



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 AM UTC

PDB ID : 8W3W / pdb_00008w3w
Title : Crystal structure of IRAK4 in complex with compound 4
Authors : Han, S.; Knafels, J.D.
Deposited on : 2024-02-22
Resolution : 1.98 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

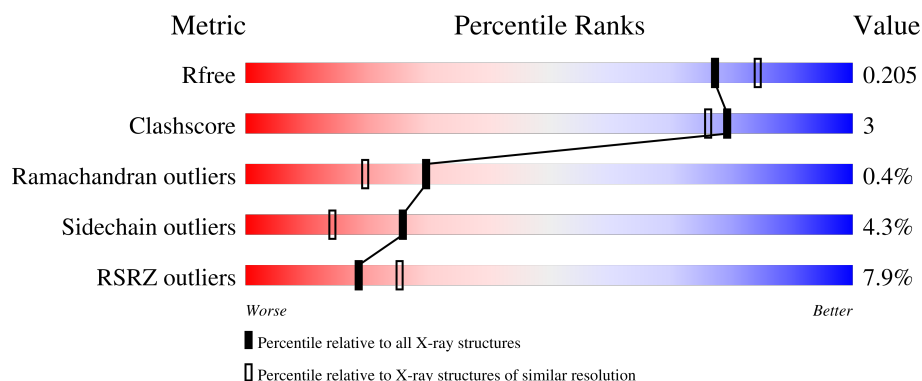
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	323	9% 84% 8% 7%
1	B	323	9% 80% 9% 11%
1	C	323	7% 81% 7% 11%
1	D	323	3% 78% 10% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9947 atoms, of which 68 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	299	Total	C	N	O	P	S	0	0	0
			2359	1476	395	470	3	15			
1	B	289	Total	C	N	O	P	S	0	2	0
			2288	1431	383	456	3	15			
1	C	288	Total	C	N	O	P	S	0	0	0
			2276	1425	383	451	3	14			
1	D	287	Total	C	N	O	P	S	0	0	0
			2268	1419	381	451	3	14			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3

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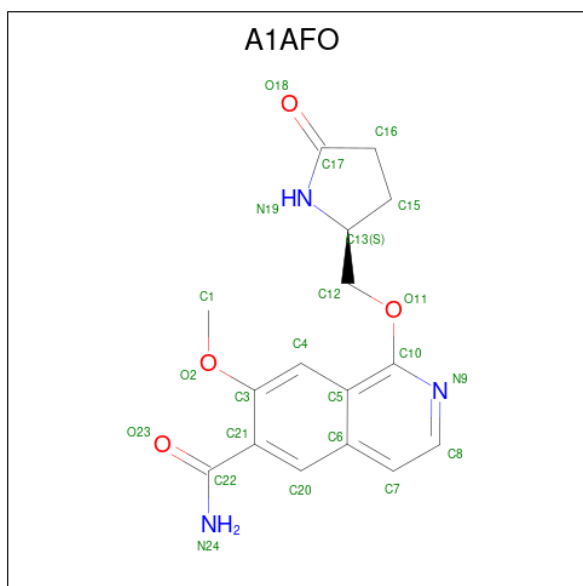
Chain	Residue	Modelled	Actual	Comment	Reference
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	138	MET	-	initiating methionine	UNP Q9NWZ3
C	139	HIS	-	expression tag	UNP Q9NWZ3
C	140	HIS	-	expression tag	UNP Q9NWZ3
C	141	HIS	-	expression tag	UNP Q9NWZ3
C	142	HIS	-	expression tag	UNP Q9NWZ3
C	143	HIS	-	expression tag	UNP Q9NWZ3
C	144	HIS	-	expression tag	UNP Q9NWZ3
C	145	GLY	-	expression tag	UNP Q9NWZ3
C	146	GLY	-	expression tag	UNP Q9NWZ3
C	147	GLU	-	expression tag	UNP Q9NWZ3
C	148	ASN	-	expression tag	UNP Q9NWZ3
C	149	LEU	-	expression tag	UNP Q9NWZ3
C	150	TYR	-	expression tag	UNP Q9NWZ3
C	151	PHE	-	expression tag	UNP Q9NWZ3
C	152	GLN	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	138	MET	-	initiating methionine	UNP Q9NWZ3
D	139	HIS	-	expression tag	UNP Q9NWZ3
D	140	HIS	-	expression tag	UNP Q9NWZ3
D	141	HIS	-	expression tag	UNP Q9NWZ3
D	142	HIS	-	expression tag	UNP Q9NWZ3
D	143	HIS	-	expression tag	UNP Q9NWZ3
D	144	HIS	-	expression tag	UNP Q9NWZ3
D	145	GLY	-	expression tag	UNP Q9NWZ3
D	146	GLY	-	expression tag	UNP Q9NWZ3
D	147	GLU	-	expression tag	UNP Q9NWZ3
D	148	ASN	-	expression tag	UNP Q9NWZ3
D	149	LEU	-	expression tag	UNP Q9NWZ3
D	150	TYR	-	expression tag	UNP Q9NWZ3
D	151	PHE	-	expression tag	UNP Q9NWZ3
D	152	GLN	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 7-methoxy-1-{[(2S)-5-oxopyrrolidin-2-yl]methoxy}isoquinoline-6-carboxamide (CCD ID: A1AFO) (formula: C₁₆H₁₇N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	17	0
			40	16	17	3	4		
2	B	1	Total	C	H	N	O	17	0
			40	16	17	3	4		
2	C	1	Total	C	H	N	O	17	0
			40	16	17	3	4		
2	D	1	Total	C	H	N	O	17	0
			40	16	17	3	4		

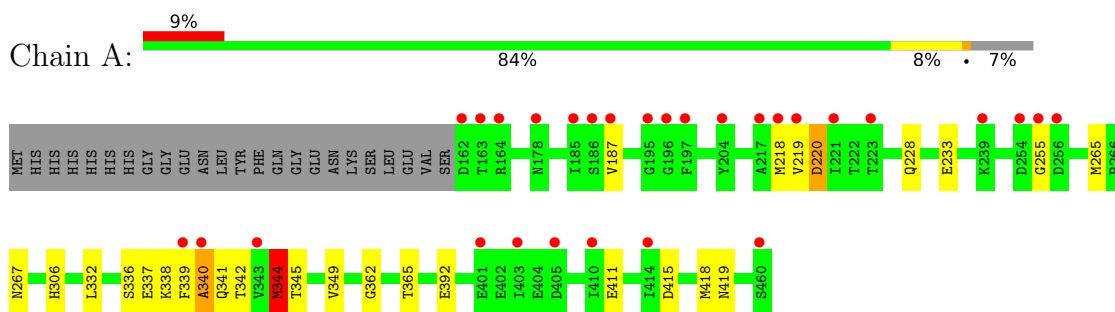
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	137	Total	O	0	0
			137	137		
3	C	146	Total	O	0	0
			146	146		
3	D	172	Total	O	0	0
			172	172		

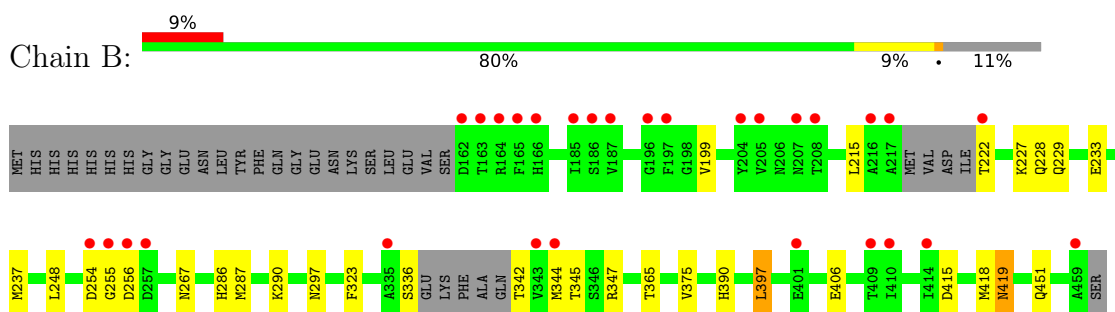
3 Residue-property plots [i](#)

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.

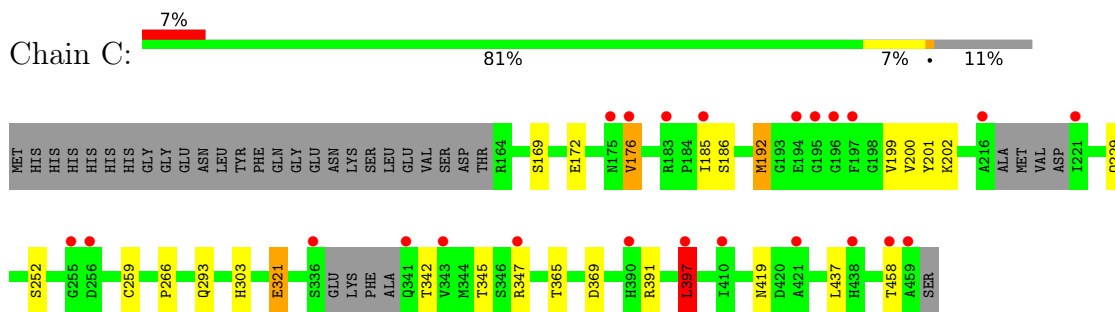
- Molecule 1: Interleukin-1 receptor-associated kinase 4



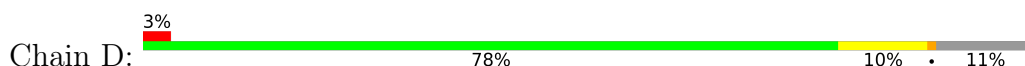
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	142.72Å 139.26Å 88.04Å 90.00° 124.84° 90.00°	Depositor
Resolution (Å)	47.09 – 1.98 47.09 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.09-1.98) 95.3 (47.09-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.98Å)	Xtriage
Refinement program	BUSTER 2.11.8 (22-FEB-2023)	Depositor
R, R_{free}	0.192 , 0.213 0.184 , 0.205	Depositor DCC
R_{free} test set	4785 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9947	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.79% 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: A1AFO, 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	0.72	3/2365 (0.1%)	1.01	3/3187 (0.1%)
1	B	0.70	0/2300	1.00	3/3098 (0.1%)
1	C	0.74	2/2279 (0.1%)	0.95	0/3068
1	D	0.79	2/2272 (0.1%)	0.98	0/3060
All	All	0.74	7/9216 (0.1%)	0.98	6/12413 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	192	MET	SD-CE	-16.69	1.37	1.79
1	C	192	MET	SD-CE	-13.70	1.45	1.79
1	D	327	ILE	CG1-CD1	-7.56	1.22	1.51
1	A	344	MET	SD-CE	-6.63	1.62	1.79
1	A	340	ALA	CA-C	6.17	1.61	1.52
1	A	265	MET	SD-CE	-5.68	1.65	1.79
1	C	397	LEU	CB-CG	-5.17	1.43	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	GLY	CA-C-N	6.61	131.70	121.19
1	A	255	GLY	C-N-CA	6.61	131.70	121.19
1	A	267	ASN	CA-CB-CG	-5.94	106.66	112.60
1	B	255	GLY	CA-C-N	5.06	131.20	121.54
1	B	255	GLY	C-N-CA	5.06	131.20	121.54
1	B	267	ASN	CA-CB-CG	-5.00	107.59	112.60

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	2359	0	2315	7	0
1	B	2288	0	2247	15	0
1	C	2276	0	2237	18	0
1	D	2268	0	2226	13	0
2	A	23	17	0	0	0
2	B	23	17	0	0	0
2	C	23	17	0	0	0
2	D	23	17	0	0	0
3	A	141	0	0	0	0
3	B	137	0	0	0	0
3	C	146	0	0	0	0
3	D	172	0	0	0	0
All	All	9879	68	9025	50	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 (50) 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:C:185:ILE:HD12	1:C:192:MET:HG2	1.47	0.94
1:C:185:ILE:CD1	1:C:192:MET:HG2	2.00	0.92
1:C:397:LEU:HD21	1:C:437:LEU:HD22	1.49	0.90
1:D:229:GLN:HE21	1:D:347:ARG:HH22	1.29	0.81
1:B:237:MET:HG2	1:B:248:LEU:HB2	1.69	0.75
1:C:192:MET:HE3	1:C:200:VAL:HG12	1.67	0.75
1:A:306:HIS:HD2	1:A:339:PHE:HB2	1.54	0.72
1:B:237:MET:HG2	1:B:248:LEU:CB	2.20	0.71
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.38	0.71
1:B:297:ASN:ND2	1:B:451:GLN:HE21	1.89	0.69
1:B:229:GLN:NE2	1:B:347:ARG:HH22	1.90	0.69
1:C:229:GLN:NE2	1:C:347:ARG:HH22	1.92	0.66
1:C:321:GLU:H	1:C:321:GLU:CD	2.04	0.64
1:B:375:VAL:HG22	1:B:397:LEU:HD13	1.78	0.64
1:C:266:PRO:HG2	1:C:321:GLU:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:HIS:HD2	1:D:311:ASP:H	1.47	0.62
1:D:192:MET:HE3	1:D:200:VAL:HG12	1.84	0.59
1:D:303:HIS:HE1	1:D:369:ASP:OD2	1.86	0.59
1:C:303:HIS:HE1	1:C:369:ASP:OD2	1.86	0.58
1:C:185:ILE:HD11	1:C:192:MET:HG2	1.82	0.58
1:C:172:GLU:O	1:C:176:VAL:HG13	2.03	0.58
1:A:187:VAL:HG22	1:A:187:VAL:O	2.04	0.57
1:B:286:HIS:HE1	1:D:247:GLU:OE2	1.88	0.57
1:C:185:ILE:HD11	1:C:202:LYS:HB2	1.85	0.57
1:B:237:MET:HG2	1:B:248:LEU:HB3	1.92	0.51
1:D:229:GLN:NE2	1:D:347:ARG:HH22	2.02	0.50
1:B:287[B]:MET:HE2	1:B:323:PHE:HB3	1.95	0.48
1:C:293:GLN:HE22	1:C:458:THR:CG2	2.27	0.48
1:D:183:ARG:HB2	1:D:189:GLY:HA3	1.95	0.48
1:B:390:HIS:O	1:C:391:ARG:HA	2.15	0.47
1:A:306:HIS:CD2	1:A:339:PHE:HB2	2.42	0.47
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.97	0.46
1:B:287[B]:MET:HE2	1:B:323:PHE:CB	2.45	0.46
1:D:306:HIS:HB3	1:D:336:SER:O	2.15	0.46
1:D:332:LEU:HD22	1:D:349:VAL:HG21	1.97	0.46
1:B:287[B]:MET:HE1	1:B:290:LYS:HD3	1.99	0.45
1:C:229:GLN:HE22	1:C:347:ARG:HH22	1.62	0.45
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.98	0.45
1:D:181:ASP:HB3	1:D:190:ASN:HD22	1.82	0.44
1:A:332:LEU:HD22	1:A:349:VAL:HG21	2.00	0.43
1:A:344:MET:HG3	1:A:362:GLY:O	2.18	0.43
1:A:219:VAL:HG12	1:A:220:ASP:H	1.84	0.43
1:C:192:MET:HE2	1:C:201:TYR:C	2.43	0.43
1:C:293:GLN:HE22	1:C:458:THR:HG21	1.83	0.43
1:D:181:ASP:OD1	1:D:183:ARG:HD3	2.19	0.42
1:B:229:GLN:HE22	1:B:347:ARG:HH22	1.64	0.42
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.02	0.42
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.02	0.41
1:D:288:ARG:HB3	1:D:380:ILE:HG23	2.03	0.41
1:B:419:ASN:HB2	1:C:186:SER:HB2	2.04	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	294/323 (91%)	284 (97%)	8 (3%)	2 (1%)	18	9
1	B	283/323 (88%)	276 (98%)	7 (2%)	0	100	100
1	C	279/323 (86%)	275 (99%)	4 (1%)	0	100	100
1	D	279/323 (86%)	271 (97%)	6 (2%)	2 (1%)	18	9
All	All	1135/1292 (88%)	1106 (97%)	25 (2%)	4 (0%)	30	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	255	GLY
1	A	341	GLN
1	A	340	ALA
1	D	406	GLU

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	257/278 (92%)	245 (95%)	12 (5%)	23	12
1	B	250/278 (90%)	236 (94%)	14 (6%)	19	8
1	C	248/278 (89%)	241 (97%)	7 (3%)	38	29
1	D	247/278 (89%)	237 (96%)	10 (4%)	28	17
All	All	1002/1112 (90%)	959 (96%)	43 (4%)	26	14

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	MET
1	A	220	ASP
1	A	228	GLN
1	A	233	GLU
1	A	336	SER
1	A	337	GLU
1	A	338	LYS
1	A	344	MET
1	A	365	THR
1	A	392	GLU
1	A	411	GLU
1	A	419	ASN
1	B	199	VAL
1	B	215	LEU
1	B	222	THR
1	B	227	LYS
1	B	228	GLN
1	B	233	GLU
1	B	254	ASP
1	B	256	ASP
1	B	336	SER
1	B	344	MET
1	B	365	THR
1	B	397	LEU
1	B	406	GLU
1	B	419	ASN
1	C	169	SER
1	C	176	VAL
1	C	199	VAL
1	C	321	GLU
1	C	365	THR
1	C	397	LEU
1	C	419	ASN
1	D	169	SER
1	D	183	ARG
1	D	222	THR
1	D	227	LYS
1	D	228	GLN
1	D	256	ASP
1	D	365	THR
1	D	407	GLU
1	D	408	LYS

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Mol	Chain	Res	Type
1	D	419	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	229	GLN
1	A	293	GLN
1	A	305	ASN
1	A	306	HIS
1	A	390	HIS
1	A	394	GLN
1	A	438	HIS
1	B	229	GLN
1	B	286	HIS
1	B	293	GLN
1	B	297	ASN
1	B	305	ASN
1	B	390	HIS
1	B	394	GLN
1	B	419	ASN
1	C	175	ASN
1	C	179	ASN
1	C	229	GLN
1	C	303	HIS
1	C	305	ASN
1	C	390	HIS
1	C	419	ASN
1	D	190	ASN
1	D	229	GLN
1	D	303	HIS
1	D	305	ASN
1	D	309	HIS
1	D	394	GLN
1	D	419	ASN
1	D	438	HIS

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	C	345	1	8,10,11	1.33	1 (12%)	10,14,16	1.67	3 (30%)
1	TPO	D	342	1	8,10,11	1.14	1 (12%)	10,14,16	1.76	1 (10%)
1	TPO	D	345	1	8,10,11	1.05	0	10,14,16	1.55	2 (20%)
1	SEP	A	346	1	8,9,10	0.85	0	7,12,14	0.85	0
1	TPO	B	345	1	8,10,11	1.65	2 (25%)	10,14,16	1.61	2 (20%)
1	TPO	B	342	1	8,10,11	1.26	1 (12%)	10,14,16	1.79	1 (10%)
1	SEP	B	346	1	8,9,10	0.88	0	7,12,14	0.88	0
1	SEP	C	346	1	8,9,10	0.86	0	7,12,14	0.87	0
1	TPO	C	342	1	8,10,11	1.08	1 (12%)	10,14,16	1.79	2 (20%)
1	TPO	A	345	1	8,10,11	1.43	1 (12%)	10,14,16	1.73	3 (30%)
1	TPO	A	342	1	8,10,11	0.97	1 (12%)	10,14,16	1.92	1 (10%)
1	SEP	D	346	1	8,9,10	0.80	0	7,12,14	0.99	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	C	345	1	-	4/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	D	345	1	-	5/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	C	342	1	-	2/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	342	1	-	2/9/11/13	-
1	SEP	D	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	B	345	TPO	P-OG1	-3.51	1.53	1.59
1	B	342	TPO	P-OG1	-3.13	1.54	1.59
1	A	345	TPO	P-OG1	-2.94	1.54	1.59
1	D	342	TPO	P-OG1	-2.63	1.54	1.59
1	C	342	TPO	P-OG1	-2.52	1.55	1.59
1	C	345	TPO	P-OG1	-2.11	1.55	1.59
1	B	345	TPO	CB-CA	2.10	1.58	1.53
1	A	342	TPO	P-OG1	-2.06	1.55	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	P-OG1-CB	-4.69	110.59	123.33
1	A	342	TPO	P-OG1-CB	-4.52	111.03	123.33
1	D	342	TPO	P-OG1-CB	-4.47	111.17	123.33
1	C	342	TPO	P-OG1-CB	-4.38	111.41	123.33
1	A	345	TPO	O2P-P-OG1	3.83	120.79	105.85
1	B	345	TPO	O3P-P-OG1	3.46	119.35	105.85
1	D	345	TPO	O3P-P-OG1	3.30	118.73	105.85
1	C	345	TPO	OG1-P-O1P	2.86	119.53	109.33
1	C	345	TPO	O3P-P-O2P	2.52	117.25	107.80
1	A	345	TPO	P-OG1-CB	-2.37	116.88	123.33
1	C	345	TPO	O3P-P-O1P	-2.31	101.85	110.83
1	B	345	TPO	P-OG1-CB	-2.21	117.31	123.33
1	A	345	TPO	O2P-P-O1P	-2.07	102.77	110.83
1	D	345	TPO	OG1-P-O1P	-2.06	101.99	109.33
1	C	342	TPO	O2P-P-OG1	2.01	113.69	105.85

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1

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

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	A1AFO	C	501	-	25,25,25	0.65	1 (4%)	31,35,35	1.45	1 (3%)
2	A1AFO	D	501	-	25,25,25	0.75	1 (4%)	31,35,35	1.37	1 (3%)
2	A1AFO	A	501	-	25,25,25	0.80	1 (4%)	31,35,35	1.41	1 (3%)
2	A1AFO	B	501	-	25,25,25	0.70	1 (4%)	31,35,35	1.45	1 (3%)

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	A1AFO	C	501	-	-	0/11/20/20	0/3/3/3
2	A1AFO	D	501	-	-	0/11/20/20	0/3/3/3
2	A1AFO	A	501	-	-	0/11/20/20	0/3/3/3
2	A1AFO	B	501	-	-	0/11/20/20	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1AFO	C10-N9	3.53	1.37	1.31
2	D	501	A1AFO	C10-N9	3.09	1.36	1.31
2	B	501	A1AFO	C10-N9	2.86	1.36	1.31
2	C	501	A1AFO	C10-N9	2.41	1.35	1.31

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	A1AFO	C12-O11-C10	7.17	125.28	117.64
2	B	501	A1AFO	C12-O11-C10	7.12	125.23	117.64
2	A	501	A1AFO	C12-O11-C10	6.89	124.99	117.64
2	D	501	A1AFO	C12-O11-C10	6.56	124.63	117.64

There are no chirality outliers.

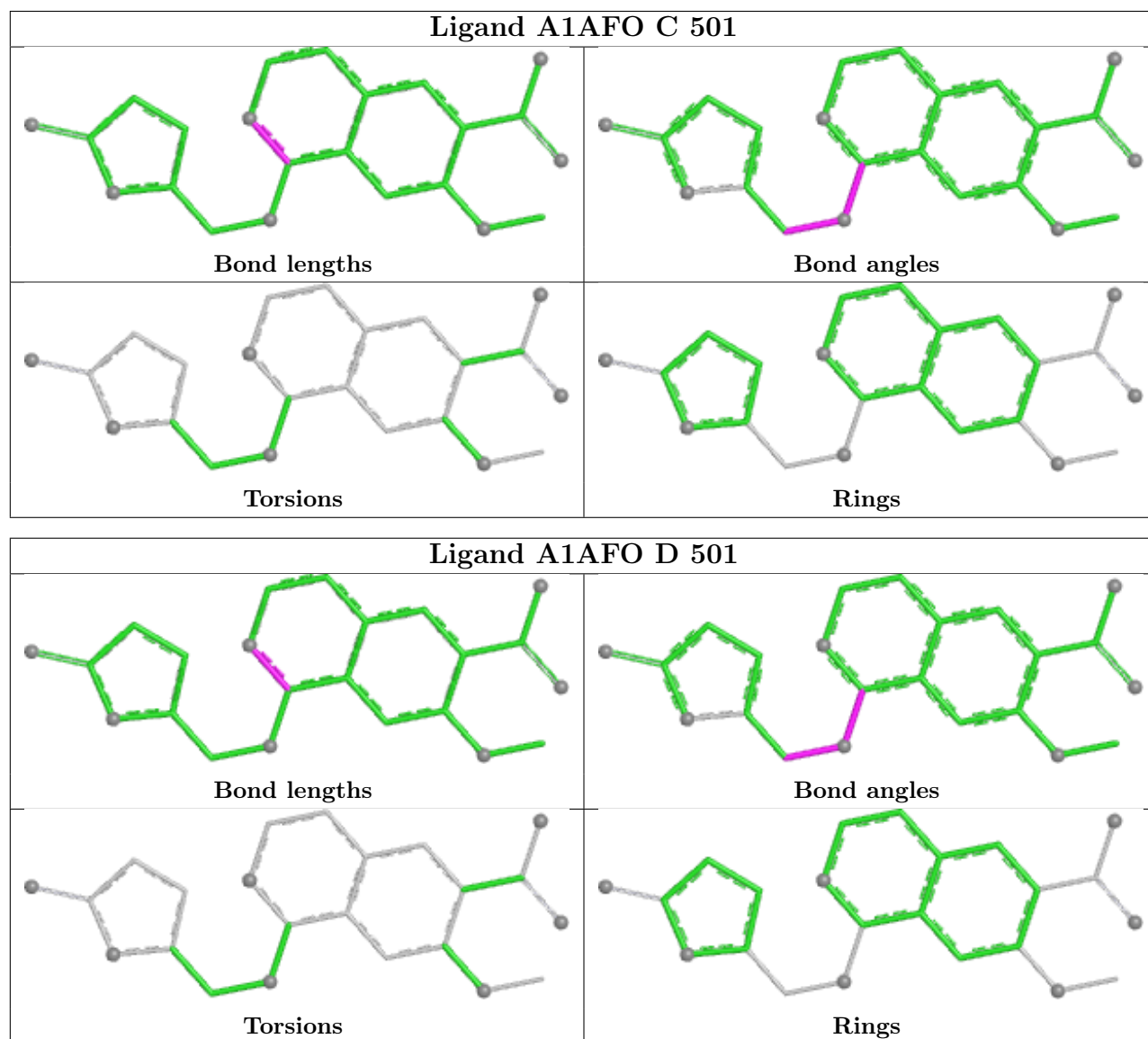
There are no torsion outliers.

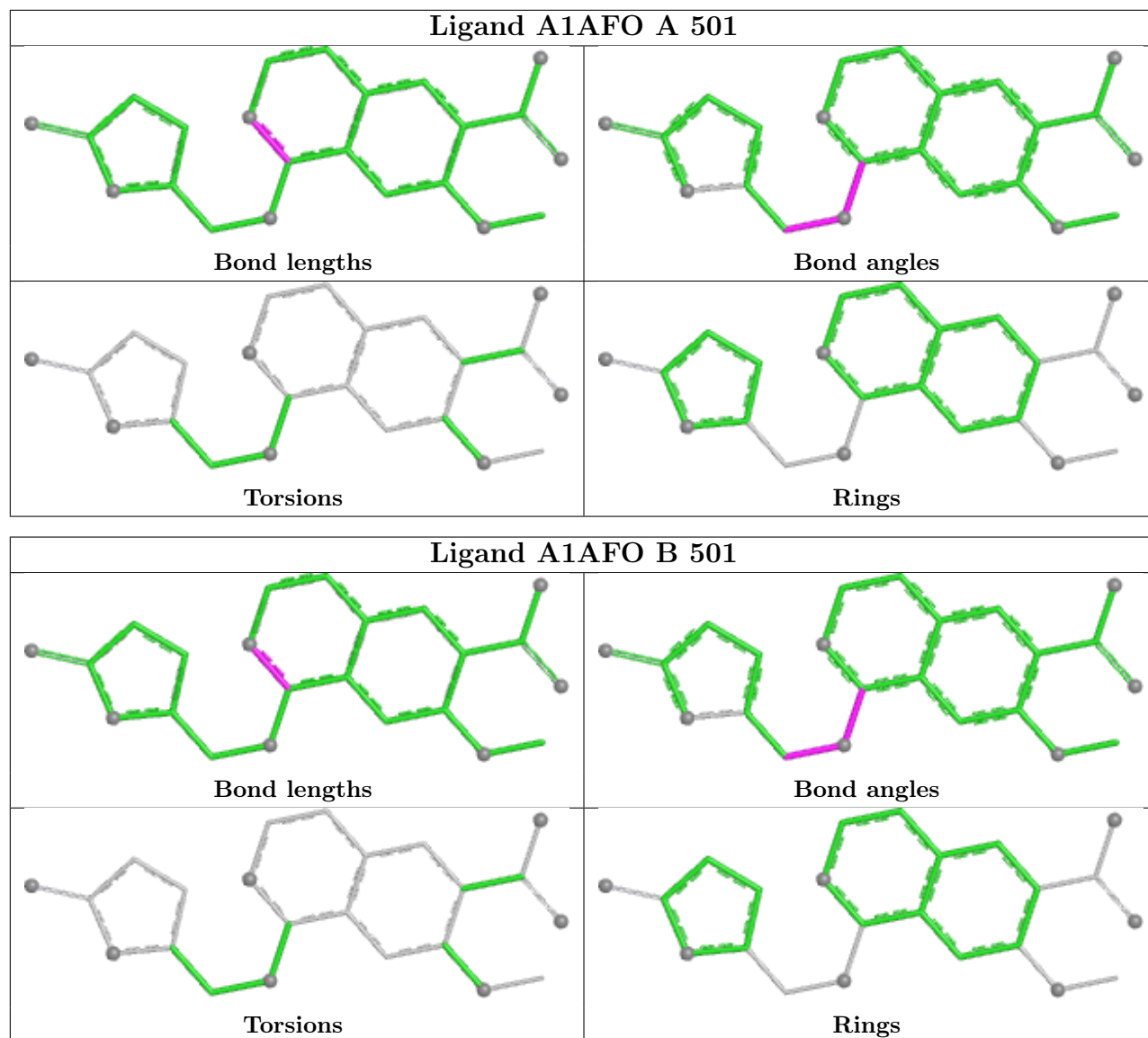
There are no ring outliers.

No monomer is involved in short contacts.

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	296/323 (91%)	0.54	29 (9%) 13 18	26, 44, 74, 87	0
1	B	286/323 (88%)	0.51	29 (10%) 12 17	21, 43, 71, 83	2 (0%)
1	C	285/323 (88%)	0.42	23 (8%) 18 25	27, 40, 64, 77	0
1	D	284/323 (87%)	0.19	10 (3%) 47 57	24, 36, 61, 75	0
All	All	1151/1292 (89%)	0.41	91 (7%) 18 25	21, 41, 70, 87	2 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	255	GLY	6.3
1	D	216	ALA	6.0
1	C	197	PHE	5.2
1	A	163	THR	4.9
1	C	195	GLY	4.9
1	D	222	THR	4.8
1	A	340	ALA	4.7
1	B	255	GLY	4.5
1	B	217	ALA	4.5
1	B	165	PHE	4.5
1	B	196	GLY	4.5
1	C	196	GLY	4.4
1	B	197	PHE	4.0
1	A	204	TYR	3.9
1	B	222	THR	3.8
1	C	221	ILE	3.8
1	A	339	PHE	3.8
1	C	458	THR	3.5
1	B	163	THR	3.4
1	C	421	ALA	3.4
1	C	255	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	410	ILE	3.3
1	B	162	ASP	3.3
1	A	219	VAL	3.3
1	C	397	LEU	3.2
1	A	196	GLY	3.2
1	D	459	ALA	3.1
1	C	256	ASP	3.1
1	C	336	SER	3.1
1	A	217	ALA	3.1
1	A	343	VAL	3.0
1	D	256	ASP	2.8
1	A	185	ILE	2.7
1	C	341	GLN	2.7
1	A	401	GLU	2.7
1	B	410	ILE	2.6
1	D	407	GLU	2.6
1	B	204	TYR	2.6
1	C	175	ASN	2.6
1	A	254	ASP	2.6
1	A	256	ASP	2.6
1	A	187	VAL	2.6
1	A	255	GLY	2.5
1	A	197	PHE	2.5
1	A	239	LYS	2.5
1	C	216	ALA	2.5
1	A	410	ILE	2.5
1	D	257	ASP	2.5
1	C	185	ILE	2.4
1	B	216	ALA	2.4
1	C	390	HIS	2.4
1	B	164	ARG	2.4
1	B	256	ASP	2.3
1	B	459	ALA	2.3
1	C	194	GLU	2.3
1	B	185	ILE	2.3
1	D	164	ARG	2.3
1	B	257	ASP	2.3
1	A	218	MET	2.3
1	A	162	ASP	2.3
1	B	187	VAL	2.3
1	A	195	GLY	2.2
1	B	254	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	205	VAL	2.2
1	D	344	MET	2.2
1	A	186	SER	2.2
1	C	347	ARG	2.2
1	C	176	VAL	2.2
1	D	406	GLU	2.2
1	A	460	SER	2.2
1	A	221	ILE	2.2
1	B	166	HIS	2.2
1	B	208	THR	2.2
1	A	405	ASP	2.2
1	C	459	ALA	2.2
1	B	401	GLU	2.1
1	A	403	ILE	2.1
1	B	186	SER	2.1
1	C	438	HIS	2.1
1	A	414	ILE	2.1
1	B	344	MET	2.1
1	A	164	ARG	2.1
1	A	223	THR	2.1
1	B	207	ASN	2.1
1	C	343	VAL	2.1
1	B	409	THR	2.0
1	A	178	ASN	2.0
1	B	343	VAL	2.0
1	B	335	ALA	2.0
1	B	414	ILE	2.0
1	C	183	ARG	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	TPO	A	342	11/12	0.82	0.14	76,79,97,98	0
1	SEP	A	346	10/11	0.84	0.13	60,63,81,82	0
1	SEP	B	346	10/11	0.84	0.12	53,57,85,91	0
1	SEP	C	346	10/11	0.84	0.12	54,58,90,92	0
1	SEP	D	346	10/11	0.84	0.14	49,54,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	B	342	11/12	0.85	0.11	65,67,88,94	0
1	TPO	D	342	11/12	0.87	0.11	58,59,83,83	0
1	TPO	C	342	11/12	0.87	0.11	62,66,88,89	0
1	TPO	C	345	11/12	0.95	0.08	50,54,55,56	0
1	TPO	A	345	11/12	0.96	0.07	54,61,63,65	0
1	TPO	B	345	11/12	0.96	0.07	54,55,57,57	0
1	TPO	D	345	11/12	0.97	0.06	42,49,53,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

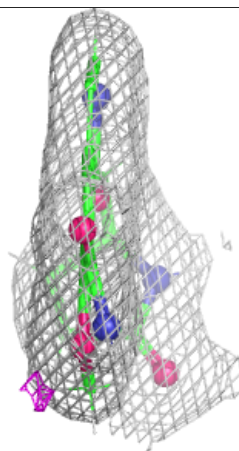
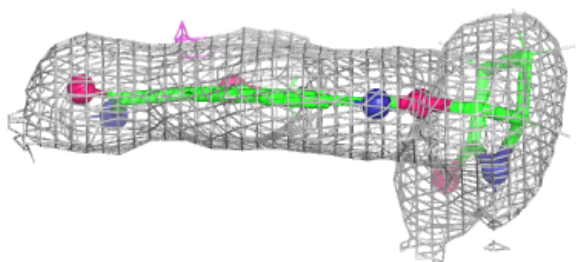
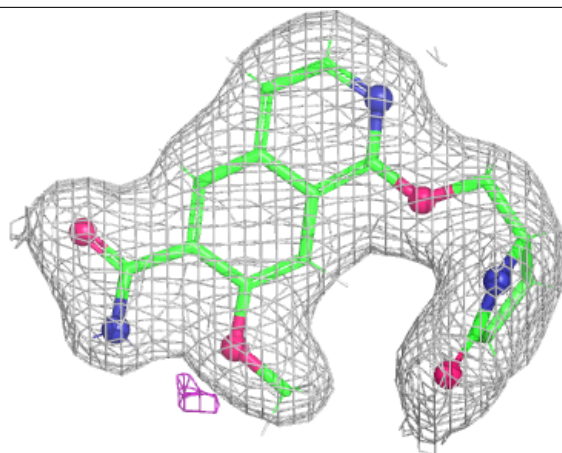
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1AFO	B	501	23/23	0.97	0.05	17,29,31,31	17
2	A1AFO	C	501	23/23	0.97	0.05	14,27,30,30	17
2	A1AFO	D	501	23/23	0.97	0.06	12,27,28,29	17
2	A1AFO	A	501	23/23	0.98	0.05	16,29,30,30	17

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.

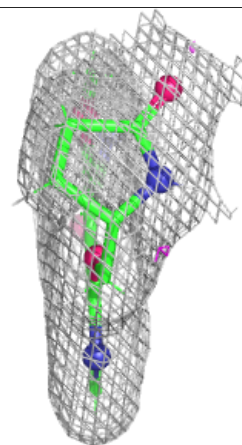
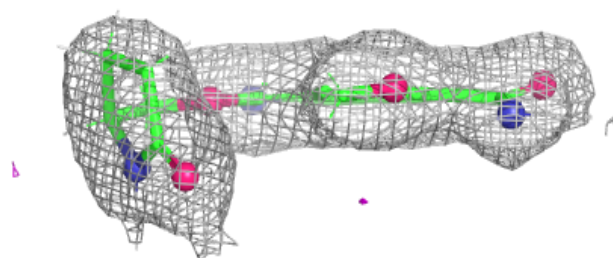
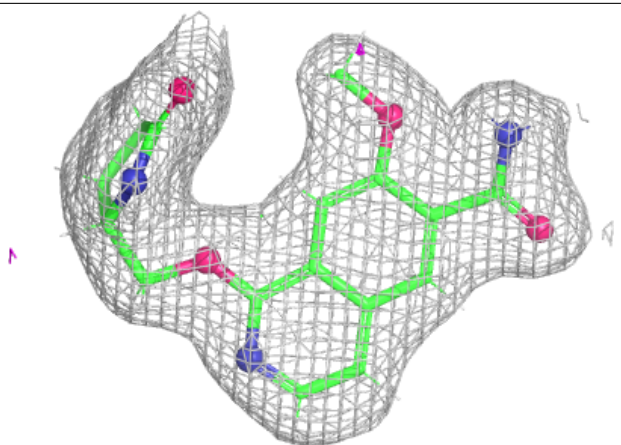
Electron density around A1AFO B 501:

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



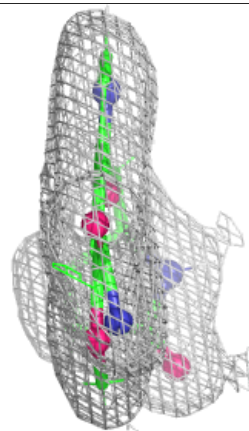
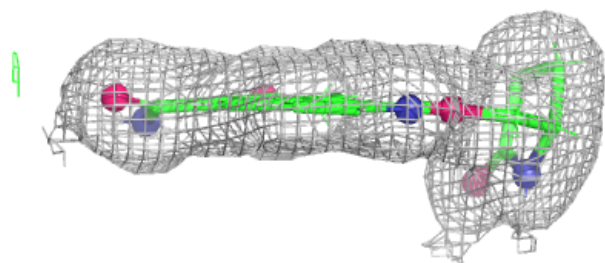
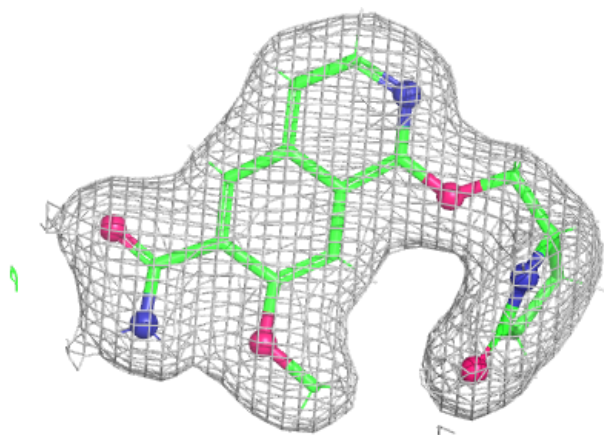
Electron density around A1AFO C 501:

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



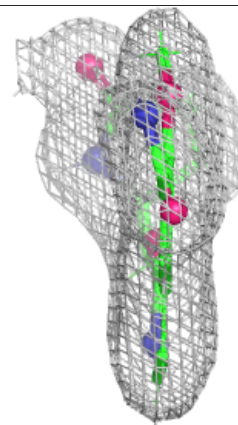
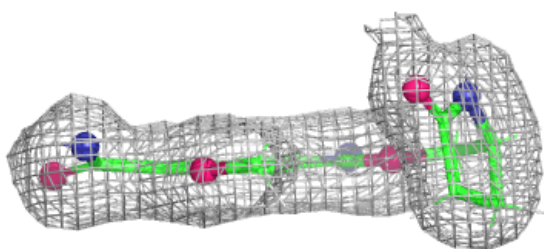
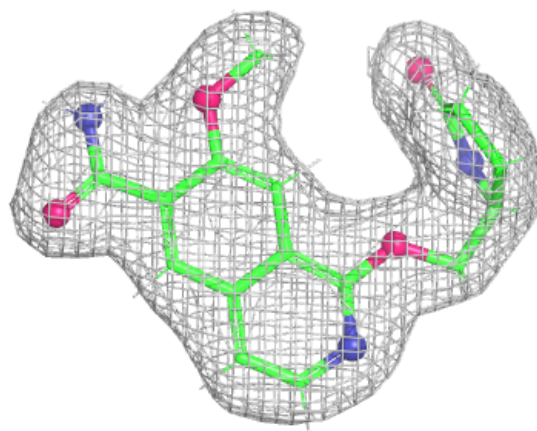
Electron density around A1AFO D 501:

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



Electron density around A1AFO 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.