



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 4ZTL / pdb_00004ztl
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2015-05-14
Resolution : 2.39 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

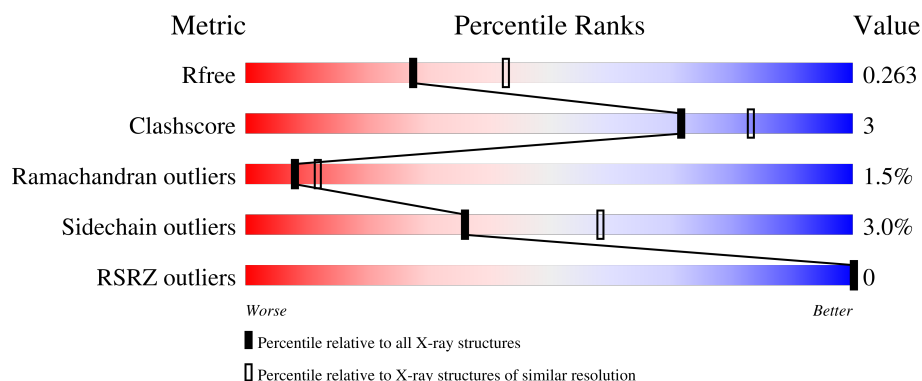
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

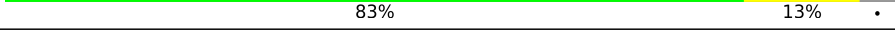
The reported resolution of this entry is 2.39 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	
1	B	301	
1	C	301	
1	D	301	

2 Entry composition [i](#)

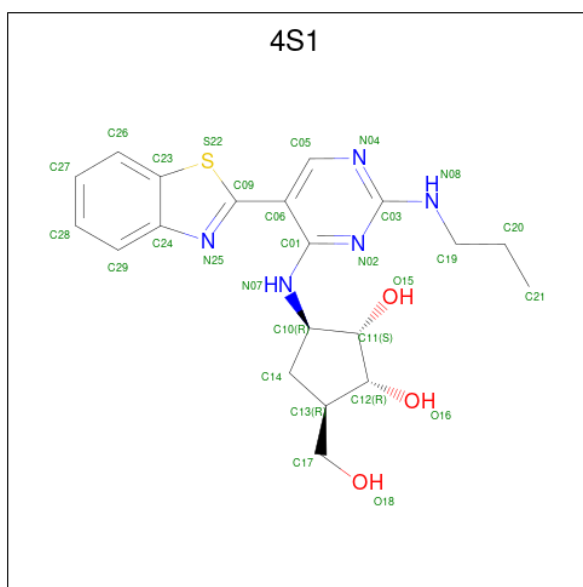
There are 3 unique types of molecules in this entry. The entry contains 9076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	283	Total	C	N	O	P	S	0	1	3
			2230	1398	372	442	3	15			
1	B	272	Total	C	N	O	P	S	0	1	4
			2124	1332	355	419	3	15			
1	C	285	Total	C	N	O	P	S	0	0	2
			2239	1405	378	439	3	14			
1	D	288	Total	C	N	O	P	S	0	0	4
			2259	1414	382	446	3	14			

- Molecule 2 is (1R,2S,3R,5R)-3-{[5-(1,3-benzothiazol-2-yl)-2-(propylamino)pyrimidin-4-yl]amino}-5-(hydroxymethyl)cyclopentane-1,2-diol (CCD ID: 4S1) (formula: C₂₀H₂₅N₅O₃S).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			29	20	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			29	20	5	3	1		

- Molecule 3 is water.

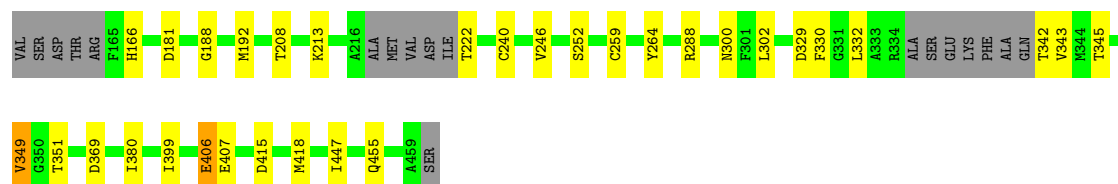
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	19	Total	O	0	0
			19	19		
3	C	35	Total	O	0	0
			35	35		
3	D	35	Total	O	0	0
			35	35		

3 Residue-property plots

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.

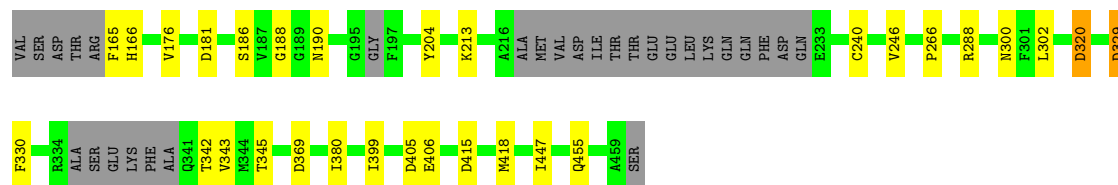
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A: 



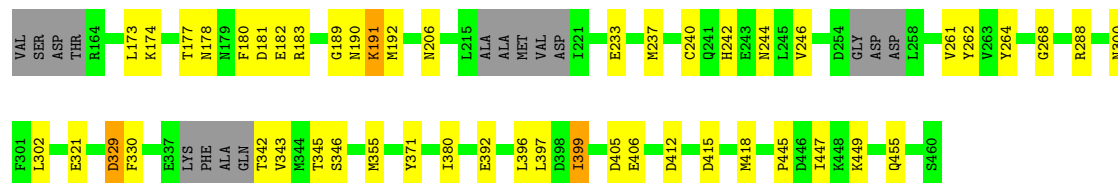
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B: 



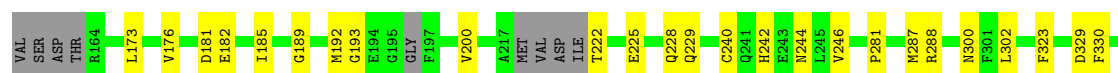
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C: 



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

Chain D: 



E337	LYS	T342	V343	K344	T345	D369	I370	Y371	I380	E392	L397	D405	E406	I447	K448	K449	Q455	A459	S460
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.18Å 139.39Å 87.98Å 90.00° 125.93° 90.00°	Depositor
Resolution (Å)	28.31 – 2.39 28.31 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.31-2.39) 92.4 (28.31-2.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.225 , 0.251 0.237 , 0.263	Depositor DCC
R_{free} test set	2817 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.317 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4411e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 4S1, SEP

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	0.82	0/2234	1.34	5/3010 (0.2%)
1	B	0.83	0/2124	1.34	5/2860 (0.2%)
1	C	0.89	0/2242	1.36	8/3019 (0.3%)
1	D	0.88	0/2262	1.35	6/3047 (0.2%)
All	All	0.85	0/8862	1.35	24/11936 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	GLU	N-CA-C	-7.50	103.08	112.90
1	C	412	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	240	CYS	N-CA-C	5.85	118.29	107.99
1	B	369	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	405	ASP	CA-C-N	5.73	132.48	121.54
1	B	405	ASP	C-N-CA	5.73	132.48	121.54
1	A	240	CYS	N-CA-C	5.70	118.04	108.23
1	C	405	ASP	CA-C-N	5.68	132.39	121.54
1	C	405	ASP	C-N-CA	5.68	132.39	121.54
1	D	405	ASP	CA-C-N	5.64	132.32	121.54
1	D	405	ASP	C-N-CA	5.64	132.32	121.54
1	C	240	CYS	N-CA-C	5.49	117.65	107.99
1	C	174	LYS	N-CA-C	-5.34	105.46	111.28
1	C	177	THR	N-CA-C	5.34	119.90	113.17
1	A	369	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	240	CYS	N-CA-C	5.17	117.10	107.99
1	D	369	ASP	CA-CB-CG	5.17	117.77	112.60
1	C	355	MET	N-CA-C	5.12	117.86	110.28
1	D	229	GLN	CA-C-N	5.08	127.35	120.44
1	D	229	GLN	C-N-CA	5.08	127.35	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	351	THR	CA-C-N	5.05	128.40	120.82
1	A	351	THR	C-N-CA	5.05	128.40	120.82
1	C	178	ASN	N-CA-C	-5.03	105.19	111.92

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	2230	0	2186	11	0
1	B	2124	0	2084	9	0
1	C	2239	0	2207	22	0
1	D	2259	0	2218	17	0
2	A	29	0	25	2	0
2	B	29	0	25	2	0
2	C	29	0	25	3	0
2	D	29	0	25	3	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	35	0	0	0	0
3	D	35	0	0	0	0
All	All	9076	0	8795	58	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 (58) 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:192:MET:HE1	1:A:264:TYR:HE1	1.52	0.72
1:A:192:MET:HE1	1:A:264:TYR:CE1	2.28	0.68
1:D:242:HIS:CD2	1:D:244:ASN:H	2.17	0.62
1:C:192:MET:HE1	1:C:264:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:HIS:CD2	1:C:244:ASN:H	2.21	0.58
1:B:181:ASP:HB3	1:B:190:ASN:HB2	1.87	0.57
1:C:246:VAL:HG21	2:C:501:4S1:H22	1.87	0.57
1:C:192:MET:HE1	1:C:264:TYR:HE1	1.69	0.56
1:D:242:HIS:HD2	1:D:244:ASN:H	1.54	0.56
1:B:246:VAL:HG21	2:B:501:4S1:H22	1.87	0.56
1:C:182:GLU:HA	1:C:191:LYS:HB2	1.92	0.51
1:D:222:THR:HB	1:D:225:GLU:HB2	1.92	0.51
1:D:246:VAL:HG21	2:D:501:4S1:H22	1.92	0.51
1:A:332:LEU:HD13	1:A:349:VAL:HG13	1.93	0.50
1:D:288:ARG:HB3	1:D:380:ILE:HG23	1.93	0.50
1:C:237:MET:HE3	1:C:262:TYR:HE2	1.76	0.49
1:C:268:GLY:HA2	2:C:501:4S1:H16	1.93	0.49
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.94	0.49
1:C:246:VAL:HG21	2:C:501:4S1:C26	2.42	0.49
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.78	0.48
1:D:193:GLY:HA3	2:D:501:4S1:H8	1.95	0.48
1:C:242:HIS:HD2	1:C:244:ASN:H	1.60	0.48
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.97	0.47
1:A:246:VAL:HG21	2:A:501:4S1:C26	2.45	0.47
1:C:181:ASP:HB3	1:C:190:ASN:HB2	1.96	0.46
1:B:302:LEU:HD11	1:B:330:PHE:HE1	1.81	0.46
1:B:246:VAL:HG21	2:B:501:4S1:C26	2.46	0.46
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.97	0.46
1:B:266:PRO:HD2	1:B:320:ASP:HA	1.98	0.45
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.98	0.45
1:C:445:PRO:HB3	1:C:449:LYS:HD3	1.97	0.45
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.45
1:C:321:GLU:HG3	1:D:281:PRO:HD3	1.98	0.45
1:D:287:MET:HE2	1:D:323:PHE:CB	2.47	0.45
1:C:183:ARG:HB3	1:C:189:GLY:HA3	1.99	0.45
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.98	0.44
1:C:302:LEU:HD11	1:C:330:PHE:HE1	1.82	0.44
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.83	0.44
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.99	0.44
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.99	0.44
1:A:246:VAL:HG21	2:A:501:4S1:H22	1.99	0.44
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.99	0.44
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.99	0.43
1:D:287:MET:HE2	1:D:323:PHE:HB3	2.00	0.43
1:D:185:ILE:HD11	1:D:192:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD22	1:A:349:VAL:HG11	2.02	0.42
1:B:176:VAL:HB	1:B:204:TYR:H	1.84	0.42
1:C:371:TYR:OH	1:C:397:LEU:HD22	2.20	0.42
1:D:246:VAL:HG21	2:D:501:4S1:C26	2.50	0.41
1:C:173:LEU:HD21	1:C:261:VAL:HG21	2.02	0.41
1:C:192:MET:CE	1:C:264:TYR:HE1	2.33	0.41
1:C:396:LEU:O	1:C:399:ILE:HB	2.20	0.41
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.03	0.41
1:D:185:ILE:HA	1:D:189:GLY:O	2.21	0.41
1:A:288:ARG:HB3	1:A:380:ILE:HG23	2.02	0.41
1:D:173:LEU:HA	1:D:176:VAL:HG22	2.02	0.41
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.04	0.40
1:D:371:TYR:OH	1:D:397:LEU:HD22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	276/301 (92%)	266 (96%)	7 (2%)	3 (1%)	11	18
1	B	262/301 (87%)	247 (94%)	11 (4%)	4 (2%)	8	12
1	C	275/301 (91%)	260 (94%)	10 (4%)	5 (2%)	6	9
1	D	278/301 (92%)	265 (95%)	9 (3%)	4 (1%)	9	13
All	All	1091/1204 (91%)	1038 (95%)	37 (3%)	16 (2%)	8	12

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU

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Mol	Chain	Res	Type
1	C	406	GLU
1	D	406	GLU
1	D	459	ALA
1	D	181	ASP
1	A	329	ASP
1	B	329	ASP
1	C	191	LYS
1	C	329	ASP
1	D	329	ASP
1	A	188	GLY
1	B	188	GLY
1	C	206	ASN
1	C	180	PHE
1	B	186	SER

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	244/259 (94%)	234 (96%)	10 (4%)	27	46
1	B	232/259 (90%)	225 (97%)	7 (3%)	36	58
1	C	244/259 (94%)	238 (98%)	6 (2%)	42	64
1	D	246/259 (95%)	240 (98%)	6 (2%)	43	65
All	All	966/1036 (93%)	937 (97%)	29 (3%)	36	58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	181	ASP
1	A	208	THR
1	A	213	LYS
1	A	222	THR
1	A	343	VAL
1	A	349	VAL

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Mol	Chain	Res	Type
1	A	399	ILE
1	A	406	GLU
1	A	455	GLN
1	B	165	PHE
1	B	166	HIS
1	B	213	LYS
1	B	329	ASP
1	B	343	VAL
1	B	399	ILE
1	B	455	GLN
1	C	233	GLU
1	C	329	ASP
1	C	343	VAL
1	C	392	GLU
1	C	399	ILE
1	C	455	GLN
1	D	182	GLU
1	D	228	GLN
1	D	343	VAL
1	D	392	GLU
1	D	449	LYS
1	D	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	242	HIS
1	A	244	ASN
1	A	394	GLN
1	A	451	GLN
1	B	190	ASN
1	B	242	HIS
1	B	297	ASN
1	B	394	GLN
1	B	452	GLN
1	C	242	HIS
1	C	394	GLN
1	C	451	GLN
1	D	166	HIS
1	D	178	ASN
1	D	190	ASN

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Mol	Chain	Res	Type
1	D	228	GLN
1	D	232	GLN
1	D	242	HIS
1	D	390	HIS
1	D	394	GLN
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	342	1	8,10,11	1.02	0	10,14,16	1.58	1 (10%)
1	SEP	D	346	1	8,9,10	1.05	0	7,12,14	0.82	0
1	TPO	A	345	1	8,10,11	1.28	1 (12%)	10,14,16	1.37	2 (20%)
1	TPO	A	342	1	8,10,11	1.13	1 (12%)	10,14,16	1.53	1 (10%)
1	TPO	C	345	1	8,10,11	1.42	2 (25%)	10,14,16	1.27	1 (10%)
1	TPO	D	342	1	8,10,11	1.23	1 (12%)	10,14,16	1.50	1 (10%)
1	TPO	C	342	1	8,10,11	1.22	1 (12%)	10,14,16	1.49	1 (10%)
1	TPO	B	345	1	8,10,11	1.12	1 (12%)	10,14,16	1.41	2 (20%)
1	SEP	B	346	1	8,9,10	0.89	0	7,12,14	0.88	0
1	SEP	C	346	1	8,9,10	0.92	0	7,12,14	1.25	1 (14%)
1	TPO	D	345	1	8,10,11	1.04	1 (12%)	10,14,16	1.43	2 (20%)
1	SEP	A	346	1	8,9,10	0.97	0	7,12,14	0.87	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	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	TPO	A	342	1	-	2/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	TPO	D	342	1	-	2/9/11/13	-
1	TPO	C	342	1	-	2/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	D	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	TPO	P-OG1	-2.71	1.54	1.59
1	A	345	TPO	P-OG1	-2.71	1.54	1.59
1	C	342	TPO	P-OG1	-2.50	1.55	1.59
1	C	345	TPO	CB-CA	2.43	1.59	1.53
1	A	342	TPO	P-OG1	-2.24	1.55	1.59
1	C	345	TPO	P-OG1	-2.22	1.55	1.59
1	B	345	TPO	P-OG1	-2.18	1.55	1.59
1	D	345	TPO	P-OG1	-2.04	1.56	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	P-OG1-CB	-4.11	112.16	123.33
1	A	342	TPO	P-OG1-CB	-4.04	112.35	123.33
1	C	342	TPO	P-OG1-CB	-3.84	112.89	123.33
1	D	342	TPO	P-OG1-CB	-3.82	112.93	123.33
1	C	346	SEP	OG-CB-CA	2.83	110.89	108.14
1	D	345	TPO	P-OG1-CB	-2.65	116.13	123.33
1	B	345	TPO	P-OG1-CB	-2.53	116.45	123.33
1	A	345	TPO	P-OG1-CB	-2.46	116.65	123.33
1	D	345	TPO	O3P-P-OG1	2.19	114.37	105.85
1	C	345	TPO	P-OG1-CB	-2.14	117.52	123.33
1	A	345	TPO	O3P-P-OG1	2.06	113.87	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	TPO	O3P-P-OG1	2.05	113.83	105.85

There are no chirality outliers.

All (17) 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	C	345	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
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	342	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	D	342	TPO	O-C-CA-CB
1	D	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 oligosaccharides 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	4S1	B	501	-	32,32,32	1.83	12 (37%)	43,45,45	1.30	7 (16%)
2	4S1	D	501	-	32,32,32	1.65	6 (18%)	43,45,45	1.58	10 (23%)
2	4S1	A	501	-	32,32,32	1.77	11 (34%)	43,45,45	1.14	3 (6%)
2	4S1	C	501	-	32,32,32	1.70	10 (31%)	43,45,45	1.39	5 (11%)

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	4S1	B	501	-	-	0/14/30/30	0/4/4/4
2	4S1	D	501	-	-	0/14/30/30	0/4/4/4
2	4S1	A	501	-	-	0/14/30/30	0/4/4/4
2	4S1	C	501	-	-	1/14/30/30	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4S1	C03-N08	3.72	1.40	1.34
2	D	501	4S1	C06-C01	3.68	1.47	1.42
2	B	501	4S1	C06-C01	3.64	1.47	1.42
2	C	501	4S1	C03-N08	3.63	1.40	1.34
2	D	501	4S1	C03-N08	3.39	1.40	1.34
2	B	501	4S1	C11-C10	3.38	1.57	1.53
2	D	501	4S1	C05-C06	3.36	1.46	1.40
2	D	501	4S1	C03-N04	3.25	1.39	1.34
2	C	501	4S1	C10-N07	3.20	1.50	1.45
2	A	501	4S1	C29-C24	3.10	1.44	1.40
2	A	501	4S1	C28-C29	2.86	1.43	1.38
2	C	501	4S1	C29-C24	2.78	1.44	1.40
2	B	501	4S1	C28-C27	2.75	1.44	1.38
2	B	501	4S1	C03-N08	2.74	1.38	1.34
2	C	501	4S1	C06-C01	2.70	1.46	1.42
2	B	501	4S1	C05-N04	2.68	1.39	1.34
2	D	501	4S1	C29-C24	2.67	1.44	1.40
2	A	501	4S1	C05-C06	2.66	1.45	1.40
2	A	501	4S1	C27-C26	2.59	1.43	1.38
2	B	501	4S1	C05-C06	2.58	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	4S1	C17-C13	2.56	1.57	1.52
2	A	501	4S1	C11-C10	2.52	1.56	1.53
2	B	501	4S1	C24-C23	2.49	1.44	1.40
2	A	501	4S1	C28-C27	2.45	1.43	1.38
2	A	501	4S1	C01-N07	2.44	1.38	1.35
2	C	501	4S1	C11-C10	2.43	1.56	1.53
2	B	501	4S1	C28-C29	2.39	1.43	1.38
2	C	501	4S1	C03-N04	2.35	1.37	1.34
2	B	501	4S1	C29-C24	2.29	1.43	1.40
2	B	501	4S1	C27-C26	2.26	1.42	1.38
2	C	501	4S1	C28-C27	2.25	1.43	1.38
2	A	501	4S1	C01-N02	2.24	1.38	1.34
2	D	501	4S1	C28-C27	2.22	1.43	1.38
2	B	501	4S1	C01-N02	2.19	1.38	1.34
2	A	501	4S1	C06-C01	2.09	1.45	1.42
2	B	501	4S1	C09-S22	2.07	1.80	1.76
2	C	501	4S1	C05-C06	2.07	1.43	1.40
2	C	501	4S1	C28-C29	2.05	1.42	1.38
2	C	501	4S1	C27-C26	2.00	1.42	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4S1	C19-N08-C03	4.23	131.15	123.82
2	B	501	4S1	C19-N08-C03	3.75	130.31	123.82
2	C	501	4S1	C19-N08-C03	3.64	130.13	123.82
2	C	501	4S1	N07-C01-N02	-3.52	111.78	118.55
2	D	501	4S1	C13-C12-C11	3.33	107.79	103.87
2	C	501	4S1	N08-C03-N04	3.32	121.68	117.21
2	D	501	4S1	C06-C05-N04	-3.06	120.01	124.32
2	B	501	4S1	C13-C12-C11	2.76	107.12	103.87
2	A	501	4S1	C13-C12-C11	2.74	107.09	103.87
2	B	501	4S1	C06-C05-N04	-2.66	120.58	124.32
2	A	501	4S1	C13-C14-C10	2.57	107.14	103.55
2	A	501	4S1	C01-N07-C10	2.56	128.70	123.05
2	D	501	4S1	O18-C17-C13	-2.55	105.45	111.26
2	D	501	4S1	N08-C03-N04	2.45	120.50	117.21
2	B	501	4S1	O18-C17-C13	-2.38	105.83	111.26
2	B	501	4S1	C05-N04-C03	2.34	119.02	115.81
2	D	501	4S1	C05-N04-C03	2.32	118.99	115.81
2	D	501	4S1	C01-N07-C10	2.31	128.13	123.05
2	D	501	4S1	N07-C01-N02	-2.28	114.16	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	4S1	C01-N07-C10	2.21	127.93	123.05
2	C	501	4S1	O16-C12-C11	2.18	118.82	111.82
2	C	501	4S1	N04-C03-N02	-2.11	124.38	126.42
2	D	501	4S1	C13-C14-C10	2.04	106.39	103.55
2	D	501	4S1	C28-C27-C26	-2.01	117.76	120.24
2	B	501	4S1	N07-C01-N02	-2.01	114.68	118.55

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	4S1	N08-C19-C20-C21

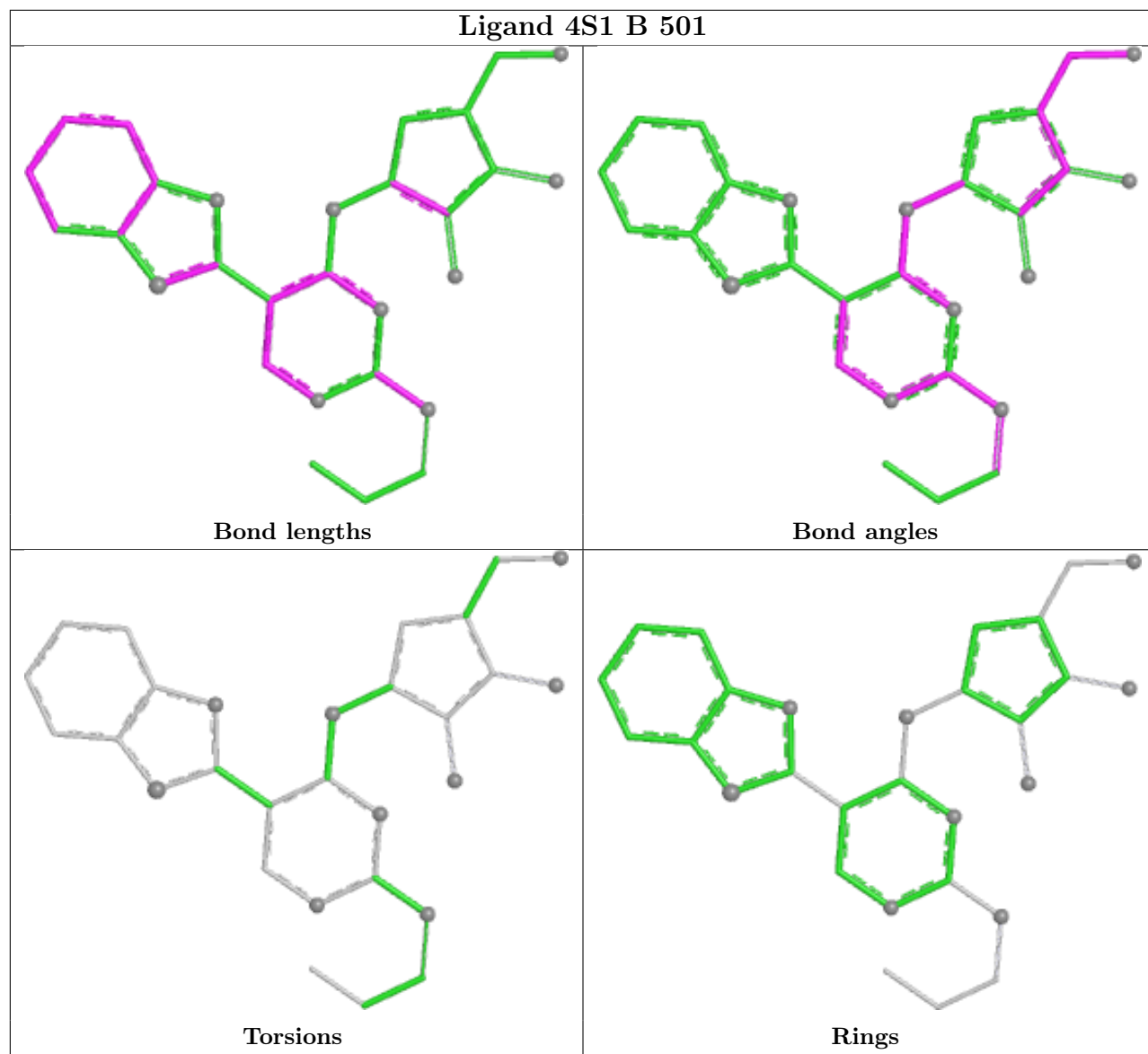
There are no ring outliers.

4 monomers are involved in 10 short contacts:

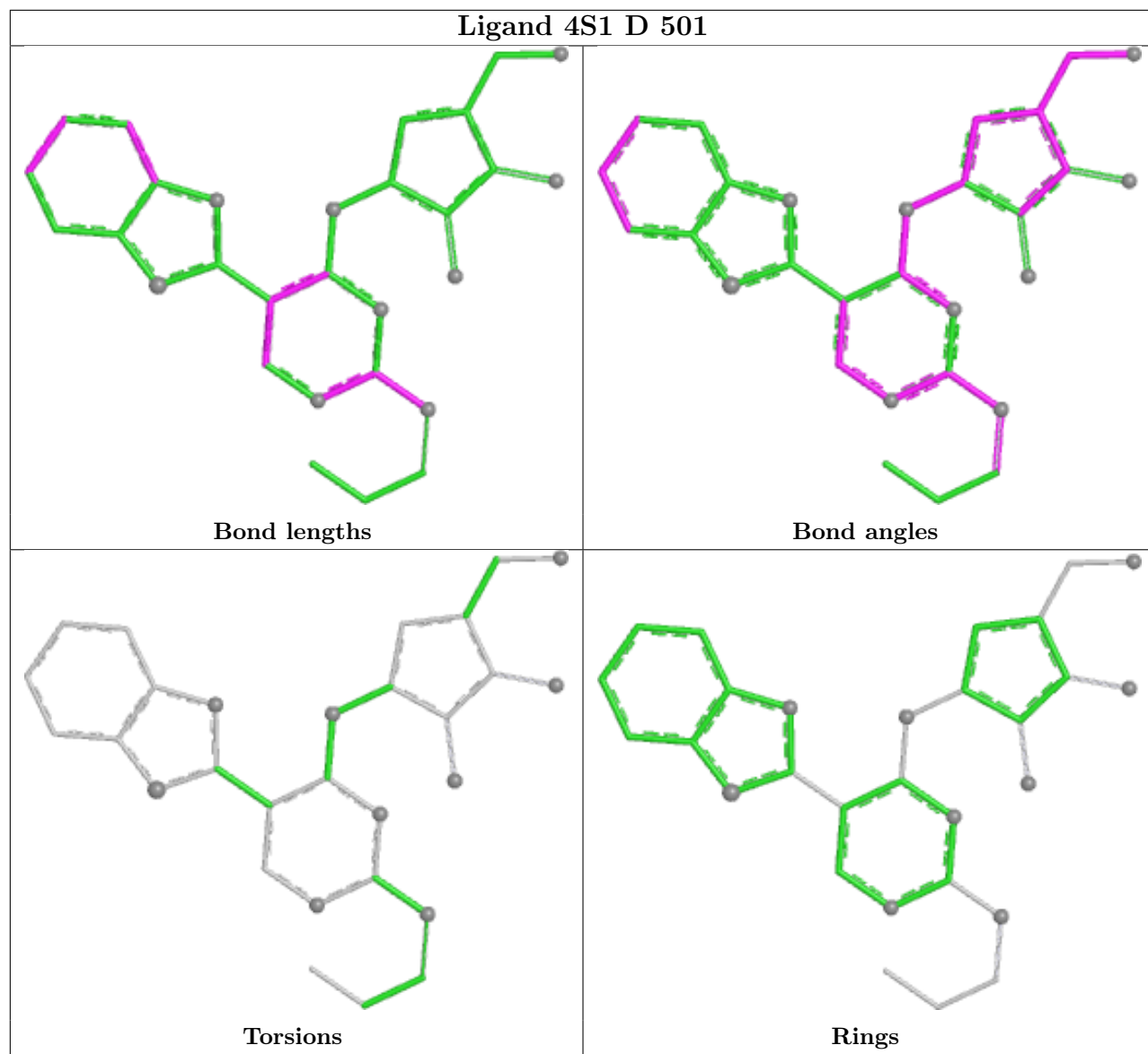
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	4S1	2	0
2	D	501	4S1	3	0
2	A	501	4S1	2	0
2	C	501	4S1	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

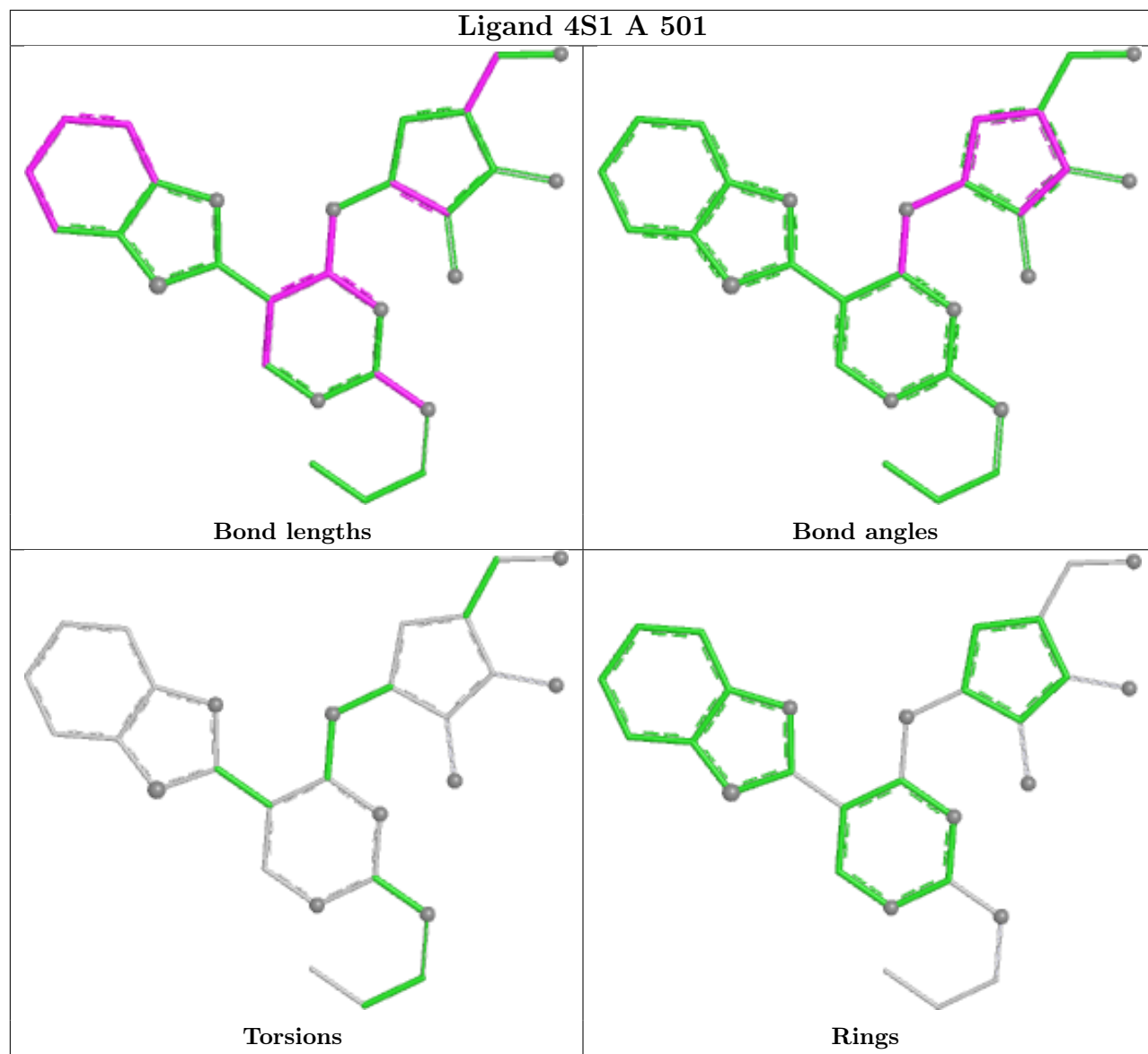
Ligand 4S1 B 501

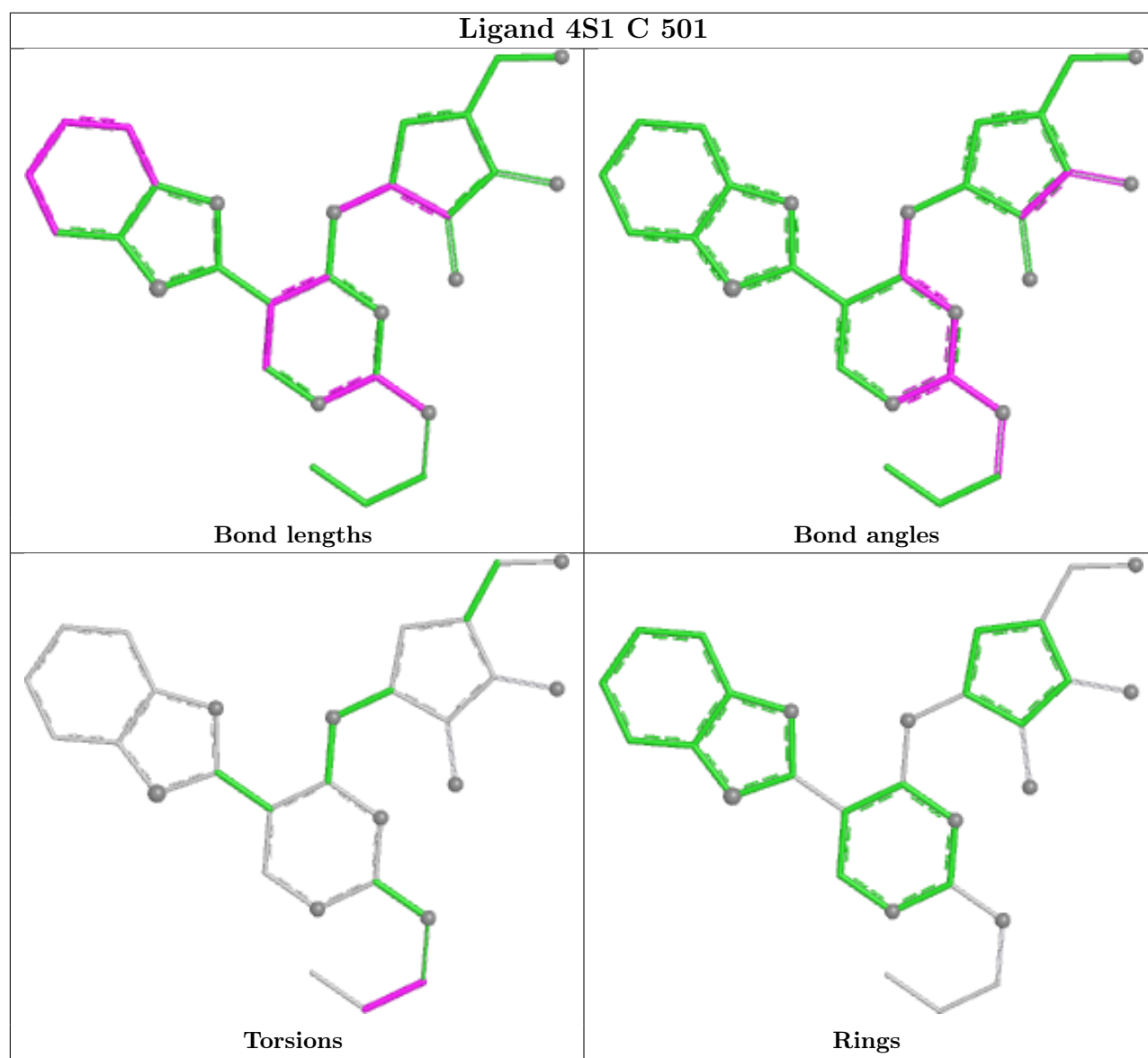


Ligand 4S1 D 501



Ligand 4S1 A 501





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	280/301 (93%)	-0.68	0 100 100	23, 73, 148, 178	1 (0%)
1	B	269/301 (89%)	-0.71	0 100 100	22, 69, 145, 162	1 (0%)
1	C	282/301 (93%)	-0.79	0 100 100	33, 64, 126, 155	0
1	D	285/301 (94%)	-0.82	0 100 100	35, 63, 111, 153	0
All	All	1116/1204 (92%)	-0.75	0 100 100	22, 66, 141, 178	2 (0%)

There are no RSRZ outliers to report.

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

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	0.95	0.06	108,112,117,118	0
1	SEP	D	346	10/11	0.95	0.09	90,95,103,103	0
1	SEP	A	346	10/11	0.97	0.05	107,110,117,117	0
1	TPO	B	342	11/12	0.98	0.07	111,113,116,117	0
1	TPO	B	345	11/12	0.98	0.04	104,104,108,109	0
1	TPO	A	345	11/12	0.98	0.04	102,103,108,109	0
1	TPO	C	342	11/12	0.98	0.07	99,100,106,106	0
1	SEP	C	346	10/11	0.98	0.06	88,94,102,102	0
1	TPO	D	342	11/12	0.98	0.06	98,100,107,107	0
1	TPO	A	342	11/12	0.98	0.06	114,116,120,120	0
1	TPO	D	345	11/12	0.99	0.06	86,89,91,91	0
1	TPO	C	345	11/12	0.99	0.04	86,87,89,90	0

6.3 Carbohydrates [i](#)

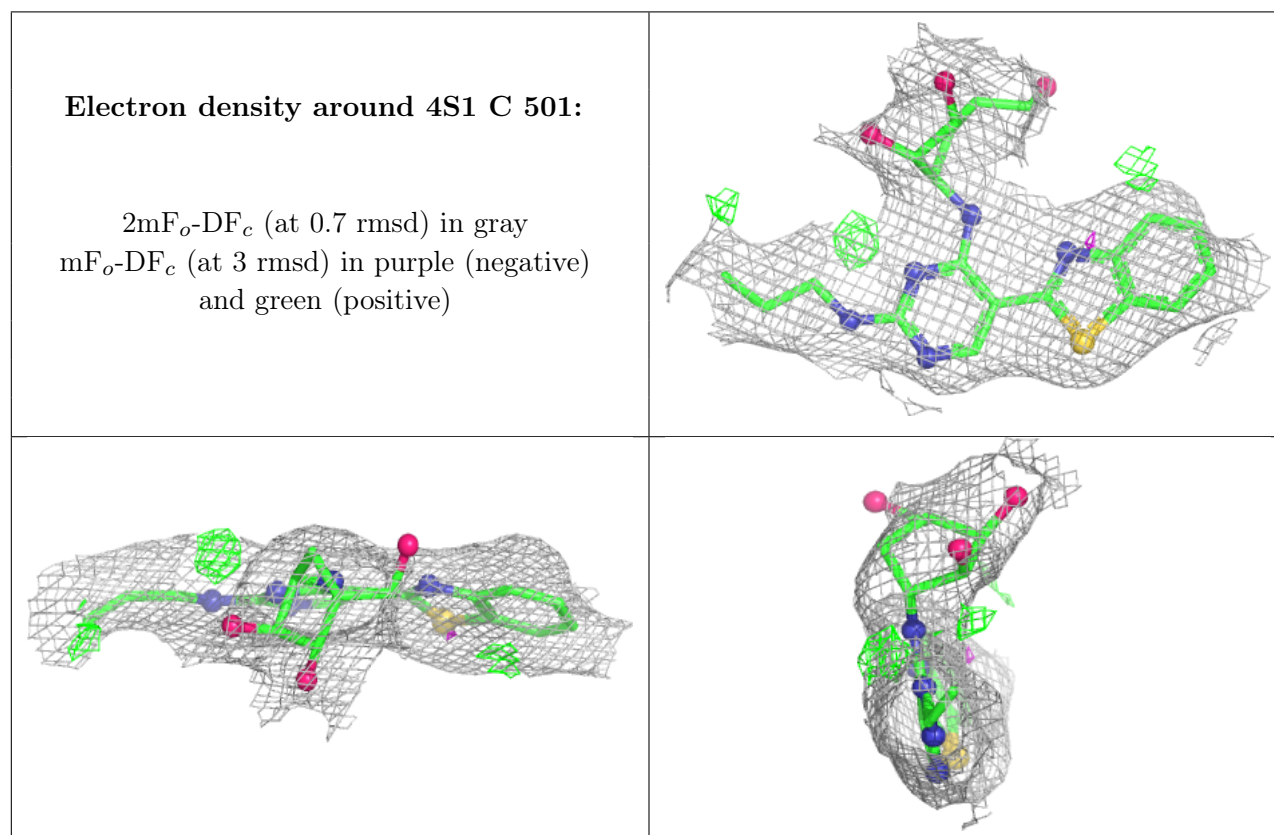
There are no oligosaccharides in this entry.

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.

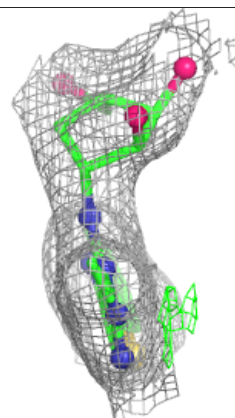
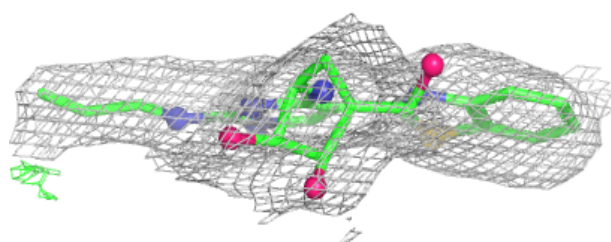
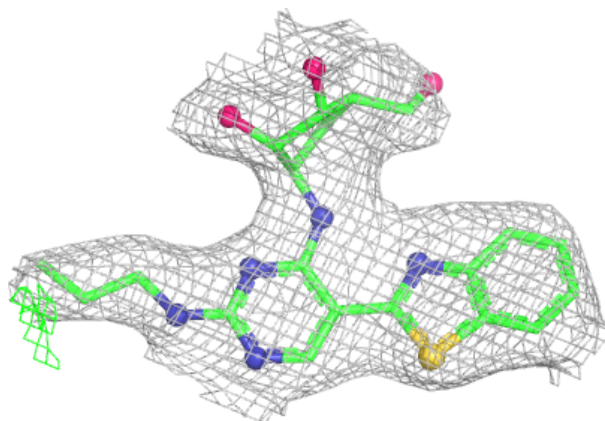
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	4S1	C	501	29/29	0.97	0.06	63,71,79,80	0
2	4S1	B	501	29/29	0.98	0.05	70,73,81,88	0
2	4S1	A	501	29/29	0.98	0.05	75,77,82,84	0
2	4S1	D	501	29/29	0.99	0.04	54,60,72,75	0

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.

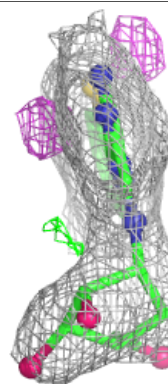
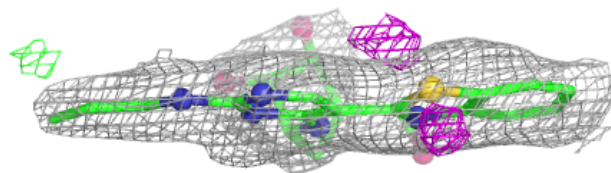
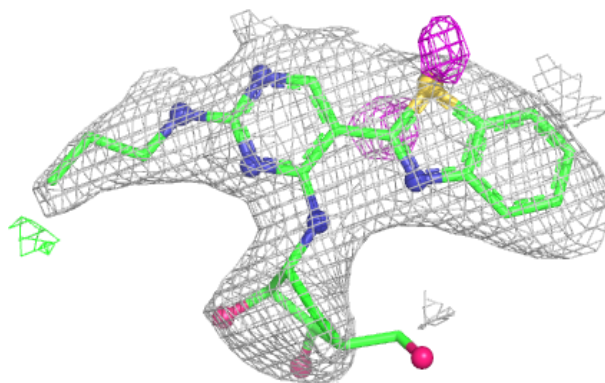


Electron density around 4S1 B 501:

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

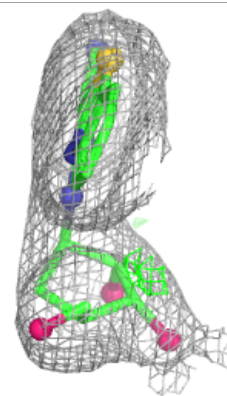
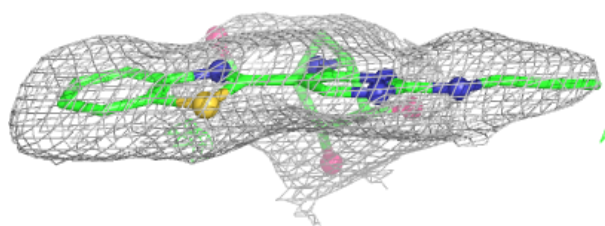
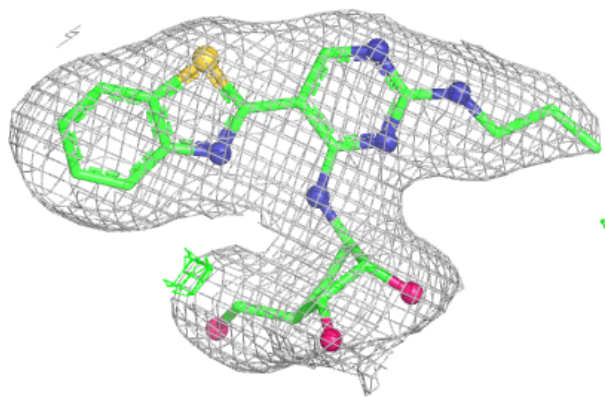
**Electron density around 4S1 A 501:**

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



Electron density around 4S1 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.