



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:16 AM UTC

PDB ID : 6IMO / pdb\_00006imo  
Title : Crystal structure of PDE4D complexed with a novel inhibitor  
Authors : Zhang, X.L.; Su, H.X.; Xu, Y.C.  
Deposited on : 2018-10-23  
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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<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>.

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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)  
Xtrriage (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

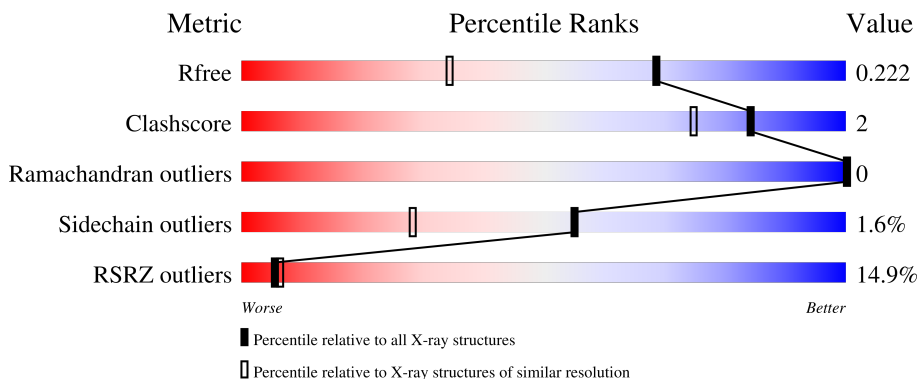
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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  $\geq 3$ , 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	
1	B	349	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 5637 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
			Total	C	N	O	S			
1	A	324	2591	1643	440	494	14	0	0	0
1	B	320	2522	1605	428	475	14	0	0	0

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

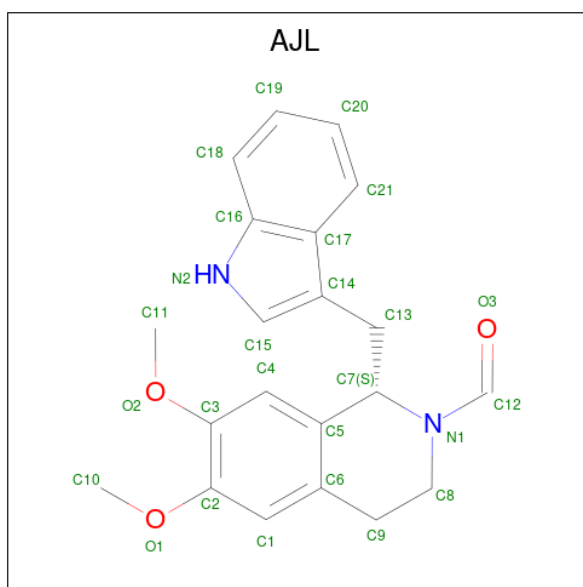
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is (1S)-1-[(1H-indol-3-yl)methyl]-6,7-dimethoxy-3,4-dihydroisoquinoline-2(1H)-carbaldehyde (CCD ID: AJL) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	A	1	26	21	2	3	0	0
4	B	1	26	21	2	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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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	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
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	244	Total O 244 244	0	0
6	B	175	Total O 175 175	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.55Å 80.48Å 163.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.27 – 1.55 29.27 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.27-1.55) 97.4 (29.27-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 1.55Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.206 , 0.225 0.207 , 0.222	Depositor DCC
$R_{free}$ test set	5439 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5637	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.14	36/2645 (1.4%)	0.70	1/3600 (0.0%)
1	B	1.71	77/2574 (3.0%)	1.01	12/3510 (0.3%)
All	All	1.45	113/5219 (2.2%)	0.87	13/7110 (0.2%)

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	ILE	C-O	-9.16	1.14	1.24
1	B	254	LYS	C-O	-8.61	1.14	1.24
1	A	312	ASN	C-O	-8.33	1.13	1.24
1	B	292	VAL	C-O	-8.18	1.14	1.23
1	B	165	ALA	C-O	-8.00	1.14	1.24
1	B	359	ASP	C-O	-7.96	1.14	1.23
1	B	364	SER	C-O	-7.96	1.14	1.23
1	A	352	MET	C-O	-7.87	1.13	1.23
1	B	276	HIS	C-O	-7.76	1.15	1.24
1	B	362	ASN	CA-CB	-7.72	1.45	1.53
1	A	314	VAL	C-O	-7.71	1.14	1.24
1	A	290	LYS	C-O	-7.70	1.14	1.23
1	B	110	ALA	C-O	-7.68	1.15	1.24
1	B	298	LEU	C-O	-7.64	1.14	1.23
1	B	175	LEU	C-O	-7.43	1.14	1.24
1	A	165	ALA	C-O	-7.33	1.15	1.24
1	A	280	LEU	C-O	-7.21	1.15	1.24
1	A	316	CYS	C-O	-7.16	1.15	1.24
1	B	196	ALA	C-O	-7.13	1.15	1.24
1	A	287	VAL	C-O	-7.06	1.16	1.24
1	B	171	SER	C-O	-7.05	1.16	1.24
1	B	100	ASN	C-O	-7.05	1.14	1.24
1	A	283	LEU	C-O	-7.03	1.15	1.24
1	A	197	SER	C-O	-7.00	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	ILE	C-O	-7.00	1.16	1.24
1	B	302	ASN	C-O	-7.00	1.14	1.23
1	A	169	VAL	C-O	-7.00	1.16	1.24
1	B	195	PHE	C-O	-6.92	1.15	1.24
1	B	200	HIS	C-O	-6.92	1.15	1.24
1	B	266	ASP	C-O	-6.91	1.16	1.24
1	A	298	LEU	C-O	-6.89	1.15	1.23
1	B	154	HIS	C-O	-6.87	1.15	1.24
1	A	167	ASP	C-O	-6.85	1.16	1.24
1	A	278	ASN	C-O	-6.84	1.16	1.24
1	B	137	ILE	C-O	-6.80	1.16	1.24
1	B	109	ILE	C-O	-6.73	1.16	1.24
1	B	133	LYS	C-O	-6.70	1.15	1.24
1	B	101	LYS	C-O	-6.66	1.15	1.24
1	B	174	VAL	C-O	-6.63	1.16	1.24
1	B	199	ILE	C-O	-6.58	1.15	1.24
1	B	155	ALA	C-O	-6.53	1.15	1.24
1	B	314	VAL	C-O	-6.48	1.15	1.24
1	A	364	SER	C-O	-6.46	1.16	1.23
1	B	169	VAL	C-O	-6.42	1.16	1.24
1	B	280	LEU	C-O	-6.38	1.16	1.24
1	B	315	HIS	C-O	-6.34	1.16	1.24
1	B	275	LYS	C-O	-6.31	1.15	1.23
1	A	359	ASP	C-O	-6.29	1.16	1.24
1	A	315	HIS	C-O	-6.28	1.16	1.24
1	B	145	TYR	C-O	-6.27	1.16	1.24
1	A	198	ALA	C-O	-6.27	1.16	1.24
1	A	406	TYR	C-O	-6.27	1.16	1.24
1	B	279	LEU	C-O	-6.26	1.16	1.24
1	B	106	VAL	C-O	-6.25	1.16	1.24
1	B	321	ASN	C-O	-6.21	1.18	1.24
1	A	313	MET	C-O	-6.19	1.17	1.24
1	B	246	CYS	C-O	-6.19	1.15	1.24
1	B	108	ARG	C-O	-6.13	1.16	1.24
1	A	410	ILE	C-O	-6.12	1.16	1.24
1	A	91	VAL	C-O	-6.08	1.17	1.24
1	A	93	ALA	C-O	-6.04	1.17	1.24
1	B	304	SER	C-O	-5.97	1.17	1.24
1	B	149	LEU	C-O	-5.96	1.17	1.24
1	B	319	LEU	C-O	-5.96	1.14	1.23
1	A	90	ASP	C-O	-5.96	1.17	1.24
1	A	355	SER	C-O	-5.95	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	HIS	C-O	-5.92	1.17	1.23
1	B	151	ASP	C-O	-5.91	1.16	1.24
1	B	388	VAL	N-CA	-5.88	1.37	1.46
1	B	389	HIS	CA-C	-5.87	1.46	1.53
1	B	310	LEU	C-O	-5.87	1.17	1.24
1	A	311	GLN	C-O	-5.87	1.17	1.24
1	B	172	THR	C-O	-5.83	1.17	1.24
1	B	126	PHE	C-O	-5.81	1.17	1.24
1	B	287	VAL	C-O	-5.78	1.17	1.24
1	A	405	TRP	C-O	-5.77	1.17	1.24
1	A	166	ALA	C-O	-5.74	1.17	1.24
1	B	278	ASN	C-O	-5.73	1.17	1.24
1	B	363	ALA	C-O	-5.68	1.16	1.23
1	B	256	GLN	CD-NE2	-5.66	1.21	1.33
1	A	282	ASP	C-O	-5.58	1.17	1.24
1	A	350	ARG	C-O	-5.56	1.16	1.24
1	A	358	CYS	C-O	-5.54	1.16	1.23
1	B	164	HIS	C-O	-5.54	1.17	1.24
1	A	170	GLN	C-O	-5.54	1.17	1.24
1	B	125	ILE	C-O	-5.53	1.17	1.24
1	B	318	ASP	CG-OD1	-5.50	1.15	1.25
1	B	185	PHE	C-O	-5.49	1.17	1.24
1	B	307	ILE	C-O	-5.41	1.17	1.24
1	B	306	ARG	C-O	-5.38	1.17	1.24
1	B	181	LEU	C-O	-5.37	1.16	1.24
1	B	311	GLN	C-O	-5.35	1.18	1.24
1	B	168	VAL	C-O	-5.34	1.17	1.24
1	B	281	ALA	C-O	-5.34	1.17	1.24
1	B	156	ASP	C-O	-5.34	1.17	1.24
1	B	283	LEU	N-CA	-5.33	1.39	1.46
1	B	357	MET	C-O	-5.33	1.14	1.24
1	B	316	CYS	C-O	-5.32	1.17	1.24
1	B	303	TYR	C-O	-5.32	1.17	1.24
1	B	362	ASN	N-CA	-5.28	1.38	1.46
1	B	143	ILE	C-O	-5.27	1.17	1.24
1	B	256	GLN	C-O	-5.27	1.17	1.24
1	A	312	ASN	CG-OD1	-5.20	1.13	1.23
1	B	244	GLU	C-O	-5.19	1.17	1.23
1	B	122	MET	C-O	-5.17	1.18	1.24
1	B	317	ALA	C-O	-5.17	1.18	1.24
1	A	407	GLN	C-O	-5.15	1.18	1.24
1	B	359	ASP	CG-OD2	-5.13	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	GLU	C-O	-5.11	1.17	1.23
1	B	289	THR	CA-C	-5.08	1.46	1.52
1	B	142	LEU	C-O	-5.05	1.18	1.24
1	A	284	LYS	C-O	-5.05	1.18	1.24
1	B	184	VAL	C-O	-5.03	1.17	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ILE	CA-C-N	10.76	131.20	119.90
1	B	137	ILE	C-N-CA	10.76	131.20	119.90
1	B	90	ASP	N-CA-C	-6.83	103.96	112.90
1	B	290	LYS	N-CA-C	6.24	119.28	110.23
1	B	393	GLN	N-CA-C	6.10	118.43	111.11
1	A	200	HIS	N-CA-C	5.96	119.65	112.38
1	B	289	THR	N-CA-CB	-5.61	102.44	110.80
1	B	106	VAL	N-CA-C	5.61	116.39	110.72
1	B	174	VAL	N-CA-C	5.51	116.24	110.62
1	B	301	ASP	CA-C-N	-5.35	113.50	122.92
1	B	301	ASP	C-N-CA	-5.35	113.50	122.92
1	B	200	HIS	N-CA-C	5.21	118.74	112.38
1	B	308	GLN	CB-CG-CD	5.12	121.30	112.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	2591	0	2519	14	0
1	B	2522	0	2433	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	0	0	0
5	A	32	0	48	3	0
5	B	16	0	24	0	0
6	A	244	0	0	2	0
6	B	175	0	0	1	0
All	All	5637	0	5024	23	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 (23) 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:293:THR:HG22	1:A:299:LEU:CD2	1.86	1.05
1:A:293:THR:HG22	1:A:299:LEU:HD23	1.03	1.02
1:A:293:THR:CG2	1:A:299:LEU:HD23	1.91	1.00
1:B:249:PHE:O	1:B:257:ARG:NH1	2.22	0.72
1:A:282:ASP:HB3	1:A:308:GLN:OE1	1.97	0.64
5:A:510:EDO:O1	5:A:511:EDO:O1	2.16	0.63
1:A:336:ILE:HG23	1:A:337:MET:HE3	1.87	0.56
1:A:293:THR:CG2	1:A:299:LEU:CD2	2.64	0.56
5:A:511:EDO:H11	6:A:702:HOH:O	2.11	0.50
1:A:358:CYS:SG	5:A:508:EDO:H12	2.53	0.48
1:B:292:VAL:HA	1:B:297:VAL:O	2.17	0.45
1:A:308:GLN:NE2	6:A:608:HOH:O	2.48	0.45
1:B:289:THR:O	1:B:289:THR:HG23	2.16	0.44
1:A:337:MET:HE1	1:A:340:PHE:CD2	2.53	0.44
1:B:286:MET:HE2	1:B:286:MET:HB2	1.91	0.44
1:A:348:ARG:HB2	1:A:354:ILE:HD11	2.02	0.42
1:A:299:LEU:HA	1:A:299:LEU:HD22	1.80	0.42
1:B:104:LEU:HD22	1:B:170:GLN:HG3	2.02	0.42
1:A:336:ILE:HG23	1:A:337:MET:CE	2.50	0.41
1:A:338:GLU:O	1:A:342:ARG:HG3	2.19	0.41
1:A:337:MET:CE	1:A:340:PHE:CD2	3.03	0.41
1:B:300:LEU:HD11	1:B:309:VAL:HG21	2.03	0.41
1:B:282:ASP:OD2	6:B:601:HOH:O	2.21	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	322/349 (92%)	318 (99%)	4 (1%)	0	100	100
1	B	316/349 (90%)	312 (99%)	4 (1%)	0	100	100
All	All	638/698 (91%)	630 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	287/318 (90%)	285 (99%)	2 (1%)	76	59
1	B	274/318 (86%)	267 (97%)	7 (3%)	40	13
All	All	561/636 (88%)	552 (98%)	9 (2%)	55	28

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	LEU
1	A	299	LEU
1	B	91	VAL
1	B	253	THR
1	B	258	GLN
1	B	286	MET
1	B	289	THR
1	B	308	GLN

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Mol	Chain	Res	Type
1	B	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	321	ASN
1	B	250	GLN
1	B	258	GLN
1	B	278	ASN
1	B	407	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 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	A	507	-	3,3,3	0.40	0	2,2,2	0.57	0
4	AJL	A	504	-	29,29,29	0.44	0	36,41,41	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	511	-	3,3,3	0.46	0	2,2,2	0.51	0
5	EDO	A	508	-	3,3,3	0.40	0	2,2,2	0.77	0
5	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.43	0
5	EDO	B	506	-	3,3,3	0.42	0	2,2,2	0.50	0
5	EDO	B	507	-	3,3,3	0.40	0	2,2,2	0.70	0
4	AJL	B	503	-	29,29,29	0.42	0	36,41,41	0.58	0
5	EDO	A	505	-	3,3,3	0.39	0	2,2,2	0.71	0
5	EDO	A	509	-	3,3,3	0.39	0	2,2,2	0.50	0
5	EDO	A	506	-	3,3,3	0.36	0	2,2,2	0.55	0
5	EDO	A	512	-	3,3,3	0.43	0	2,2,2	0.75	0
5	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.51	0
5	EDO	A	510	-	3,3,3	0.41	0	2,2,2	0.58	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	A	507	-	-	1/1/1/1	-
4	AJL	A	504	-	-	2/10/23/23	0/4/4/4
5	EDO	A	511	-	-	0/1/1/1	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
5	EDO	B	506	-	-	0/1/1/1	-
5	EDO	B	507	-	-	1/1/1/1	-
4	AJL	B	503	-	-	2/10/23/23	0/4/4/4
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	A	512	-	-	1/1/1/1	-
5	EDO	B	504	-	-	0/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	AJL	C14-C13-C7-N1

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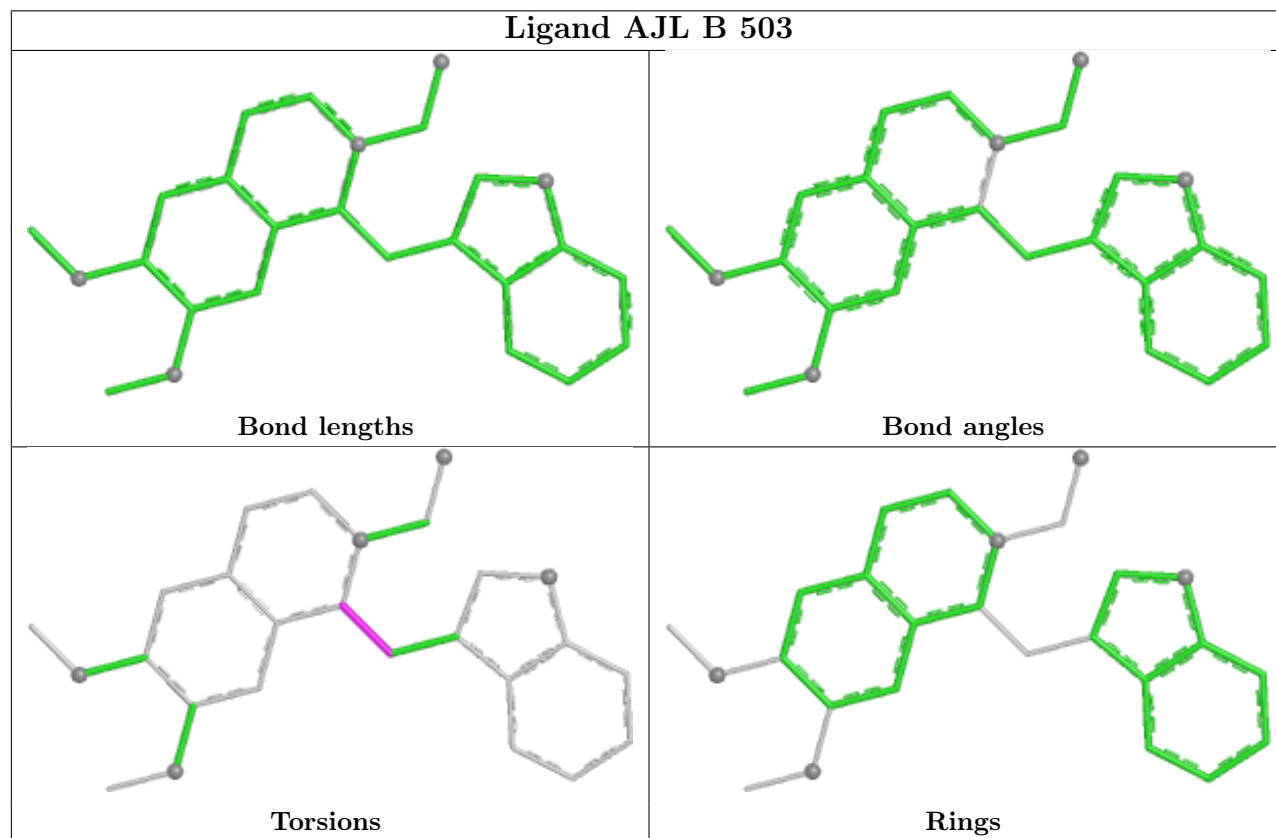
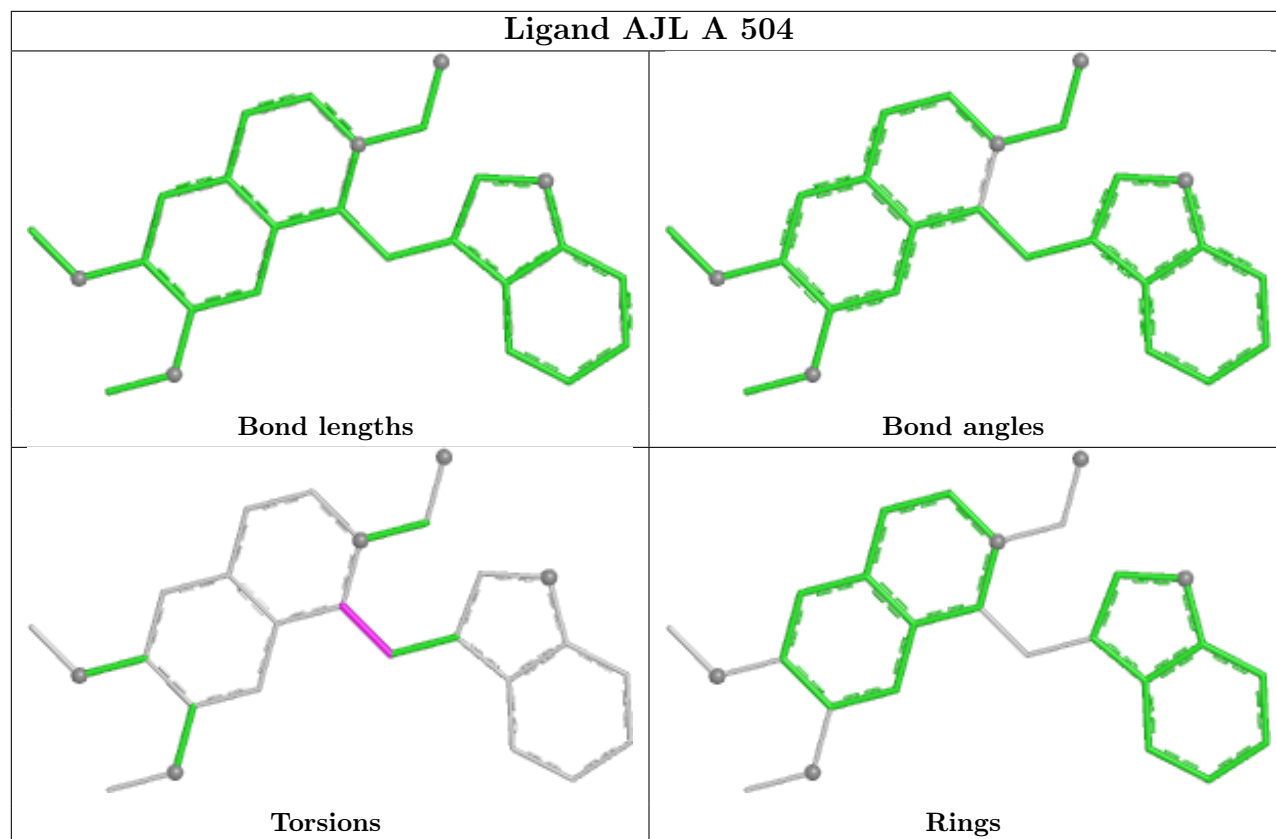
Mol	Chain	Res	Type	Atoms
5	A	510	EDO	O1-C1-C2-O2
4	A	504	AJL	C14-C13-C7-C5
4	B	503	AJL	C14-C13-C7-C5
4	A	504	AJL	C14-C13-C7-N1
5	A	512	EDO	O1-C1-C2-O2
5	A	507	EDO	O1-C1-C2-O2
5	B	507	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	511	EDO	2	0
5	A	508	EDO	1	0
5	A	510	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	324/349 (92%)	0.33	21 (6%) 25 29	5, 15, 30, 46	0
1	B	320/349 (91%)	1.18	75 (23%) 2 2	8, 21, 35, 52	0
All	All	644/698 (92%)	0.75	96 (14%) 5 6	5, 18, 34, 52	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	VAL	5.2
1	B	93	ALA	4.8
1	A	292	VAL	4.6
1	B	390	PRO	4.6
1	B	91	VAL	4.6
1	B	183	ALA	4.6
1	B	392	ALA	4.5
1	B	292	VAL	4.4
1	B	298	LEU	4.3
1	B	293	THR	4.3
1	A	296	GLY	4.2
1	B	354	ILE	3.8
1	B	131	LEU	3.8
1	B	289	THR	3.7
1	B	89	GLU	3.6
1	B	90	ASP	3.6
1	B	184	VAL	3.6
1	B	179	PRO	3.5
1	B	92	LEU	3.5
1	B	130	ASP	3.5
1	B	362	ASN	3.4
1	A	349	GLU	3.3
1	B	186	THR	3.3
1	B	181	LEU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	410	ILE	3.3
1	B	178	THR	3.3
1	B	96	LEU	3.2
1	A	294	SER	3.2
1	A	293	THR	3.2
1	B	253	THR	3.2
1	B	127	GLN	3.1
1	B	139	VAL	3.1
1	B	388	VAL	3.1
1	B	132	LEU	3.1
1	B	99	VAL	3.0
1	B	387	LEU	3.0
1	A	362	ASN	2.9
1	B	112	LEU	2.9
1	B	361	HIS	2.9
1	A	299	LEU	2.9
1	A	295	SER	2.9
1	B	396	LEU	2.9
1	A	363	ALA	2.8
1	B	395	ILE	2.8
1	B	391	ASP	2.8
1	B	287	VAL	2.8
1	B	134	THR	2.8
1	A	411	PRO	2.8
1	B	389	HIS	2.8
1	B	353	GLU	2.7
1	B	137	ILE	2.7
1	B	135	PHE	2.7
1	B	286	MET	2.7
1	A	353	GLU	2.7
1	B	182	GLU	2.6
1	B	102	TRP	2.6
1	B	98	ASP	2.6
1	B	126	PHE	2.5
1	B	141	THR	2.5
1	A	354	ILE	2.5
1	A	389	HIS	2.5
1	A	351	GLY	2.5
1	B	187	ASP	2.5
1	B	185	PHE	2.5
1	B	180	ALA	2.4
1	B	363	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	288	GLU	2.4
1	B	143	ILE	2.4
1	B	300	LEU	2.4
1	B	281	ALA	2.4
1	A	298	LEU	2.4
1	B	385	ALA	2.4
1	B	386	ASP	2.4
1	B	411	PRO	2.4
1	B	375	TYR	2.4
1	B	140	ASP	2.3
1	B	188	LEU	2.3
1	B	303	TYR	2.3
1	B	133	LYS	2.3
1	B	282	ASP	2.2
1	B	351	GLY	2.2
1	A	297	VAL	2.2
1	B	190	ILE	2.2
1	A	409	THR	2.2
1	B	176	LEU	2.2
1	B	97	GLU	2.2
1	B	384	TRP	2.2
1	B	304	SER	2.1
1	B	120	VAL	2.1
1	B	350	ARG	2.1
1	B	345	ASP	2.1
1	A	375	TYR	2.0
1	A	301	ASP	2.0
1	B	177	SER	2.0
1	A	90	ASP	2.0
1	B	216	ASN	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 oligosaccharides in this entry.

## 6.4 Ligands

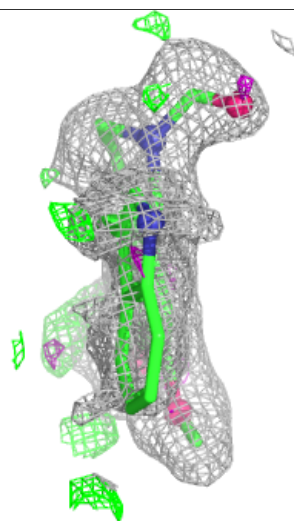
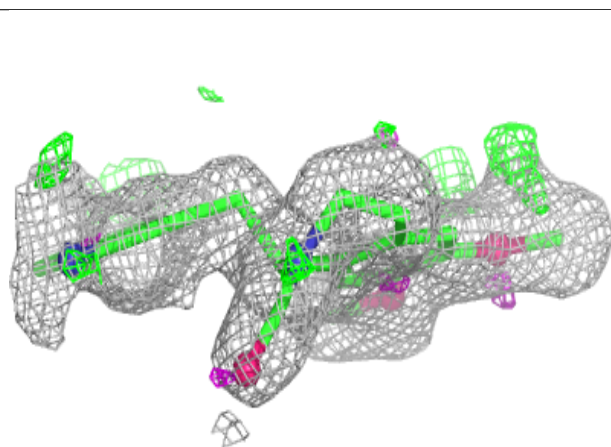
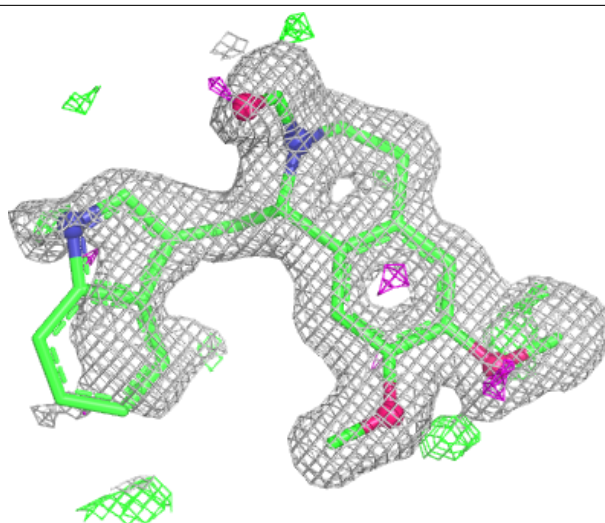
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

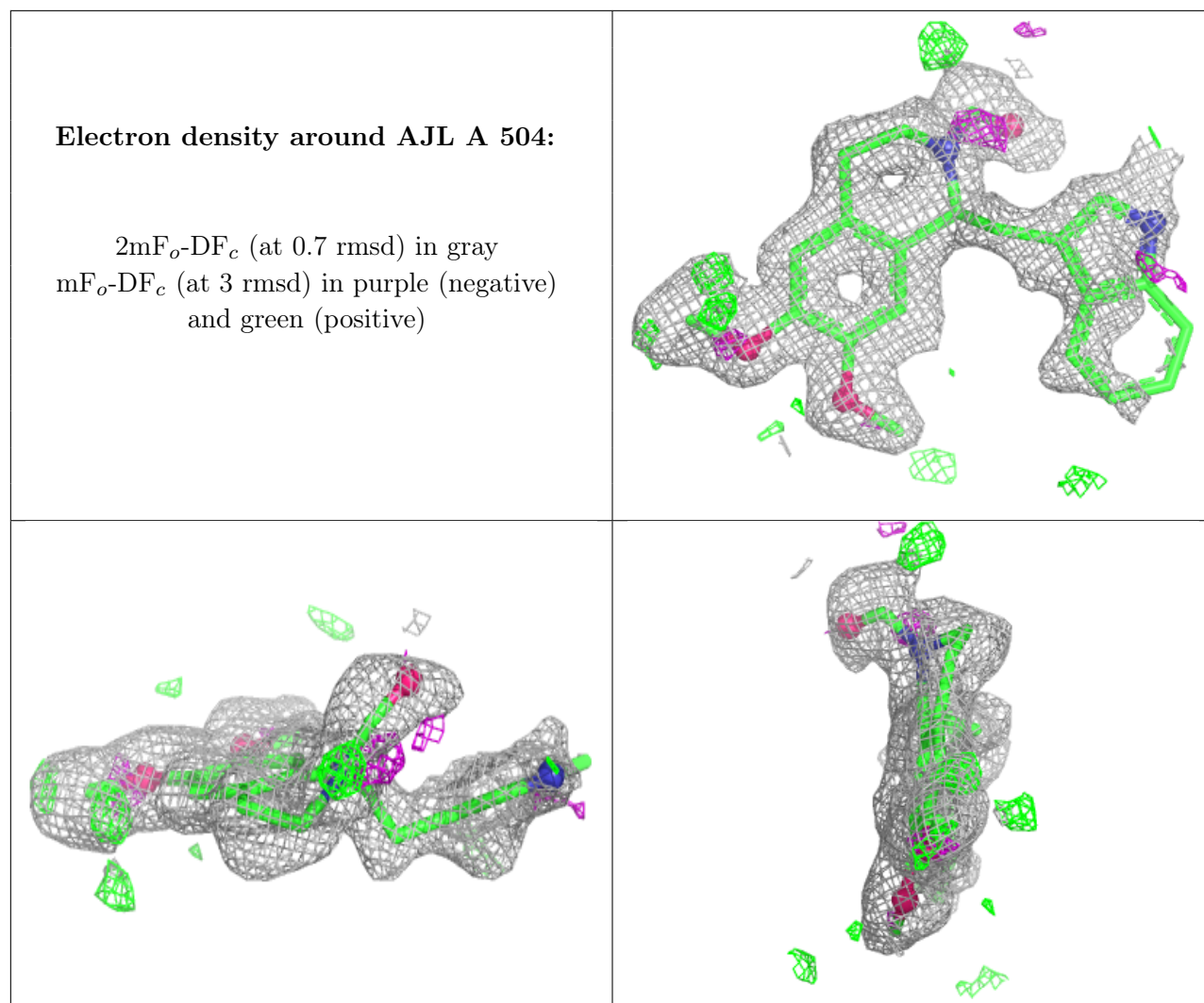
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	B	507	4/4	0.73	0.21	29,32,32,32	0
5	EDO	A	512	4/4	0.75	0.21	24,25,29,31	0
5	EDO	A	508	4/4	0.75	0.17	25,26,34,37	0
5	EDO	A	507	4/4	0.79	0.16	20,22,27,27	0
5	EDO	A	505	4/4	0.83	0.18	22,23,24,30	0
5	EDO	B	504	4/4	0.84	0.14	24,27,30,31	0
5	EDO	A	510	4/4	0.84	0.16	23,32,36,37	0
5	EDO	B	506	4/4	0.85	0.17	26,27,29,30	0
5	EDO	A	511	4/4	0.85	0.17	20,23,23,34	0
4	AJL	B	503	26/26	0.87	0.15	20,24,55,58	0
4	AJL	A	504	26/26	0.88	0.14	17,24,52,55	0
5	EDO	A	509	4/4	0.91	0.15	17,21,23,23	0
5	EDO	A	506	4/4	0.92	0.10	20,20,21,22	0
5	EDO	B	505	4/4	0.93	0.08	21,21,26,26	0
3	MG	A	503	1/1	0.97	0.12	15,15,15,15	0
2	ZN	B	501	1/1	0.99	0.05	12,12,12,12	0
3	MG	B	502	1/1	0.99	0.02	7,7,7,7	0
2	ZN	A	501	1/1	1.00	0.03	9,9,9,9	0
3	MG	A	502	1/1	1.00	0.02	6,6,6,6	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 AJL 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 [i](#)

There are no such residues in this entry.