



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:13 AM UTC

PDB ID : 6LXY / pdb_00006lxy
Title : IRAK4 in complex with inhibitor
Authors : Ghosh, K.; Bose, S.
Deposited on : 2020-02-12
Resolution : 2.19 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

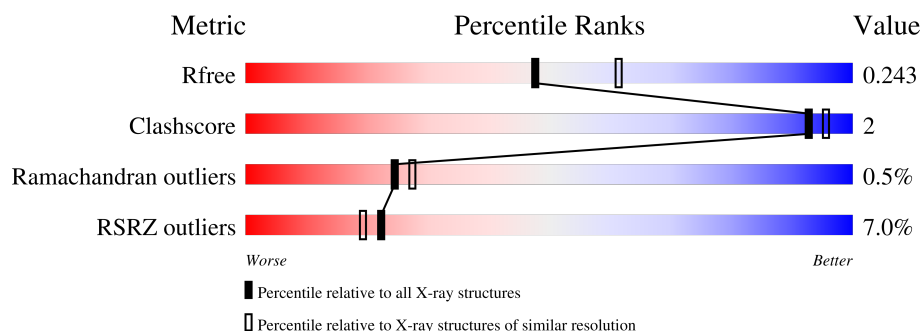
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	305	6% 91% 6% 6%
1	B	305	6% 91% 6% 6%
1	D	305	9% 93% 6% 6%
1	E	305	7% 89% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9133 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.

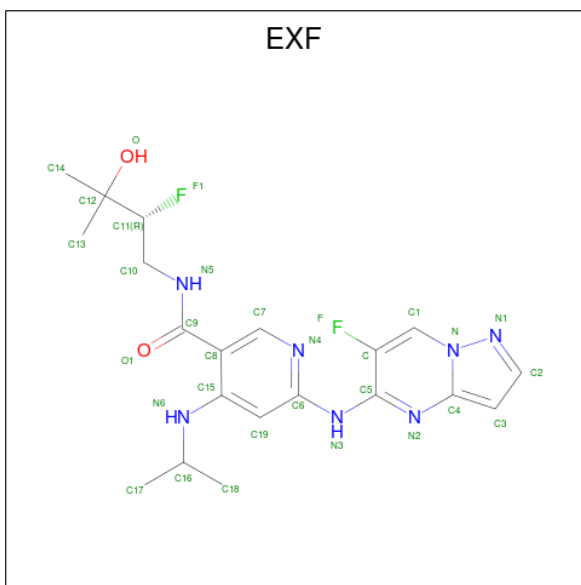
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	P	S	0	0	0
			2182	1373	370	423	2	14			
1	B	297	Total	C	N	O	P	S	0	0	0
			2221	1400	375	430	2	14			
1	D	293	Total	C	N	O	P	S	0	0	0
			2178	1373	370	419	2	14			
1	E	288	Total	C	N	O	P	S	0	0	0
			2131	1345	360	410	2	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
D	156	GLY	-	expression tag	UNP Q9NWZ3
D	157	ALA	-	expression tag	UNP Q9NWZ3
D	158	MET	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3
E	156	GLY	-	expression tag	UNP Q9NWZ3
E	157	ALA	-	expression tag	UNP Q9NWZ3
E	158	MET	-	expression tag	UNP Q9NWZ3
E	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-[(2R)-2-fluoranyl-3-methyl-3-oxidanyl-butyl]-6-[(6-fluoranylpirazolo[1,5-a]pyrimidin-5-yl)amino]-4-(propan-2-ylamino)pyridine-3-carboxamide (CCD ID: EXF) (formula: C₂₀H₂₅F₂N₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	20	2	7	2		
2	B	1	Total	C	F	N	O	0	0
			31	20	2	7	2		
2	D	1	Total	C	F	N	O	0	0
			31	20	2	7	2		
2	E	1	Total	C	F	N	O	0	0
			31	20	2	7	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

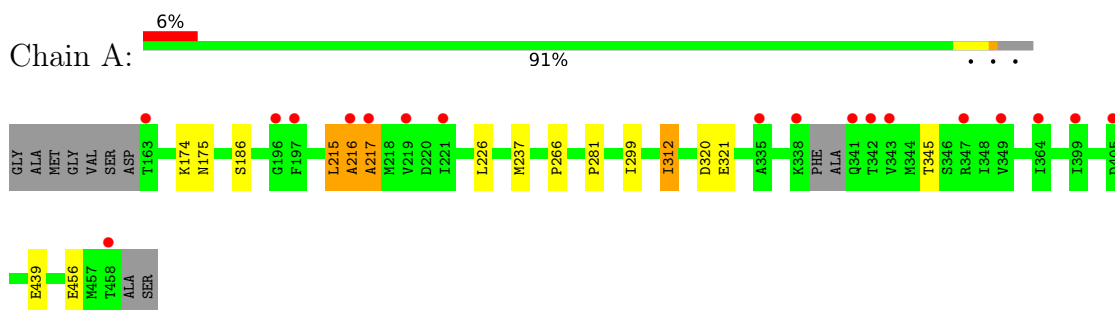
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	82	Total O 82 82	0	0
4	D	61	Total O 61 61	0	0
4	E	63	Total O 63 63	0	0

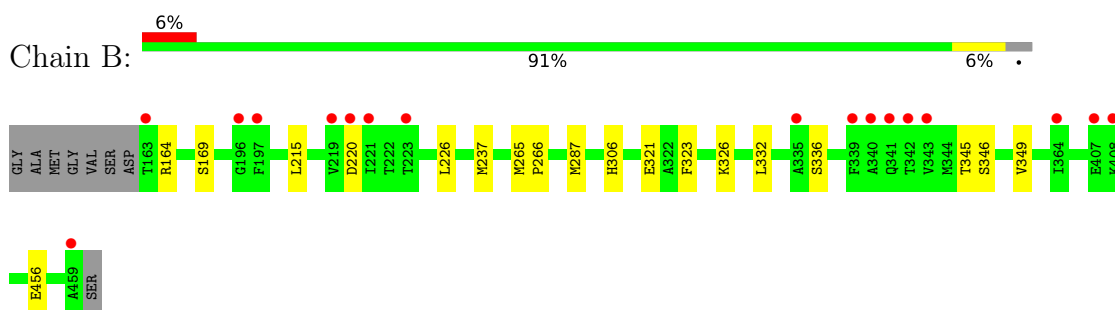
3 Residue-property plots [i](#)

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.

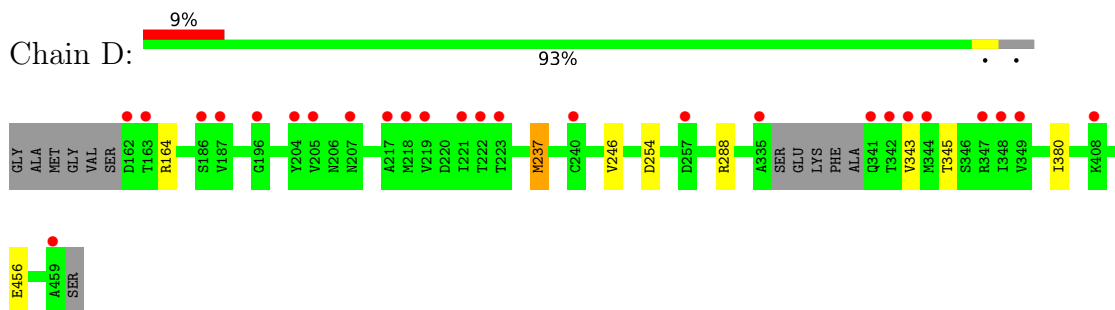
- Molecule 1: Interleukin-1 receptor-associated kinase 4



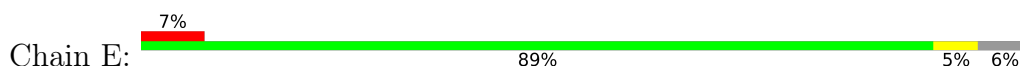
- Molecule 1: Interleukin-1 receptor-associated kinase 4

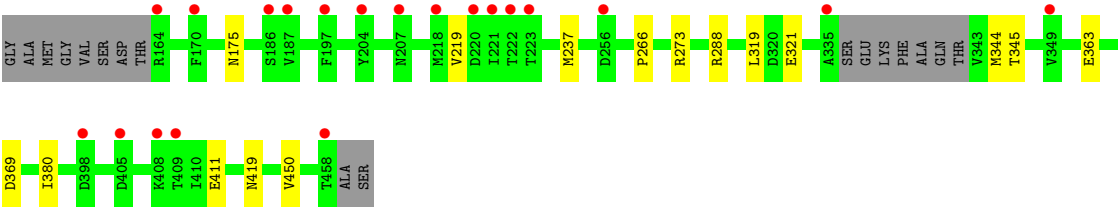


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	135.67Å 140.81Å 86.28Å 90.00° 125.70° 90.00°	Depositor
Resolution (Å)	48.08 – 2.19 48.08 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.08-2.19) 96.5 (48.08-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.20Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.201 , 0.231 (Not available) , 0.243	Depositor DCC
R_{free} test set	3255 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.9	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	0.95	EDS
Total number of atoms	9133	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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 29.46 % 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 1.5430e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SEP, SO4, TPO, EXF

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	0.85	0/2198	1.23	8/2986 (0.3%)
1	B	0.86	0/2239	1.25	3/3038 (0.1%)
1	D	0.84	1/2193 (0.0%)	1.20	3/2974 (0.1%)
1	E	0.83	0/2147	1.21	5/2915 (0.2%)
All	All	0.85	1/8777 (0.0%)	1.22	19/11913 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	237	MET	SD-CE	-6.01	1.64	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ILE	N-CA-CB	6.91	118.80	110.31
1	A	175	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	217	ALA	N-CA-C	5.77	118.60	110.23
1	E	411	GLU	CB-CG-CD	5.68	122.26	112.60
1	D	254	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	320	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	169	SER	N-CA-C	-5.27	102.68	110.48
1	E	175	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	174	LYS	N-CA-C	-5.19	105.70	111.36
1	B	456	GLU	CA-C-N	5.18	127.48	120.38
1	B	456	GLU	C-N-CA	5.18	127.48	120.38
1	D	456	GLU	CA-C-N	5.14	127.42	120.38
1	D	456	GLU	C-N-CA	5.14	127.42	120.38
1	A	215	LEU	N-CA-C	5.09	117.72	111.82
1	E	369	ASP	CA-CB-CG	5.03	117.63	112.60
1	E	450	VAL	CA-C-N	5.03	126.97	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	450	VAL	C-N-CA	5.03	126.97	120.44
1	A	456	GLU	CA-C-N	5.02	127.26	120.38
1	A	456	GLU	C-N-CA	5.02	127.26	120.38

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	2182	0	2042	9	0
1	B	2221	0	2087	10	0
1	D	2178	0	2050	2	0
1	E	2131	0	1981	7	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	D	31	0	0	0	0
2	E	31	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	76	0	0	0	0
4	B	82	0	0	0	0
4	D	61	0	0	0	0
4	E	63	0	0	0	0
All	All	9133	0	8160	26	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 2.

All (26) 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:D:237:MET:HE1	1:D:246:VAL:HG23	1.54	0.89
1:A:217:ALA:HB2	1:A:226:LEU:HD21	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:HG2	1:A:321:GLU:HG3	1.67	0.76
1:B:265:MET:HE1	1:B:326:LYS:HD2	1.72	0.71
1:E:237:MET:HA	1:E:237:MET:HE2	1.82	0.60
1:A:237:MET:HA	1:A:237:MET:HE2	1.85	0.58
1:B:237:MET:HA	1:B:237:MET:HE2	1.85	0.58
1:A:439:GLU:H	1:A:439:GLU:CD	2.16	0.54
1:A:215:LEU:O	1:A:216:ALA:C	2.51	0.54
1:B:215:LEU:HD23	1:B:226:LEU:HD22	1.92	0.51
1:B:287:MET:HE2	1:B:323:PHE:CB	2.42	0.50
1:A:186:SER:HB2	1:E:419:ASN:HB2	1.94	0.49
1:B:332:LEU:HD22	1:B:349:VAL:HG21	1.95	0.48
1:E:266:PRO:HG2	1:E:321:GLU:HB3	1.96	0.47
1:E:273:ARG:HG3	1:E:319:LEU:HD12	1.97	0.47
1:B:287:MET:CE	1:B:323:PHE:HB2	2.45	0.47
1:B:266:PRO:HG2	1:B:321:GLU:CD	2.40	0.46
1:A:321:GLU:H	1:A:321:GLU:CD	2.22	0.46
1:B:265:MET:CE	1:B:326:LYS:HD2	2.41	0.46
1:E:344:MET:CE	1:E:363:GLU:HG2	2.48	0.44
1:A:299:ILE:HD11	1:A:312:ILE:HD13	2.01	0.42
1:A:281:PRO:HD3	1:B:321:GLU:HB3	2.01	0.42
1:D:288:ARG:HB3	1:D:380:ILE:HG23	2.01	0.42
1:E:344:MET:HE2	1:E:363:GLU:HG2	2.02	0.42
1:B:306:HIS:HB3	1:B:336:SER:O	2.20	0.42
1:E:288:ARG:HB3	1:E:380:ILE:HG23	2.03	0.41

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	288/305 (94%)	284 (99%)	3 (1%)	1 (0%)	36 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	293/305 (96%)	285 (97%)	6 (2%)	2 (1%)	18	19
1	D	287/305 (94%)	277 (96%)	8 (3%)	2 (1%)	18	19
1	E	282/305 (92%)	273 (97%)	8 (3%)	1 (0%)	30	34
All	All	1150/1220 (94%)	1119 (97%)	25 (2%)	6 (0%)	24	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	ASP
1	D	343	VAL
1	B	164	ARG
1	E	219	VAL
1	A	216	ALA
1	D	164	ARG

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	D	345	1	8,10,11	1.28	2 (25%)	10,14,16	0.92	0
1	SEP	B	346	1	8,9,10	0.85	0	7,12,14	1.59	1 (14%)
1	SEP	E	346	1	8,9,10	0.96	0	7,12,14	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	E	345	1	8,10,11	1.28	2 (25%)	10,14,16	1.21	1 (10%)
1	SEP	A	346	1	8,9,10	0.87	0	7,12,14	1.19	0
1	TPO	B	345	1	8,10,11	1.07	0	10,14,16	1.16	1 (10%)
1	TPO	A	345	1	8,10,11	1.14	0	10,14,16	1.15	1 (10%)
1	SEP	D	346	1	8,9,10	0.96	0	7,12,14	0.94	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	D	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	E	346	1	-	0/6/8/10	-
1	TPO	E	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	CB-CA	2.20	1.58	1.53
1	E	345	TPO	CG2-CB	2.13	1.56	1.51
1	D	345	TPO	CG2-CB	2.07	1.56	1.51
1	E	345	TPO	CB-CA	2.06	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	O3P-P-OG	3.14	114.85	106.67
1	B	345	TPO	O2P-P-OG1	2.47	115.47	105.85
1	E	345	TPO	O2P-P-OG1	2.43	115.31	105.85
1	A	345	TPO	O2P-P-OG1	2.16	114.25	105.85

There are no chirality outliers.

All (10) 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	D	345	TPO	N-CA-CB-OG1
1	E	345	TPO	N-CA-CB-OG1
1	B	345	TPO	CB-OG1-P-O1P
1	E	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	E	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](#)

7 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	$\# Z > 2$
3	SO4	D	501	-	4,4,4	0.28	0	6,6,6	0.17	0
2	EXF	A	501	-	31,33,33	2.04	10 (32%)	37,48,48	1.54	6 (16%)
3	SO4	E	501	-	4,4,4	0.24	0	6,6,6	0.24	0
3	SO4	B	501	-	4,4,4	0.31	0	6,6,6	0.11	0
2	EXF	D	502	-	31,33,33	1.81	9 (29%)	37,48,48	1.35	5 (13%)
2	EXF	B	502	-	31,33,33	1.93	10 (32%)	37,48,48	1.35	4 (10%)
2	EXF	E	502	-	31,33,33	1.93	9 (29%)	37,48,48	1.27	5 (13%)

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	EXF	B	502	-	-	4/20/23/23	0/3/3/3
2	EXF	E	502	-	-	2/20/23/23	0/3/3/3
2	EXF	A	501	-	-	4/20/23/23	0/3/3/3
2	EXF	D	502	-	-	2/20/23/23	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EXF	C1-C	4.73	1.39	1.33
2	E	502	EXF	C1-C	4.71	1.39	1.33
2	D	502	EXF	C1-C	4.31	1.39	1.33
2	B	502	EXF	C1-C	3.99	1.38	1.33
2	A	501	EXF	C1-N	3.95	1.43	1.36
2	B	502	EXF	C19-C15	3.80	1.45	1.39
2	A	501	EXF	C5-C	3.80	1.46	1.42
2	D	502	EXF	C5-N3	3.46	1.43	1.36
2	B	502	EXF	C1-N	3.43	1.42	1.36
2	B	502	EXF	C8-C15	3.40	1.46	1.41
2	E	502	EXF	C9-N5	3.36	1.41	1.33
2	E	502	EXF	C19-C15	3.35	1.44	1.39
2	E	502	EXF	C4-N	3.30	1.44	1.38
2	A	501	EXF	C6-N4	3.17	1.39	1.34
2	D	502	EXF	C19-C15	3.11	1.44	1.39
2	A	501	EXF	C19-C15	3.06	1.44	1.39
2	A	501	EXF	C8-C15	3.01	1.45	1.41
2	E	502	EXF	O-C12	-2.84	1.39	1.44
2	D	502	EXF	F1-C11	-2.67	1.35	1.40
2	D	502	EXF	C6-N4	2.63	1.38	1.34
2	A	501	EXF	F1-C11	-2.63	1.35	1.40
2	B	502	EXF	C9-N5	2.62	1.39	1.33
2	B	502	EXF	C13-C12	2.54	1.56	1.52
2	B	502	EXF	C6-N4	2.51	1.38	1.34
2	D	502	EXF	C1-N	2.43	1.40	1.36
2	A	501	EXF	C5-N3	2.41	1.41	1.36
2	B	502	EXF	C5-N3	2.37	1.41	1.36
2	B	502	EXF	F1-C11	-2.36	1.36	1.40
2	D	502	EXF	C4-N	2.33	1.42	1.38
2	D	502	EXF	C9-N5	2.33	1.38	1.33
2	A	501	EXF	C4-N	2.29	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	502	EXF	C4-N2	2.28	1.40	1.36
2	E	502	EXF	C5-N2	2.21	1.36	1.32
2	E	502	EXF	C3-C2	2.21	1.43	1.39
2	D	502	EXF	F-C	-2.17	1.31	1.35
2	A	501	EXF	F-C	-2.08	1.31	1.35
2	B	502	EXF	O-C12	-2.06	1.41	1.44
2	E	502	EXF	C6-N4	2.03	1.37	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	EXF	C-C5-N2	4.36	123.50	119.64
2	E	502	EXF	C-C5-N2	3.93	123.12	119.64
2	A	501	EXF	N3-C5-N2	-3.79	115.71	122.71
2	A	501	EXF	C-C5-N2	3.44	122.68	119.64
2	B	502	EXF	C8-C15-N6	-3.14	118.31	121.08
2	D	502	EXF	C-C5-N2	3.07	122.36	119.64
2	A	501	EXF	C8-C15-N6	-2.97	118.46	121.08
2	D	502	EXF	F1-C11-C10	-2.71	105.55	108.06
2	B	502	EXF	N3-C5-N2	-2.67	117.79	122.71
2	D	502	EXF	N3-C5-N2	-2.62	117.88	122.71
2	A	501	EXF	C15-N6-C16	2.58	128.33	124.66
2	E	502	EXF	C8-C15-N6	-2.36	119.00	121.08
2	A	501	EXF	C14-C12-C13	-2.34	107.11	110.52
2	B	502	EXF	O-C12-C14	2.33	113.01	107.90
2	D	502	EXF	C8-C15-N6	-2.21	119.13	121.08
2	A	501	EXF	F-C-C1	-2.18	119.16	120.99
2	D	502	EXF	C15-C8-C9	2.18	123.75	120.96
2	E	502	EXF	C17-C16-C18	-2.11	106.27	111.55
2	E	502	EXF	N3-C5-N2	-2.09	118.85	122.71
2	E	502	EXF	C15-C8-C9	2.05	123.59	120.96

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EXF	C-C5-N3-C6
2	A	501	EXF	N2-C5-N3-C6
2	B	502	EXF	C-C5-N3-C6
2	B	502	EXF	N2-C5-N3-C6
2	E	502	EXF	C-C5-N3-C6
2	E	502	EXF	N2-C5-N3-C6

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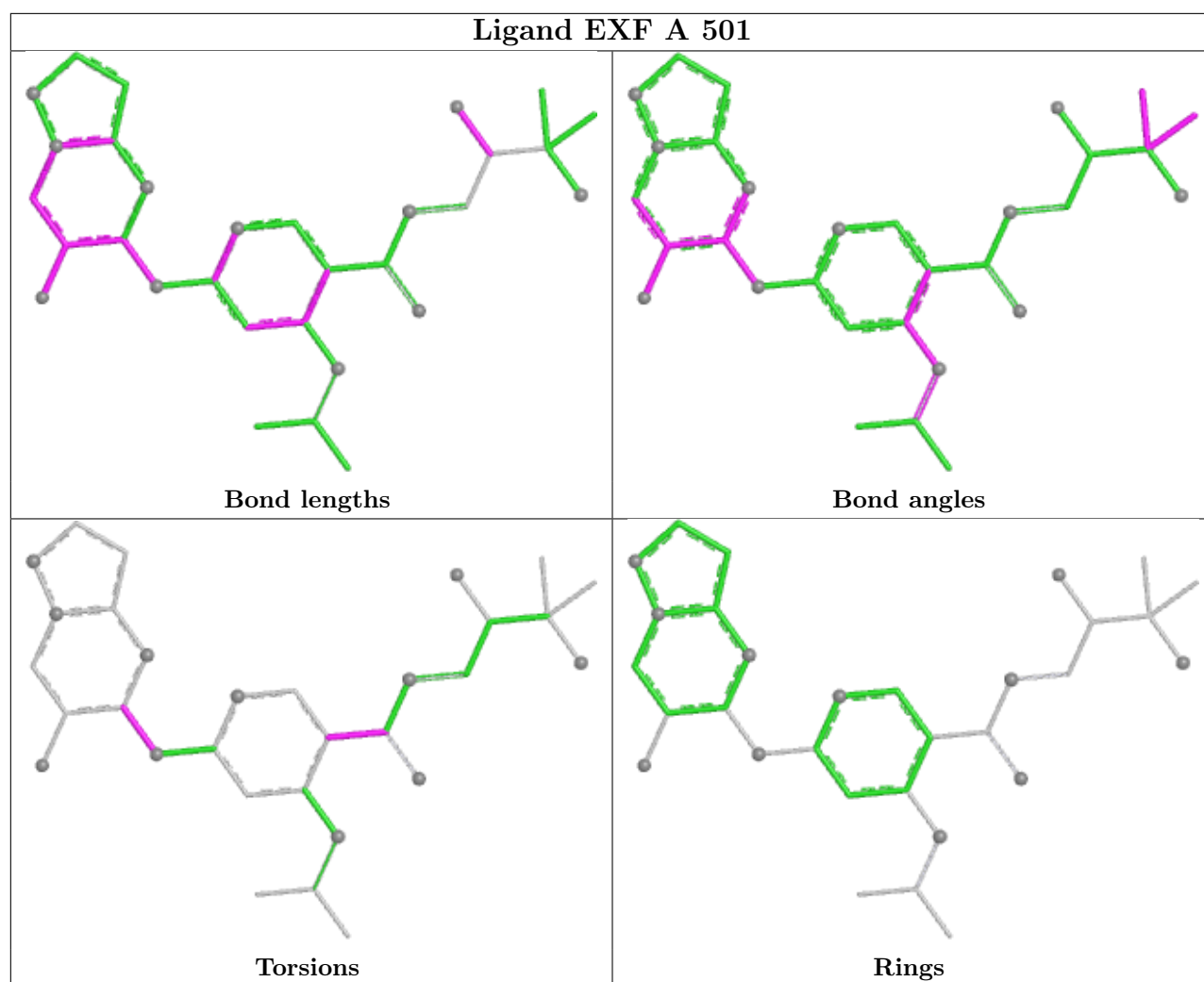
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Mol	Chain	Res	Type	Atoms
2	A	501	EXF	C7-C8-C9-O1
2	B	502	EXF	C7-C8-C9-O1
2	B	502	EXF	C7-C8-C9-N5
2	D	502	EXF	C19-C6-N3-C5
2	A	501	EXF	C7-C8-C9-N5
2	D	502	EXF	N4-C6-N3-C5

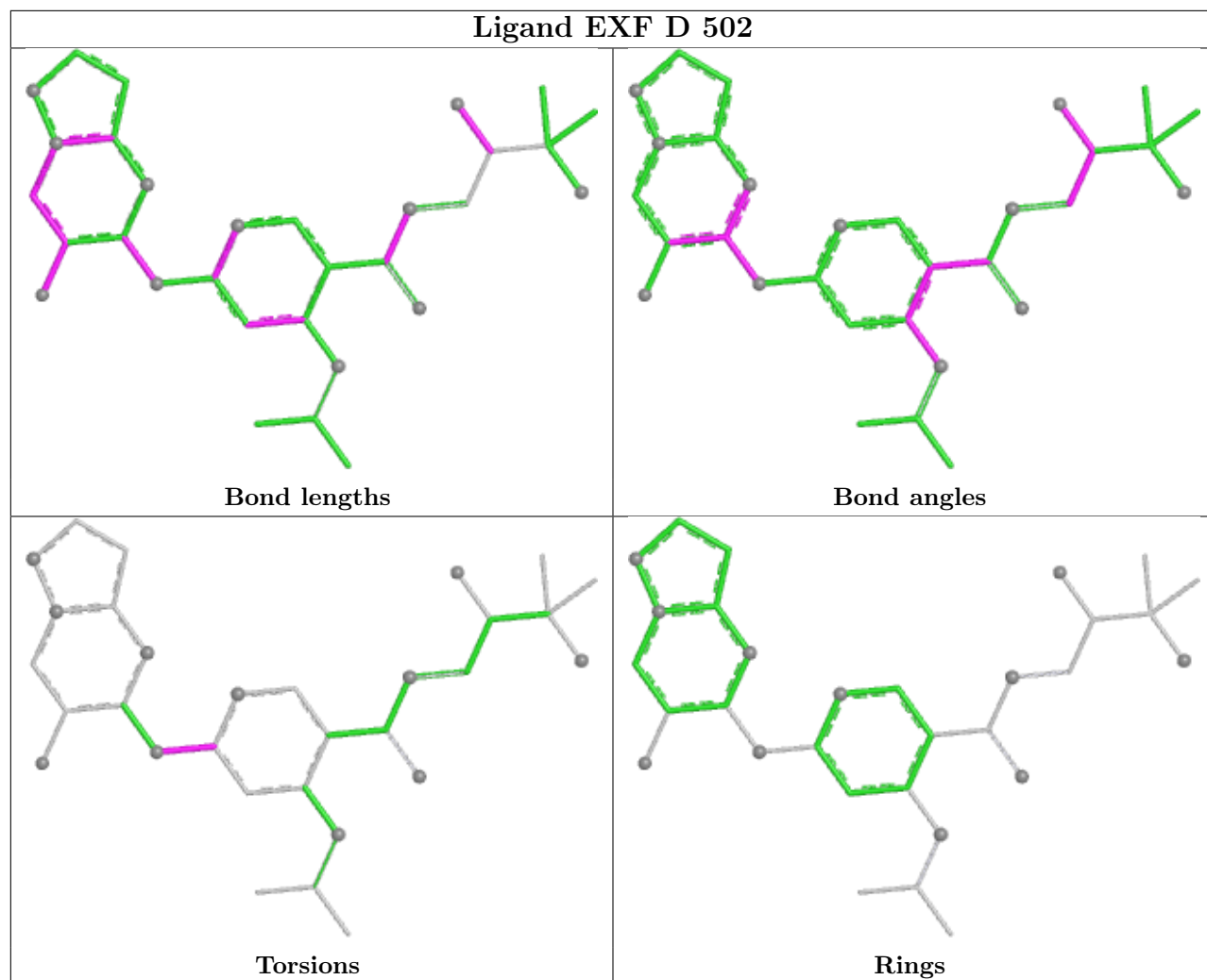
There are no ring outliers.

No monomer is involved in short contacts.

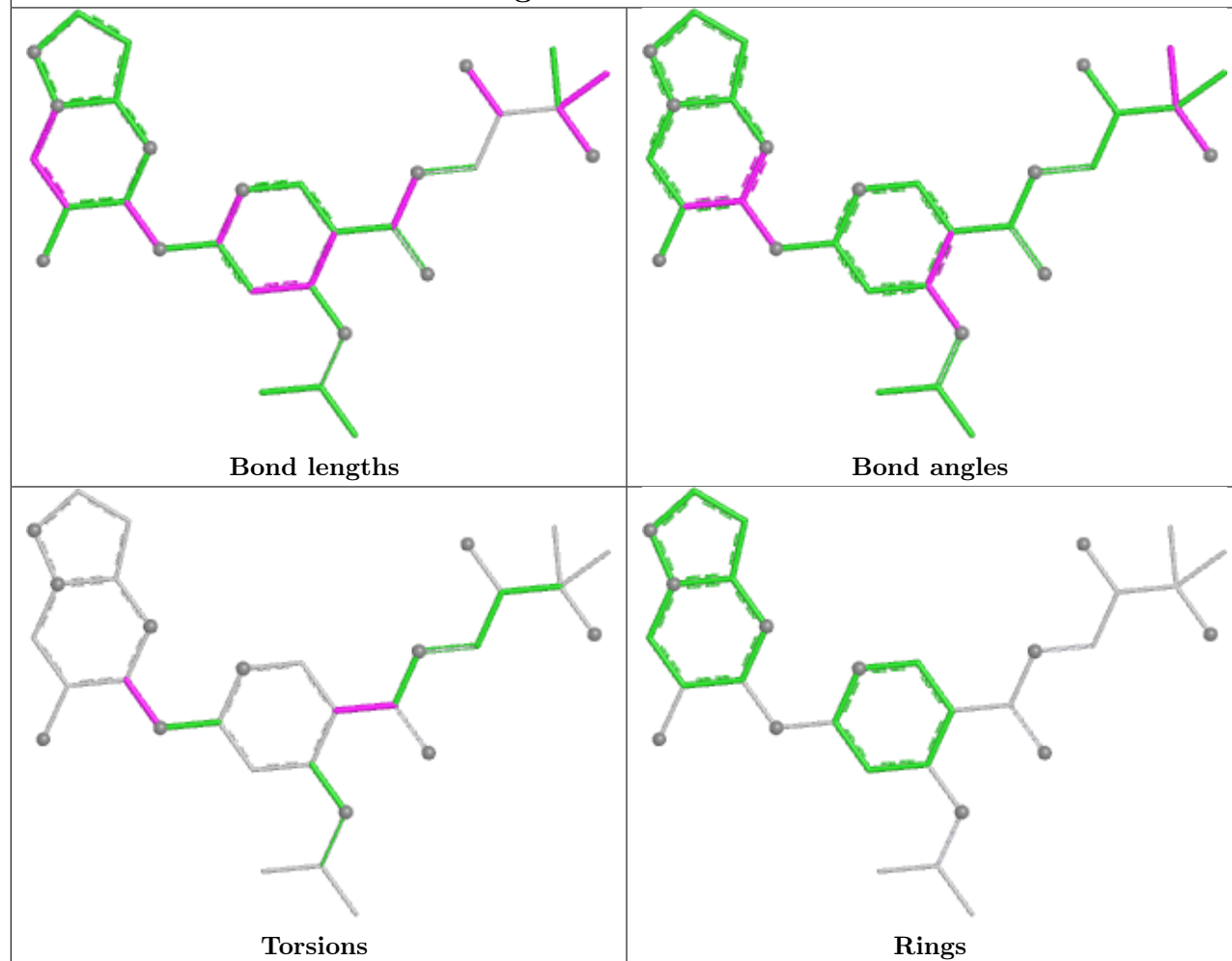
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

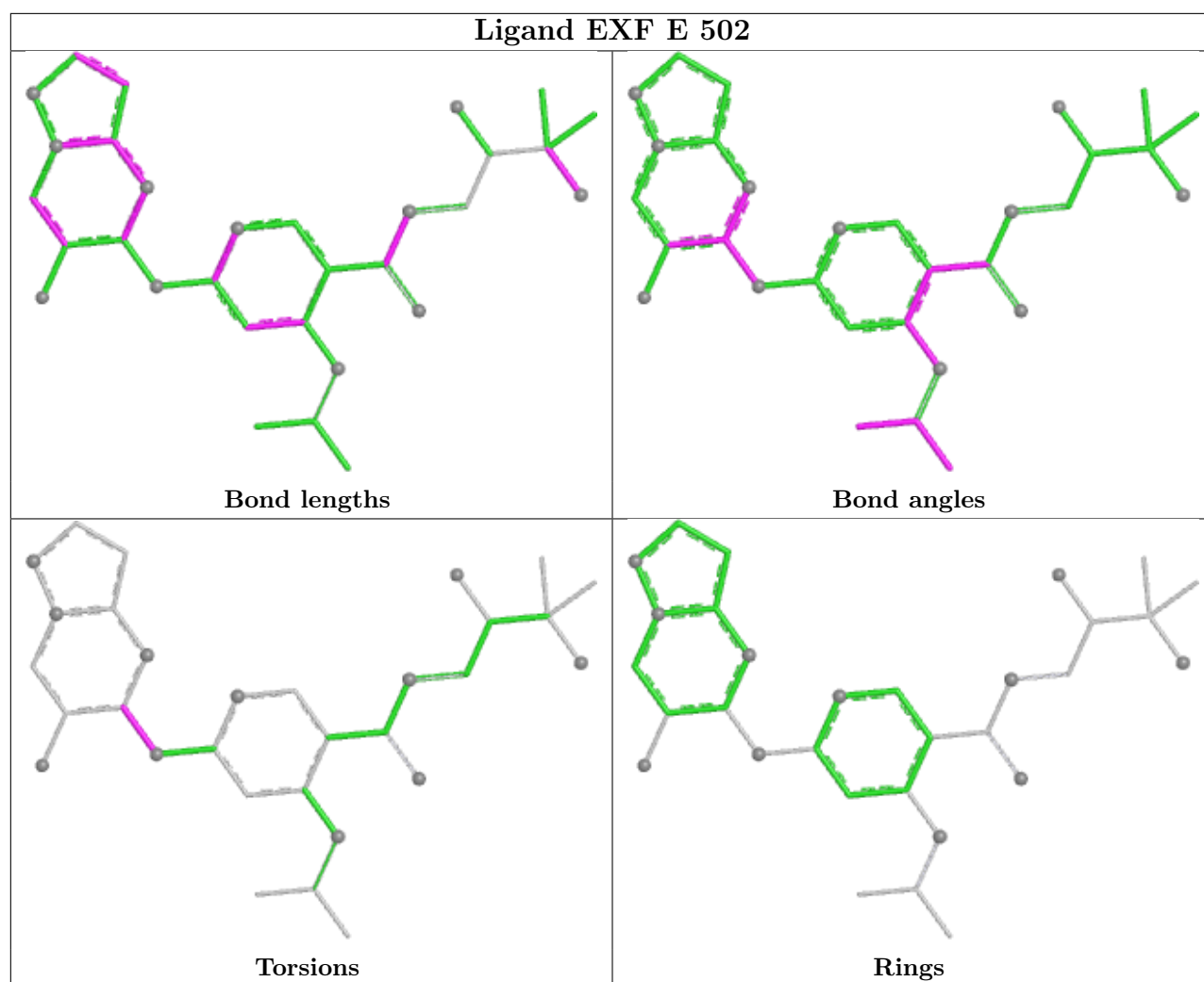


Ligand EXF D 502



Ligand EXF B 502





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	292/305 (95%)	0.37	18 (6%) 26 23	20, 39, 72, 100	0
1	B	295/305 (96%)	0.35	17 (5%) 29 25	20, 39, 71, 106	0
1	D	291/305 (95%)	0.50	26 (8%) 15 13	23, 42, 73, 86	0
1	E	286/305 (93%)	0.40	20 (6%) 22 19	21, 41, 67, 86	0
All	All	1164/1220 (95%)	0.40	81 (6%) 22 19	20, 40, 72, 106	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	6.3
1	D	219	VAL	5.3
1	B	221	ILE	5.3
1	D	459	ALA	5.0
1	B	459	ALA	4.3
1	D	163	THR	4.3
1	E	222	THR	4.2
1	A	217	ALA	3.9
1	D	342	THR	3.9
1	D	221	ILE	3.9
1	A	342	THR	3.9
1	E	335	ALA	3.8
1	A	221	ILE	3.8
1	A	196	GLY	3.8
1	B	219	VAL	3.7
1	E	221	ILE	3.7
1	B	341	GLN	3.6
1	B	342	THR	3.5
1	A	338	LYS	3.2
1	A	399	ILE	3.1
1	B	197	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	218	MET	3.0
1	E	220	ASP	3.0
1	B	364	ILE	3.0
1	D	335	ALA	3.0
1	A	341	GLN	2.9
1	D	341	GLN	2.9
1	A	405	ASP	2.9
1	A	364	ILE	2.9
1	A	458	THR	2.9
1	D	162	ASP	2.8
1	A	335	ALA	2.8
1	E	197	PHE	2.8
1	B	343	VAL	2.8
1	A	343	VAL	2.7
1	E	408	LYS	2.7
1	D	207	ASN	2.7
1	E	187	VAL	2.6
1	D	187	VAL	2.6
1	B	339	PHE	2.6
1	E	207	ASN	2.6
1	D	217	ALA	2.6
1	E	405	ASP	2.6
1	B	407	GLU	2.5
1	E	204	TYR	2.5
1	B	335	ALA	2.5
1	A	347	ARG	2.5
1	D	348	ILE	2.5
1	D	204	TYR	2.5
1	A	163	THR	2.5
1	D	343	VAL	2.4
1	E	398	ASP	2.4
1	B	163	THR	2.4
1	E	223	THR	2.4
1	D	347	ARG	2.4
1	A	219	VAL	2.4
1	D	186	SER	2.4
1	A	197	PHE	2.4
1	D	223	THR	2.4
1	D	257	ASP	2.3
1	E	218	MET	2.3
1	E	186	SER	2.3
1	E	349	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	222	THR	2.3
1	B	408	LYS	2.3
1	D	349	VAL	2.2
1	D	408	LYS	2.2
1	E	256	ASP	2.2
1	E	164	ARG	2.2
1	B	223	THR	2.2
1	A	349	VAL	2.2
1	D	240	CYS	2.2
1	E	409	THR	2.2
1	E	458	THR	2.2
1	B	196	GLY	2.1
1	D	344	MET	2.1
1	D	205	VAL	2.1
1	B	220	ASP	2.1
1	B	340	ALA	2.1
1	D	196	GLY	2.0
1	E	170	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	D	346	10/11	0.53	0.22	75,81,90,90	0
1	SEP	E	346	10/11	0.57	0.17	65,73,84,84	0
1	SEP	B	346	10/11	0.64	0.15	73,78,86,86	0
1	SEP	A	346	10/11	0.68	0.16	73,79,86,87	0
1	TPO	A	345	11/12	0.81	0.11	68,71,73,73	0
1	TPO	B	345	11/12	0.87	0.10	69,74,78,78	0
1	TPO	D	345	11/12	0.89	0.12	67,69,72,74	0
1	TPO	E	345	11/12	0.90	0.09	54,56,62,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

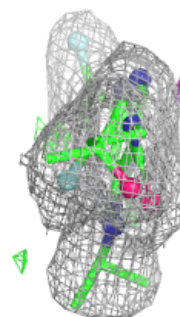
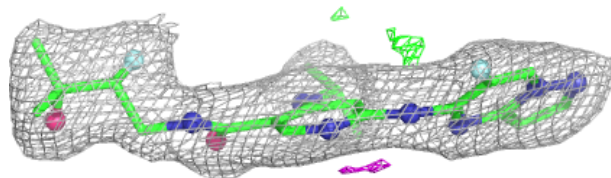
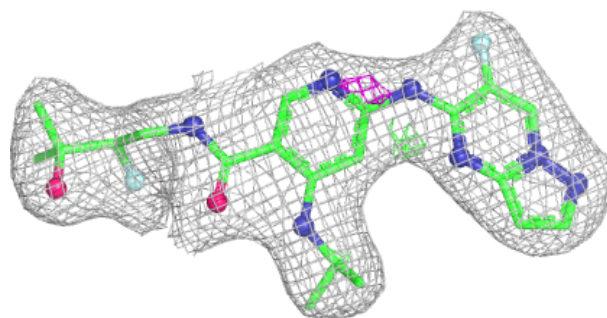
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	501	5/5	0.67	0.15	121,122,123,123	0
3	SO4	E	501	5/5	0.78	0.10	77,78,80,82	0
3	SO4	D	501	5/5	0.86	0.12	61,65,66,66	0
2	EXF	E	502	31/31	0.94	0.07	26,31,36,37	0
2	EXF	B	502	31/31	0.95	0.06	25,28,31,34	0
2	EXF	A	501	31/31	0.96	0.06	23,27,31,32	0
2	EXF	D	502	31/31	0.96	0.06	29,31,34,37	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.

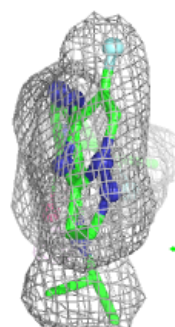
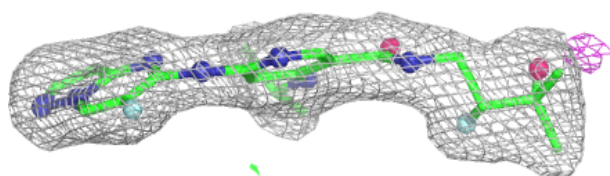
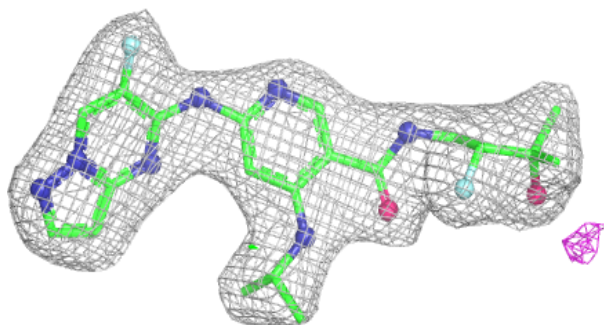
Electron density around EXF E 502:

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

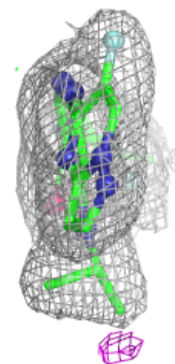
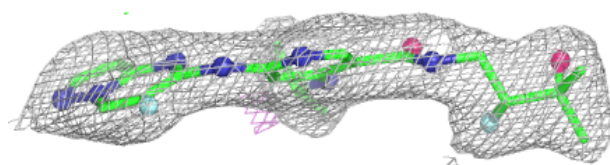
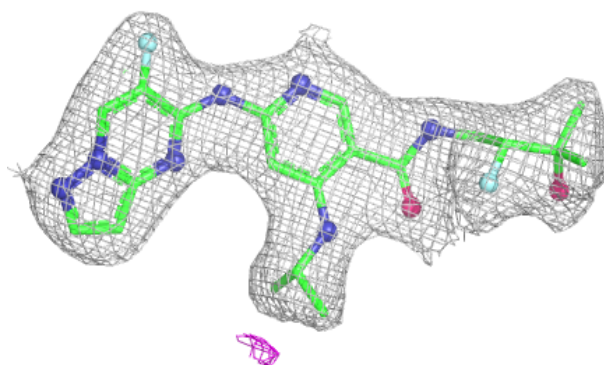


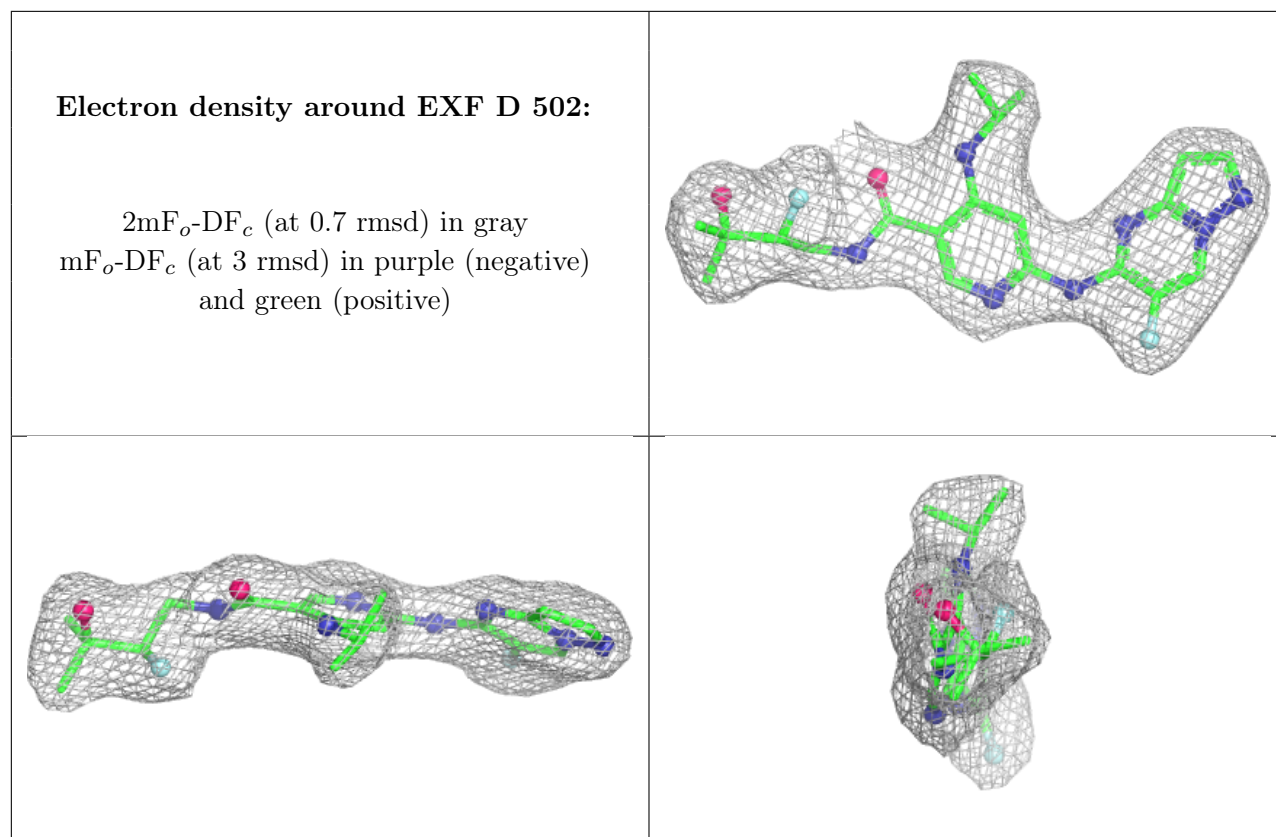
Electron density around EXF B 502:

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

**Electron density around EXF 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.