



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2021 – 06:10 PM JST

PDB ID : 7CBJ
Title : Crystal structure of PDE4D catalytic domain in complex with compound 36
Authors : Zhang, X.L.; Xu, Y.C.
Deposited on : 2020-06-12
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

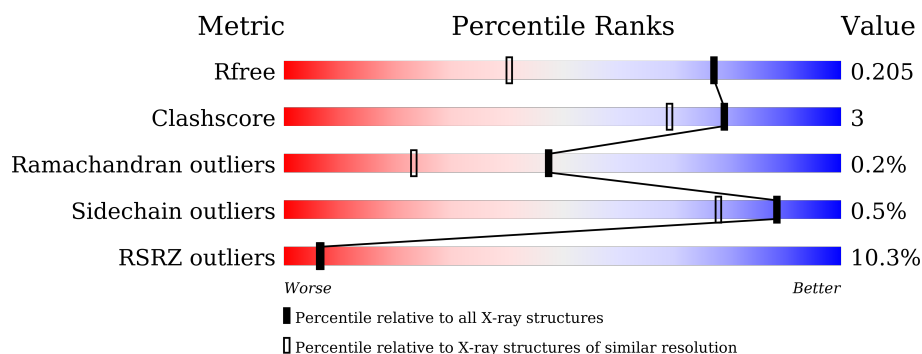
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	349	<div> <div>4%</div> <div>90%</div> <div>7%</div> </div>
1	B	349	<div> <div>15%</div> <div>86%</div> <div>6%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5657 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	3	0
			2637	1671	445	505	16			
1	B	323	Total	C	N	O	S	0	1	0
			2588	1640	435	498	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	expression tag	UNP Q08499
A	66	GLY	-	expression tag	UNP Q08499
A	67	SER	-	expression tag	UNP Q08499
A	68	SER	-	expression tag	UNP Q08499
A	69	HIS	-	expression tag	UNP Q08499
A	70	HIS	-	expression tag	UNP Q08499
A	71	HIS	-	expression tag	UNP Q08499
A	72	HIS	-	expression tag	UNP Q08499
A	73	HIS	-	expression tag	UNP Q08499
A	74	HIS	-	expression tag	UNP Q08499
A	75	SER	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	GLY	-	expression tag	UNP Q08499
A	78	LEU	-	expression tag	UNP Q08499
A	79	VAL	-	expression tag	UNP Q08499
A	80	PRO	-	expression tag	UNP Q08499
A	81	ARG	-	expression tag	UNP Q08499
A	82	GLY	-	expression tag	UNP Q08499
A	83	SER	-	expression tag	UNP Q08499
A	84	HIS	-	expression tag	UNP Q08499
A	85	MET	-	expression tag	UNP Q08499
B	65	MET	-	expression tag	UNP Q08499
B	66	GLY	-	expression tag	UNP Q08499
B	67	SER	-	expression tag	UNP Q08499
B	68	SER	-	expression tag	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
B	69	HIS	-	expression tag	UNP Q08499
B	70	HIS	-	expression tag	UNP Q08499
B	71	HIS	-	expression tag	UNP Q08499
B	72	HIS	-	expression tag	UNP Q08499
B	73	HIS	-	expression tag	UNP Q08499
B	74	HIS	-	expression tag	UNP Q08499
B	75	SER	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	GLY	-	expression tag	UNP Q08499
B	78	LEU	-	expression tag	UNP Q08499
B	79	VAL	-	expression tag	UNP Q08499
B	80	PRO	-	expression tag	UNP Q08499
B	81	ARG	-	expression tag	UNP Q08499
B	82	GLY	-	expression tag	UNP Q08499
B	83	SER	-	expression tag	UNP Q08499
B	84	HIS	-	expression tag	UNP Q08499
B	85	MET	-	expression tag	UNP Q08499

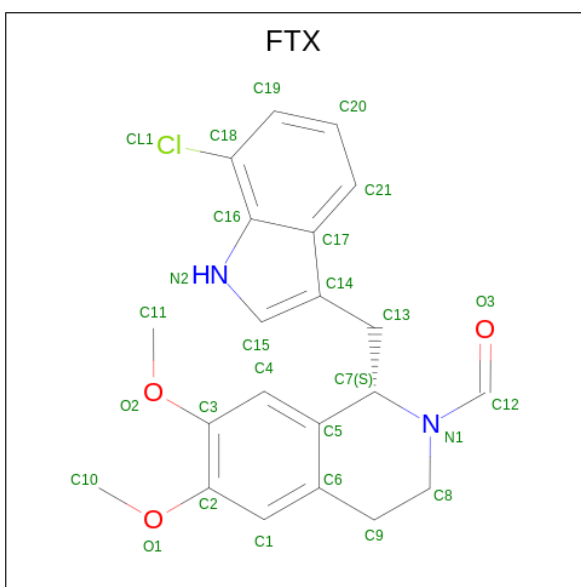
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

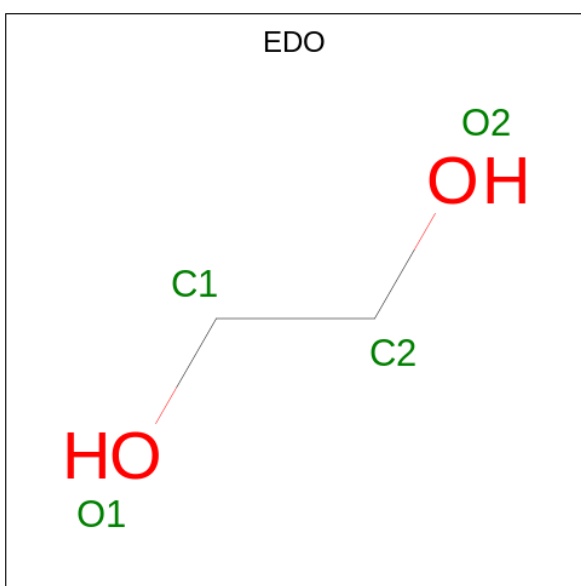
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is (1S)-1-[(7-chloranyl-1H-indol-3-yl)methyl]-6,7-dimethoxy-3,4-dihydro-1H-i soquinoline-2-carbaldehyde (three-letter code: FTX) (formula: C₂₁H₂₁ClN₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0
			27	21	1	2	3	
4	B	1	Total	C	Cl	N	O	0
			27	21	1	2	3	

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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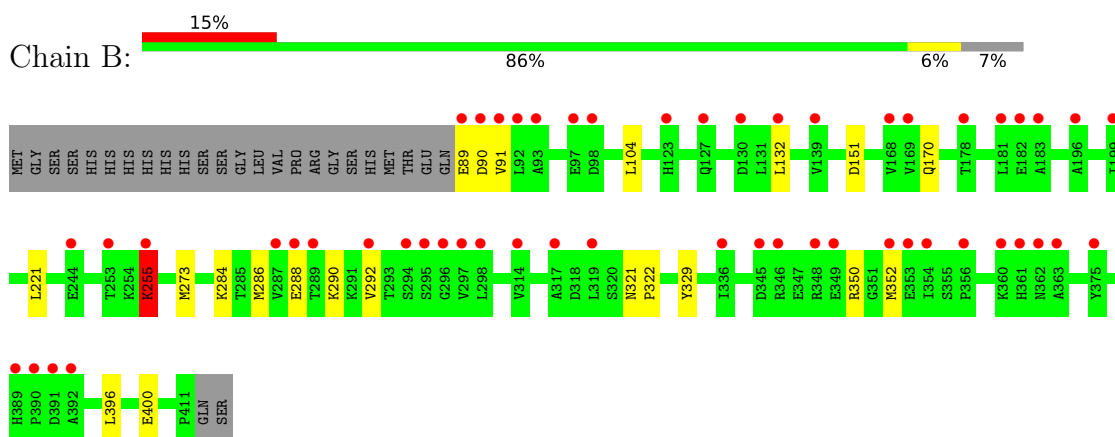
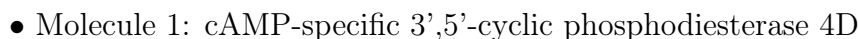
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	191	Total O 191 191	0	0
6	B	135	Total O 135 135	0	0

- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.12Å 80.46Å 164.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.52 – 1.50 33.52 – 1.50	Depositor EDS
% Data completeness (in resolution range)	91.0 (33.52-1.50) 91.0 (33.52-1.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.181 , 0.205 0.181 , 0.205	Depositor DCC
R_{free} test set	5540 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5657	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FTX, MG, ZN, EDO

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	0.86	3/2700 (0.1%)	0.83	6/3671 (0.2%)
1	B	0.96	4/2645 (0.2%)	0.78	2/3601 (0.1%)
All	All	0.91	7/5345 (0.1%)	0.80	8/7272 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	LYS	CE-NZ	34.52	2.35	1.49
1	A	244	GLU	CB-CG	17.60	1.85	1.52
1	B	255	LYS	CD-CE	15.35	1.89	1.51
1	A	244	GLU	CD-OE2	15.06	1.42	1.25
1	A	244	GLU	CD-OE1	14.94	1.42	1.25
1	B	255	LYS	CB-CG	5.58	1.67	1.52
1	B	329	TYR	CD2-CE2	-5.07	1.31	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	LYS	CD-CE-NZ	17.52	151.99	111.70
1	A	244	GLU	OE1-CD-OE2	-15.98	104.12	123.30
1	A	247	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	244	GLU	CG-CD-OE2	5.94	130.18	118.30
1	B	255	LYS	CG-CD-CE	-5.88	94.27	111.90
1	A	391	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	318	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	318	ASP	CB-CG-OD2	-5.18	113.64	118.30

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	2637	0	2579	11	1
1	B	2588	0	2511	21	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	0	0	0
4	B	27	0	0	1	0
5	A	36	0	54	0	0
5	B	12	0	18	1	0
6	A	191	0	0	2	0
6	B	135	0	0	0	0
All	All	5657	0	5162	29	1

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 (29) 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:244:GLU:CB	1:A:244:GLU:CG	1.85	1.51
1:B:255:LYS:CD	1:B:255:LYS:CE	1.89	1.46
1:B:255:LYS:HE2	1:B:255:LYS:CB	1.81	1.10
1:B:255:LYS:CE	1:B:255:LYS:HB3	1.83	1.08
1:B:255:LYS:HE2	1:B:255:LYS:HB3	0.98	0.98
1:B:255:LYS:CE	1:B:255:LYS:NZ	2.35	0.90
1:B:255:LYS:CE	1:B:255:LYS:CG	2.54	0.86
1:B:255:LYS:CE	1:B:255:LYS:CB	2.50	0.79
1:A:235:ALA:O	1:A:239:LYS:HG3	1.96	0.65
1:A:239:LYS:HG2	1:B:221:LEU:HD21	1.84	0.59
1:B:89:GLU:O	1:B:91:VAL:N	2.38	0.56
1:A:244:GLU:CG	1:A:244:GLU:CA	2.79	0.55
1:B:151:ASP:HA	5:B:506:EDO:H21	1.92	0.52
1:B:396:LEU:O	1:B:400:GLU:HG3	2.09	0.52
1:A:244:GLU:CG	1:A:244:GLU:C	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HE3	1:B:221:LEU:HG	1.95	0.49
1:B:255:LYS:CD	1:B:255:LYS:HE3	2.25	0.49
1:B:350:ARG:HD3	1:B:352:MET:CE	2.44	0.48
1:A:282:ASP:HB3	1:A:308:GLN:NE2	2.29	0.47
1:B:284:LYS:O	1:B:288:GLU:HG3	2.16	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.98	0.46
1:B:290:LYS:NZ	1:B:292:VAL:HG11	2.31	0.46
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.99	0.45
1:A:239:LYS:NZ	6:A:601:HOH:O	2.35	0.44
1:B:350:ARG:HD3	1:B:352:MET:HE1	2.02	0.42
1:A:239:LYS:HG2	1:B:221:LEU:CD2	2.50	0.41
1:A:123:HIS:NE2	1:A:127:GLN:OE1	2.54	0.41
1:A:331[B]:GLN:HG2	6:A:711:HOH:O	2.20	0.40
1:B:273:MET:HB3	4:B:503:FTX:C18	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:OE2	1:B:255:LYS:NZ[3_655]	1.92	0.28

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	327/349 (94%)	320 (98%)	7 (2%)	0	100	100
1	B	322/349 (92%)	317 (98%)	4 (1%)	1 (0%)	41	18
All	All	649/698 (93%)	637 (98%)	11 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/318 (93%)	296 (100%)	0	100	100
1	B	289/318 (91%)	286 (99%)	3 (1%)	76	57
All	All	585/636 (92%)	582 (100%)	3 (0%)	88	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	132	LEU
1	B	255	LYS
1	B	286	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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
5	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.29	0
4	FTX	A	503	-	27,30,30	0.63	1 (3%)	30,43,43	1.04	3 (10%)
4	FTX	B	503	-	27,30,30	0.60	1 (3%)	30,43,43	1.02	5 (16%)
5	EDO	A	510	-	3,3,3	0.44	0	2,2,2	0.28	0
5	EDO	A	506	-	3,3,3	0.39	0	2,2,2	0.93	0
5	EDO	A	507	-	3,3,3	0.63	0	2,2,2	0.71	0
5	EDO	B	505	-	3,3,3	0.53	0	2,2,2	0.37	0
5	EDO	A	508	-	3,3,3	0.39	0	2,2,2	0.25	0
5	EDO	A	504	-	3,3,3	0.53	0	2,2,2	0.77	0
5	EDO	A	509	-	3,3,3	0.57	0	2,2,2	0.31	0
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.23	0
5	EDO	A	512	-	3,3,3	0.43	0	2,2,2	0.87	0
5	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.59	0
5	EDO	B	506	-	3,3,3	0.42	0	2,2,2	0.54	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
5	EDO	B	504	-	-	0/1/1/1	-
4	FTX	A	503	-	-	1/9/23/23	0/4/4/4
4	FTX	B	503	-	-	1/9/23/23	0/4/4/4
5	EDO	A	510	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	507	-	-	1/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	A	512	-	-	0/1/1/1	-
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	FTX	C18-C16	-2.23	1.39	1.42
4	B	503	FTX	C18-C16	-2.12	1.39	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	FTX	C19-C18-C16	-2.48	119.19	121.03
4	A	503	FTX	C13-C7-C5	-2.48	107.39	111.66
4	B	503	FTX	C13-C7-C5	-2.43	107.47	111.66
4	A	503	FTX	C19-C18-C16	-2.30	119.32	121.03
4	B	503	FTX	C16-C18-CL1	2.27	121.05	118.97
4	B	503	FTX	C9-C8-N1	-2.11	107.86	110.39
4	B	503	FTX	C14-C13-C7	2.03	118.04	113.55
4	A	503	FTX	C16-C18-CL1	2.02	120.82	118.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	FTX	C7-C13-C14-C15
4	A	503	FTX	C7-C13-C14-C15
5	A	507	EDO	O1-C1-C2-O2

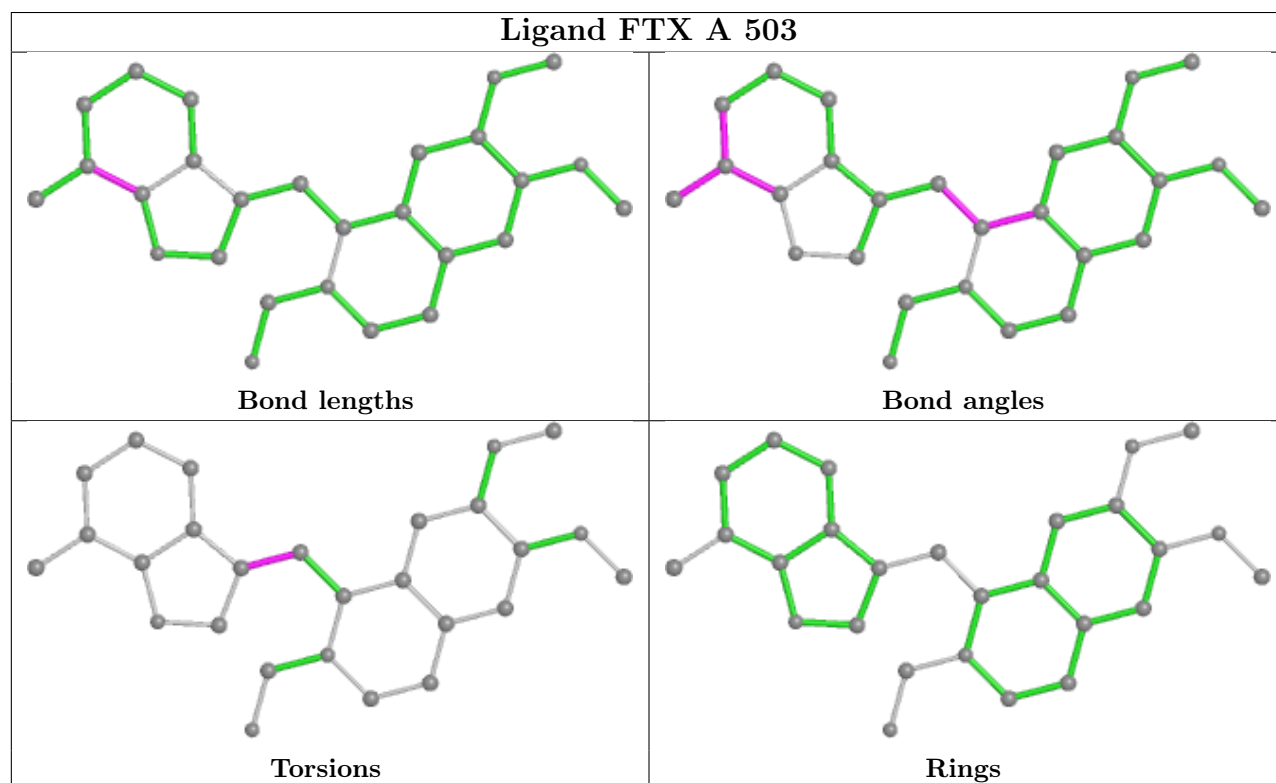
There are no ring outliers.

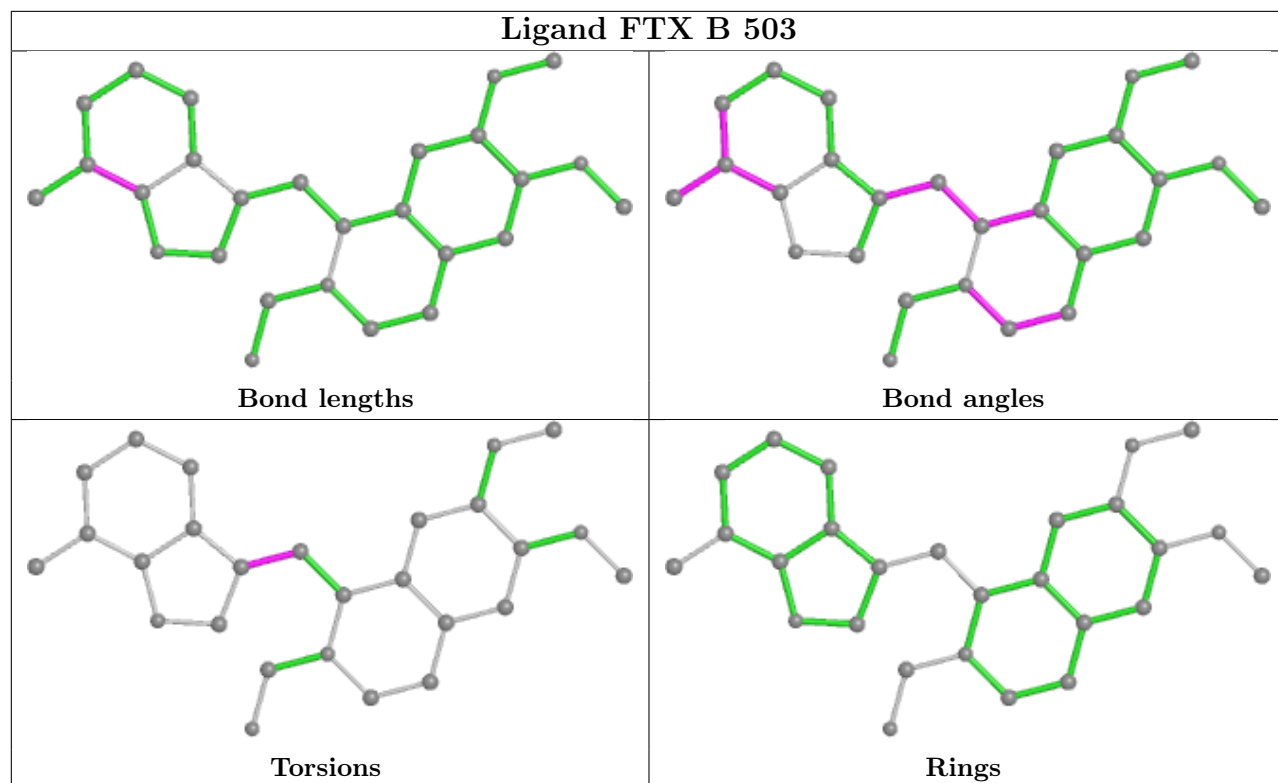
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	FTX	1	0
5	B	506	EDO	1	0

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

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





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	326/349 (93%)	0.11	14 (4%) 35 39	5, 15, 35, 56	0
1	B	323/349 (92%)	0.88	53 (16%) 1 1	7, 25, 44, 71	0
All	All	649/698 (92%)	0.50	67 (10%) 6 6	5, 20, 43, 71	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	VAL	8.2
1	B	294	SER	7.7
1	B	296	GLY	7.5
1	B	354	ILE	6.8
1	A	86	THR	5.2
1	B	183	ALA	5.1
1	B	362	ASN	5.1
1	B	89	GLU	4.9
1	B	90	ASP	4.8
1	B	295	SER	4.7
1	B	361	HIS	4.5
1	B	390	PRO	4.3
1	B	314	VAL	4.3
1	B	130	ASP	4.2
1	B	389	HIS	3.8
1	A	294	SER	3.8
1	B	297	VAL	3.7
1	B	255	LYS	3.6
1	B	352	MET	3.6
1	B	363	ALA	3.6
1	B	349	GLU	3.4
1	B	92	LEU	3.4
1	A	362	ASN	3.3
1	B	181	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLU	3.2
1	A	295	SER	3.2
1	B	93	ALA	3.2
1	B	288	GLU	3.0
1	B	139	VAL	3.0
1	B	182	GLU	3.0
1	B	289	THR	2.9
1	A	296	GLY	2.9
1	B	98	ASP	2.9
1	B	199	ILE	2.9
1	B	168	VAL	2.8
1	B	345	ASP	2.7
1	B	132	LEU	2.7
1	B	196	ALA	2.7
1	B	123	HIS	2.7
1	A	168	VAL	2.6
1	B	97	GLU	2.6
1	B	353	GLU	2.6
1	A	411	PRO	2.5
1	B	244	GLU	2.5
1	A	353	GLU	2.5
1	A	293	THR	2.4
1	A	90	ASP	2.4
1	B	298	LEU	2.4
1	B	356	PRO	2.4
1	B	360	LYS	2.4
1	B	348	ARG	2.4
1	B	178	THR	2.3
1	B	253	THR	2.3
1	A	363	ALA	2.3
1	B	346	ARG	2.3
1	B	375	TYR	2.2
1	B	292	VAL	2.2
1	A	361	HIS	2.2
1	A	88	GLN	2.2
1	B	392	ALA	2.1
1	B	336	ILE	2.1
1	B	287	VAL	2.1
1	B	317	ALA	2.1
1	B	127	GLN	2.0
1	B	169	VAL	2.0
1	B	319	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	391	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

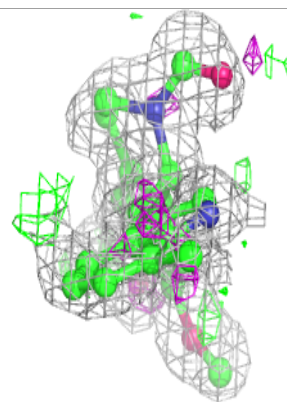
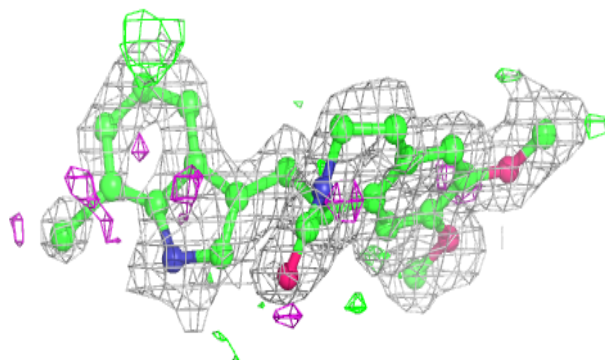
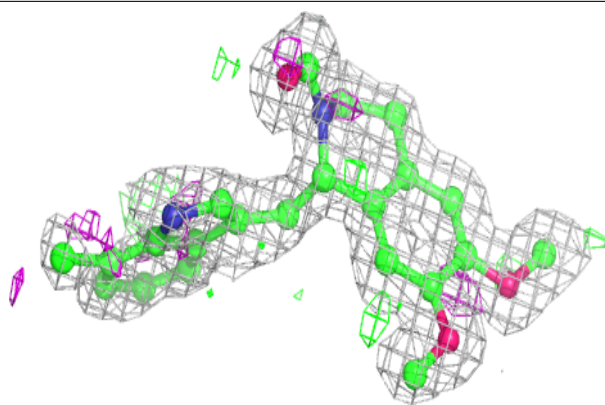
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	512	4/4	0.74	0.16	35,36,37,39	0
5	EDO	B	505	4/4	0.74	0.12	41,44,45,45	0
5	EDO	A	510	4/4	0.81	0.13	37,40,40,44	0
5	EDO	A	507	4/4	0.82	0.13	25,26,26,28	0
5	EDO	A	505	4/4	0.85	0.18	28,37,38,40	0
5	EDO	B	506	4/4	0.85	0.12	34,41,43,44	0
5	EDO	A	504	4/4	0.88	0.11	24,26,27,28	0
4	FTX	A	503	27/27	0.89	0.13	11,22,60,77	0
5	EDO	A	506	4/4	0.91	0.14	35,38,39,40	0
4	FTX	B	503	27/27	0.91	0.12	16,22,63,78	0
5	EDO	B	504	4/4	0.93	0.12	26,27,34,37	0
5	EDO	A	511	4/4	0.93	0.14	23,27,30,41	0
5	EDO	A	509	4/4	0.93	0.13	18,26,38,43	0
5	EDO	A	508	4/4	0.95	0.10	23,29,31,34	0
2	ZN	B	501	1/1	0.99	0.05	12,12,12,12	0
3	MG	B	502	1/1	0.99	0.10	7,7,7,7	0
3	MG	A	502	1/1	1.00	0.07	5,5,5,5	0
2	ZN	A	501	1/1	1.00	0.04	8,8,8,8	0

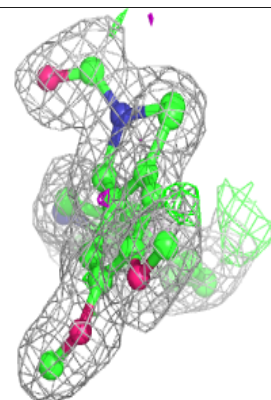
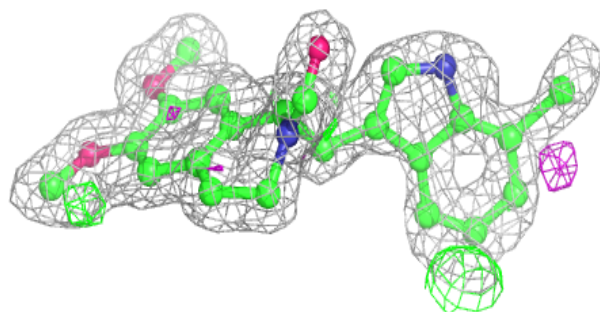
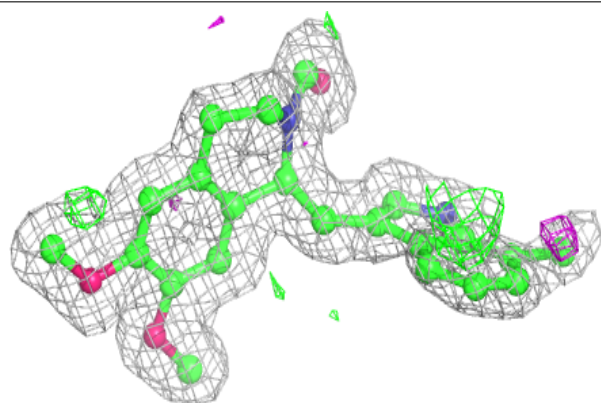
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FTX A 503:

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

**Electron density around FTX B 503:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.