bond angles



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, 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	287/301 (95%)	0.26	15 (5%) 33 25	28, 49, 93, 113	0
1	B	280/301 (93%)	0.46	31 (11%) 10 8	24, 50, 111, 127	0
1	C	282/301 (93%)	0.24	19 (6%) 24 18	25, 47, 98, 118	0
1	D	282/301 (93%)	0.13	8 (2%) 55 48	23, 45, 82, 119	0
All	All	1131/1204 (93%)	0.27	73 (6%) 25 19	23, 48, 99, 127	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	8.3
1	C	460	SER	6.3
1	D	336	SER	6.0
1	C	187	VAL	5.5
1	C	185	ILE	5.5
1	B	215	LEU	5.3
1	D	216	ALA	5.0
1	A	337	GLU	4.8
1	D	195	GLY	4.4
1	A	341	GLN	4.4
1	A	459	ALA	4.3
1	C	221	ILE	3.9
1	C	337	GLU	3.9
1	B	187	VAL	3.7
1	B	226	LEU	3.5
1	B	196	GLY	3.5
1	C	343	VAL	3.4
1	C	188	GLY	3.3
1	B	240	CYS	3.2
1	B	185	ILE	3.1
1	C	197	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	341	GLN	3.1
1	B	331	GLY	3.1
1	B	188	GLY	3.0
1	B	193	GLY	3.0
1	B	197	PHE	3.0
1	B	230	PHE	2.9
1	D	197	PHE	2.9
1	D	459	ALA	2.9
1	C	196	GLY	2.8
1	C	195	GLY	2.8
1	B	343	VAL	2.8
1	B	195	GLY	2.8
1	D	226	LEU	2.7
1	B	438	HIS	2.7
1	A	336	SER	2.7
1	B	184	PRO	2.7
1	C	184	PRO	2.7
1	D	240	CYS	2.7
1	C	254	ASP	2.7
1	C	186	SER	2.6
1	B	459	ALA	2.5
1	B	186	SER	2.5
1	B	176	VAL	2.5
1	A	256	ASP	2.4
1	A	229	GLN	2.4
1	B	227	LYS	2.4
1	A	226	LEU	2.4
1	C	183	ARG	2.4
1	C	193	GLY	2.3
1	A	197	PHE	2.3
1	A	344	MET	2.3
1	B	189	GLY	2.3
1	B	390	HIS	2.3
1	B	344	MET	2.3
1	C	179	ASN	2.3
1	D	222	THR	2.3
1	B	165	PHE	2.3
1	B	232	GLN	2.2
1	A	196	GLY	2.2
1	B	191	LYS	2.2
1	A	222	THR	2.2
1	B	192	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	190	ASN	2.2
1	B	204	TYR	2.2
1	B	334	ARG	2.1
1	A	335	ALA	2.1
1	A	343	VAL	2.1
1	C	164	ARG	2.0
1	C	336	SER	2.0
1	C	215	LEU	2.0
1	B	161	SER	2.0
1	A	215	LEU	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	SEP	B	346	10/11	0.62	0.13	83,89,97,97	0
1	SEP	D	346	10/11	0.75	0.12	77,83,91,91	0
1	TPO	A	342	11/12	0.76	0.17	89,91,96,97	0
1	SEP	C	346	10/11	0.77	0.12	72,79,88,89	0
1	SEP	A	346	10/11	0.78	0.10	75,81,89,89	0
1	TPO	C	342	11/12	0.79	0.15	81,83,90,90	0
1	TPO	D	342	11/12	0.80	0.13	87,91,98,99	0
1	TPO	B	342	11/12	0.88	0.12	81,83,86,86	0
1	TPO	B	345	11/12	0.89	0.12	77,78,83,84	0
1	TPO	D	345	11/12	0.92	0.11	71,72,76,77	0
1	TPO	A	345	11/12	0.94	0.09	73,73,77,78	0
1	TPO	C	345	11/12	0.95	0.09	64,65,70,72	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,

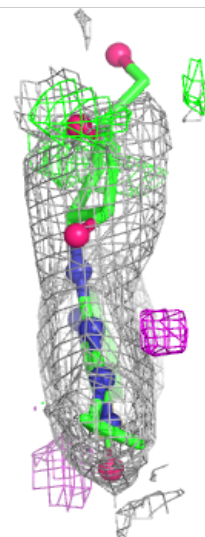
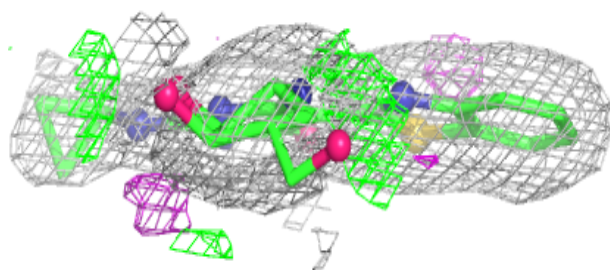
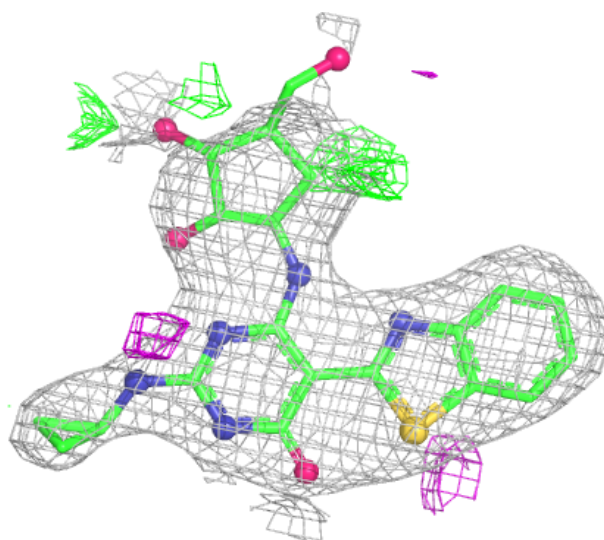
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4S2	B	501	30/30	0.83	0.15	47,57,83,89	0
2	4S2	A	501	30/30	0.85	0.15	56,65,87,89	0
2	4S2	C	501	30/30	0.87	0.12	47,61,86,86	0
2	4S2	D	501	30/30	0.90	0.12	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.

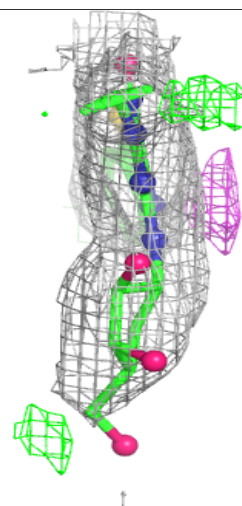
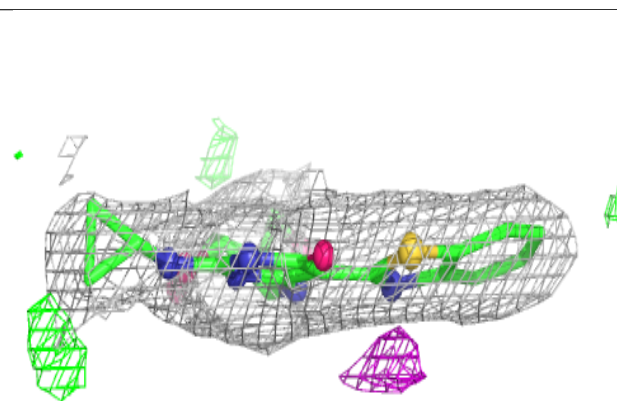
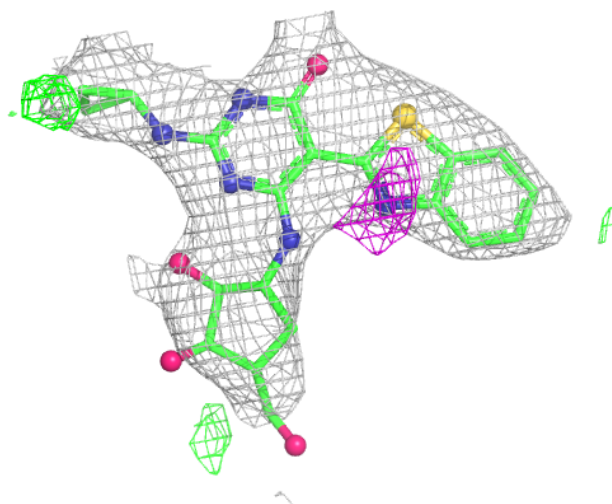
Electron density around 4S2 B 501:

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



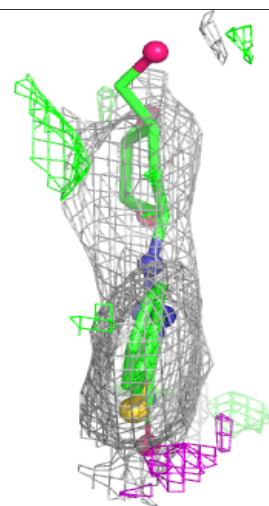
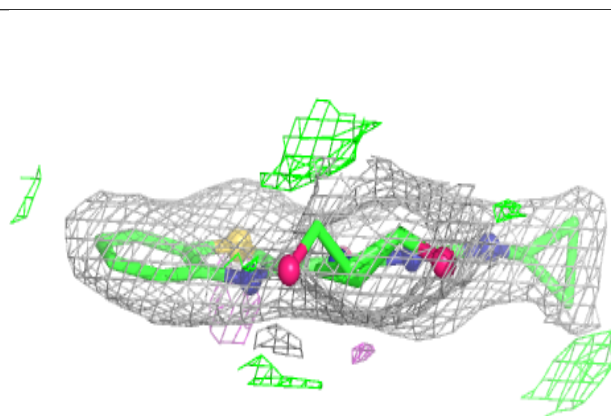
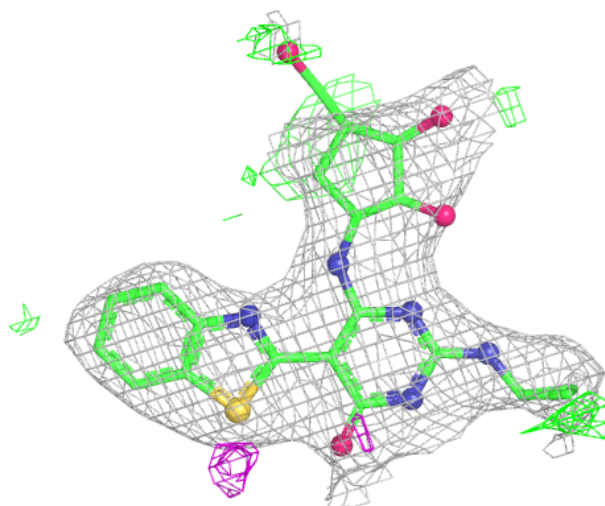
Electron density around 4S2 A 501:

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



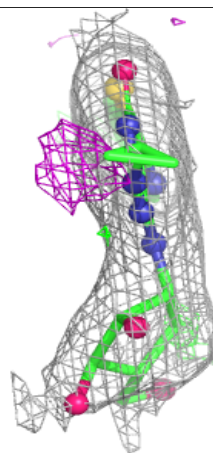
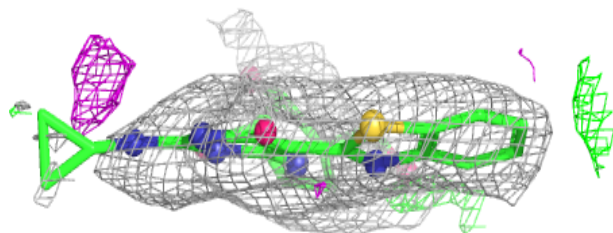
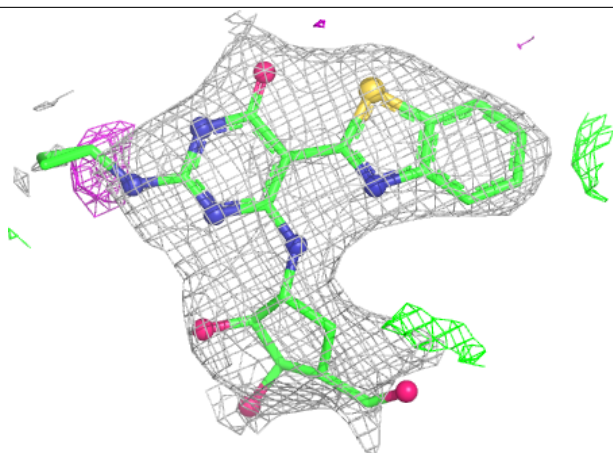
Electron density around 4S2 C 501:

$2mF_o-DF_c$ (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.