



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:16 AM UTC

PDB ID : 8K4C / pdb_00008k4c
Title : Crystal structure of PDE4D complexed with ethaverine hydrochloride
Authors : Liu, J.Y.; Li, M.J.; Xu, Y.C.
Deposited on : 2023-07-17
Resolution : 2.10 Å(reported)

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

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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

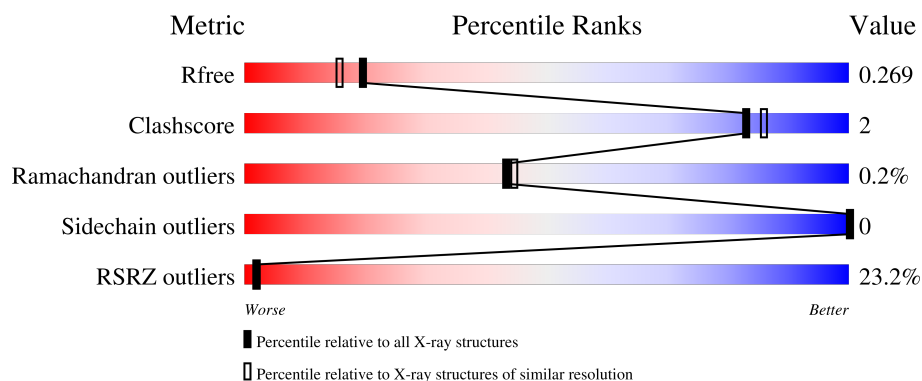
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	8% 91% 7%
1	B	349	35% 82% 10% 8%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5304 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	1	0
			2599	1647	440	497	15			
1	B	321	Total	C	N	O	S	0	1	0
			2527	1602	434	476	15			

There are 42 discrepancies between the modelled and reference sequences:

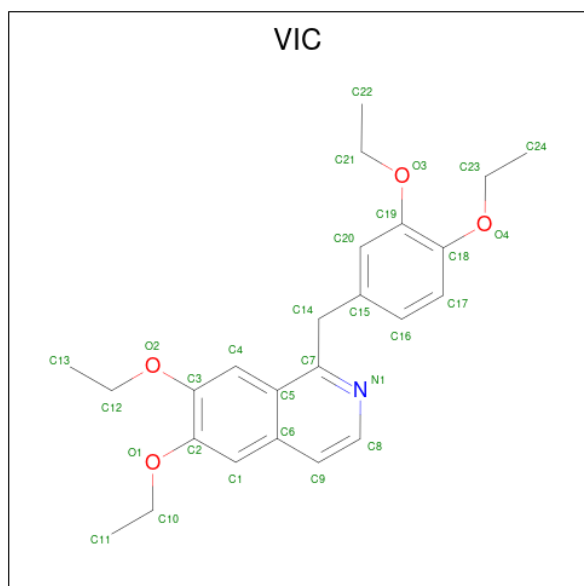
Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	expression tag	UNP Q08499
A	66	GLY	-	expression tag	UNP Q08499
A	67	SER	-	expression tag	UNP Q08499
A	68	SER	-	expression tag	UNP Q08499
A	69	HIS	-	expression tag	UNP Q08499
A	70	HIS	-	expression tag	UNP Q08499
A	71	HIS	-	expression tag	UNP Q08499
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 1-[(3,4-diethoxyphenyl)methyl]-6,7-diethoxy-isoquinoline (CCD ID: VIC) (formula: C₂₄H₂₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	24	1	4		
2	B	1	Total	C	N	O	0	0
			29	24	1	4		

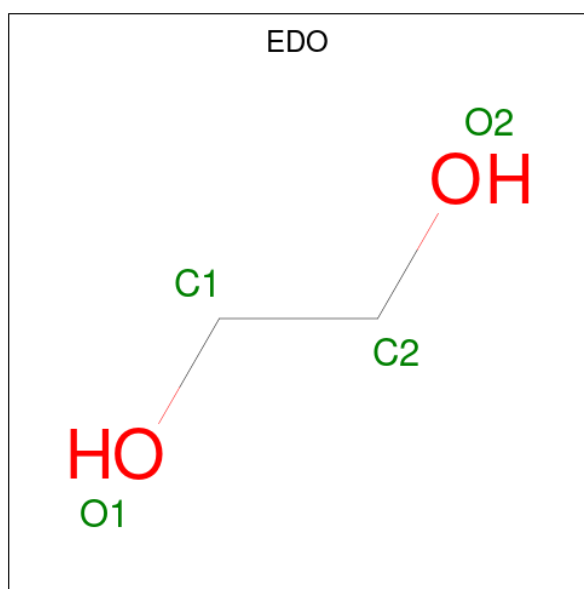
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

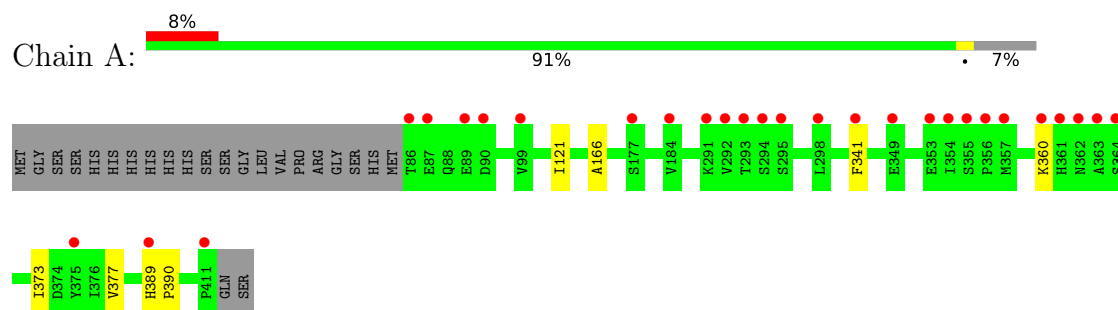
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	76	Total	O	0	0
			76	76		
6	B	36	Total	O	0	0
			36	36		

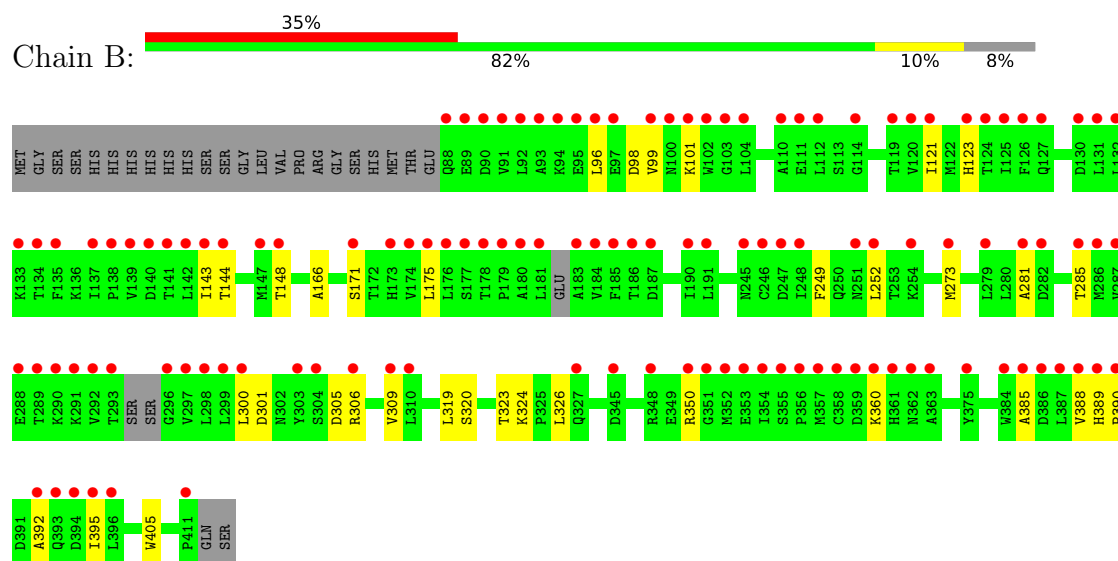
3 Residue-property plots [i](#)

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



- 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	57.69Å 79.86Å 162.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 2.10 39.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.93-2.10) 99.9 (39.93-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660)	Depositor
R, R_{free}	0.235 , 0.269 0.236 , 0.269	Depositor DCC
R_{free} test set	2208 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5304	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: VIC, ZN, EDO, MG

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	0.08	0/2653	0.28	0/3614
1	B	0.15	0/2579	0.30	0/3514
All	All	0.12	0/5232	0.29	0/7128

There are no bond length outliers.

There are no bond angle outliers.

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	2599	0	2512	4	0
1	B	2527	0	2404	20	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	6	0	0
6	A	76	0	0	0	0
6	B	36	0	0	0	0
All	All	5304	0	4922	24	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 (24) 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:B:281:ALA:O	1:B:285:THR:HG23	2.02	0.58
1:B:273:MET:HE1	1:B:319:LEU:HD11	1.87	0.57
1:B:249:PHE:HB3	1:B:252:LEU:HD12	1.86	0.57
1:B:98:ASP:HB3	1:B:101:LYS:HG3	1.89	0.54
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.90	0.53
1:B:123:HIS:ND1	1:B:143:ILE:HD11	2.27	0.50
1:B:96:LEU:O	1:B:99:VAL:HG13	2.13	0.49
1:B:301:ASP:C	1:B:306:ARG:HH12	2.21	0.48
1:A:341:PHE:CG	1:A:360:LYS:HB3	2.49	0.48
1:A:373:ILE:HA	1:A:377:VAL:HB	1.97	0.47
1:B:249:PHE:CB	1:B:252:LEU:HD12	2.45	0.47
1:B:323:THR:HB	1:B:395:ILE:HG23	2.00	0.44
1:B:350:ARG:HG3	1:B:350:ARG:HH11	1.83	0.43
1:B:388:VAL:O	1:B:388:VAL:HG23	2.18	0.43
1:B:385:ALA:HA	1:B:392:ALA:HB3	2.02	0.42
1:A:389:HIS:HA	1:A:390:PRO:HA	1.88	0.42
1:B:171:SER:O	1:B:175:LEU:HG	2.19	0.41
1:B:326:LEU:HD21	1:B:405:TRP:CD2	2.56	0.41
1:B:300:LEU:HD11	1:B:309:VAL:HG21	2.02	0.41
1:B:300:LEU:HD22	1:B:305:ASP:HB3	2.02	0.41
1:B:144:THR:O	1:B:148:THR:HG22	2.21	0.41
1:B:320:SER:O	1:B:324:LYS:HG2	2.21	0.40
1:B:389:HIS:HA	1:B:390:PRO:HA	1.85	0.40
1:A:121:ILE:HD12	1:A:166:ALA:HB1	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	325/349 (93%)	316 (97%)	9 (3%)	0	100	100
1	B	316/349 (90%)	307 (97%)	8 (2%)	1 (0%)	36	36
All	All	641/698 (92%)	623 (97%)	17 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	360	LYS

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	287/318 (90%)	287 (100%)	0	100	100
1	B	270/318 (85%)	270 (100%)	0	100	100
All	All	557/636 (88%)	557 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	210	GLN
1	A	312	ASN
1	A	361	HIS
1	B	210	GLN
1	B	302	ASN
1	B	312	ASN
1	B	331	GLN
1	B	389	HIS

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	704	-	3,3,3	0.42	0	2,2,2	0.41	0
2	VIC	B	501	-	30,31,31	0.88	1 (3%)	38,41,41	0.66	0
2	VIC	A	701	-	30,31,31	0.86	1 (3%)	38,41,41	0.68	1 (2%)

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	704	-	-	0/1/1/1	-
2	VIC	B	501	-	-	4/16/16/16	0/3/3/3
2	VIC	A	701	-	-	1/16/16/16	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	VIC	C7-N1	4.12	1.34	1.32
2	A	701	VIC	C7-N1	3.99	1.34	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	VIC	C7-C5-C6	2.47	118.96	117.77

There are no chirality outliers.

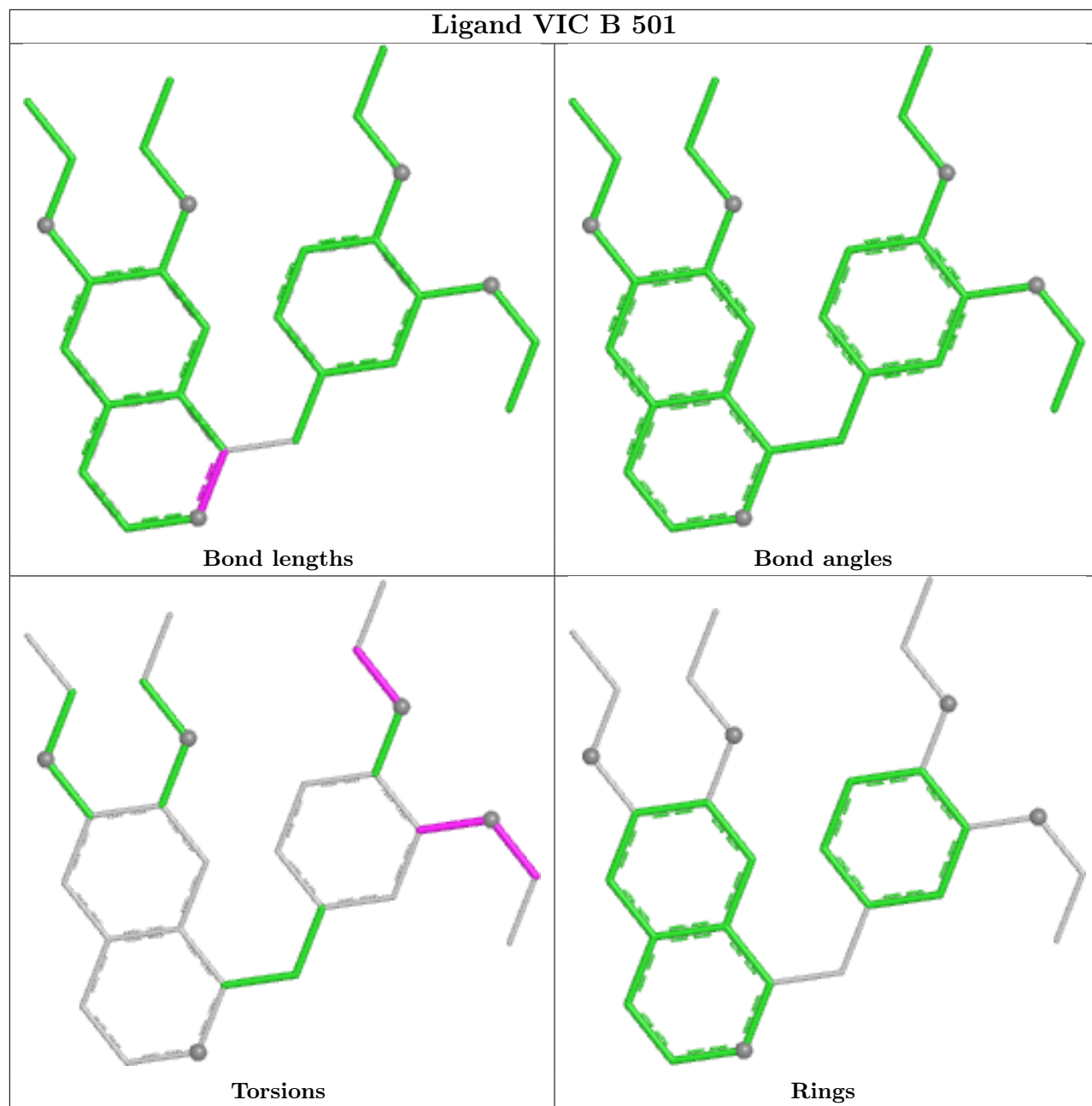
All (5) torsion outliers are listed below:

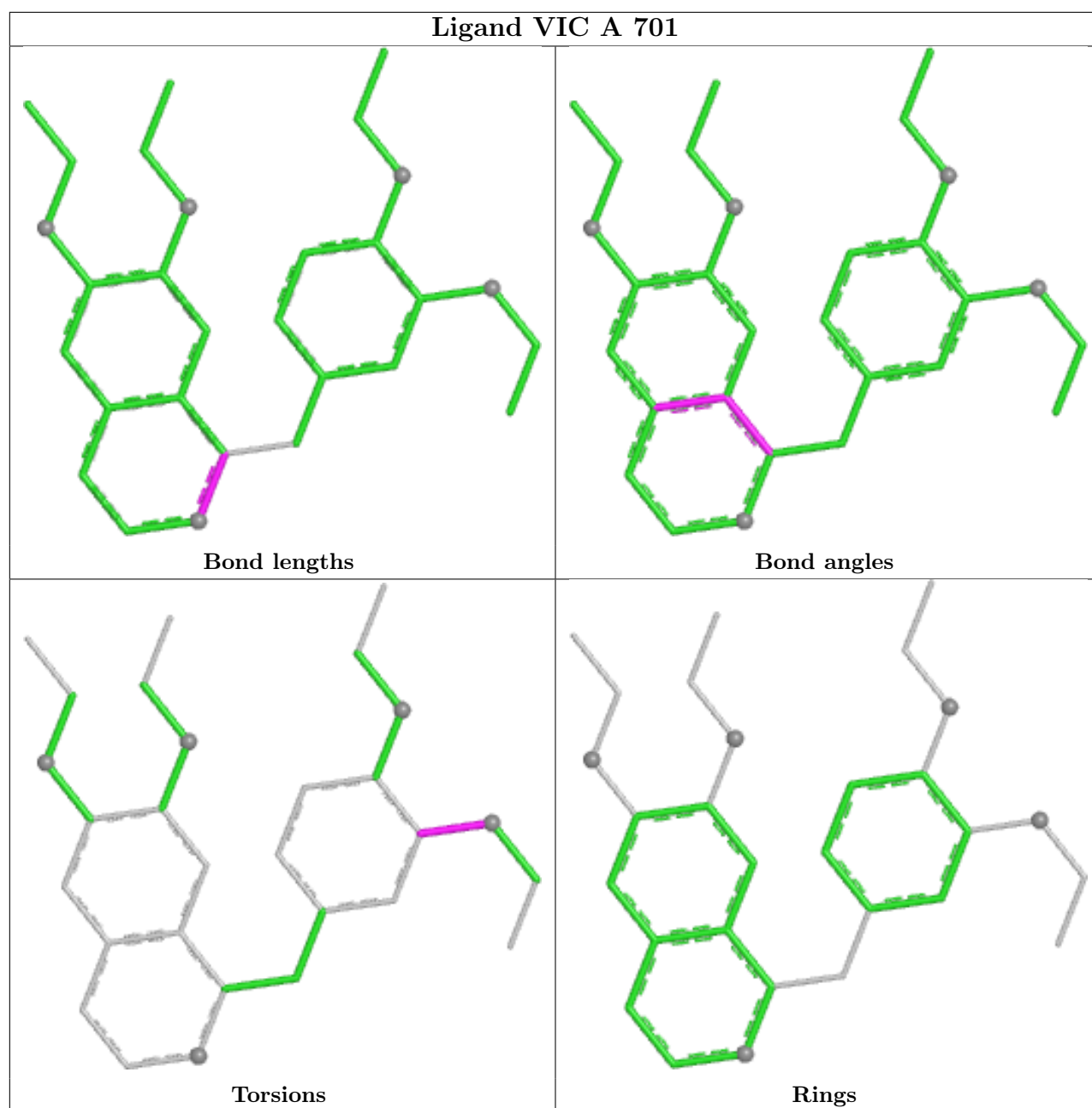
Mol	Chain	Res	Type	Atoms
2	B	501	VIC	C22-C21-O3-C19
2	B	501	VIC	C24-C23-O4-C18
2	B	501	VIC	C20-C19-O3-C21
2	B	501	VIC	C18-C19-O3-C21
2	A	701	VIC	C18-C19-O3-C21

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	326/349 (93%)	0.51	28 (8%) 16 17	14, 30, 57, 84	1 (0%)
1	B	321/349 (91%)	1.67	122 (38%) 1 1	13, 46, 76, 125	1 (0%)
All	All	647/698 (92%)	1.08	150 (23%) 2 2	13, 36, 71, 125	2 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	LEU	6.4
1	B	354	ILE	5.7
1	B	88	GLN	5.7
1	B	183	ALA	5.5
1	B	184	VAL	5.4
1	B	130	ASP	5.2
1	B	297	VAL	4.9
1	A	363	ALA	4.7
1	B	356	PRO	4.6
1	B	124	THR	4.6
1	B	246	CYS	4.6
1	B	92	LEU	4.5
1	B	361	HIS	4.5
1	A	86	THR	4.5
1	B	181	LEU	4.5
1	B	363	ALA	4.4
1	B	142	LEU	4.4
1	B	387	LEU	4.4
1	B	89	GLU	4.3
1	B	355	SER	4.3
1	B	91	VAL	4.2
1	B	390	PRO	4.1
1	B	298	LEU	4.1
1	B	176	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	289	THR	4.0
1	B	139	VAL	3.9
1	B	353	GLU	3.9
1	B	293	THR	3.9
1	B	393	GLN	3.8
1	B	296	GLY	3.8
1	B	93	ALA	3.7
1	B	125	ILE	3.6
1	B	102	TRP	3.6
1	B	177	SER	3.6
1	B	357	MET	3.6
1	B	99	VAL	3.5
1	B	131	LEU	3.5
1	B	179	PRO	3.5
1	B	135	PHE	3.5
1	B	96	LEU	3.5
1	B	411	PRO	3.4
1	B	285	THR	3.4
1	B	292	VAL	3.4
1	B	97	GLU	3.4
1	B	351	GLY	3.4
1	A	357	MET	3.4
1	A	294	SER	3.3
1	A	292	VAL	3.3
1	A	362	ASN	3.3
1	A	293	THR	3.3
1	B	137	ILE	3.3
1	A	298	LEU	3.3
1	A	87	GLU	3.2
1	B	385	ALA	3.2
1	A	361	HIS	3.2
1	B	186	THR	3.2
1	B	94	LYS	3.2
1	B	112	LEU	3.1
1	A	295	SER	3.1
1	B	358	CYS	3.1
1	A	355	SER	3.1
1	B	287	VAL	3.0
1	B	143	ILE	3.0
1	B	304	SER	3.0
1	B	147	MET	3.0
1	B	350	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	104	LEU	3.0
1	B	127	GLN	2.9
1	B	392	ALA	2.9
1	B	120	VAL	2.9
1	B	245	ASN	2.9
1	B	133	LYS	2.9
1	B	178	THR	2.9
1	B	288	GLU	2.8
1	A	375	TYR	2.8
1	B	180	ALA	2.7
1	B	327	GLN	2.7
1	B	352	MET	2.7
1	B	190	ILE	2.7
1	B	281	ALA	2.7
1	B	286	MET	2.7
1	B	375	TYR	2.7
1	B	90	ASP	2.7
1	B	386	ASP	2.7
1	B	148	THR	2.6
1	B	388	VAL	2.6
1	B	140	ASP	2.6
1	B	360	LYS	2.6
1	B	123	HIS	2.6
1	B	171	SER	2.6
1	B	141	THR	2.6
1	B	395	ILE	2.5
1	A	360	LYS	2.5
1	A	364	SER	2.5
1	A	99	VAL	2.5
1	B	248	ILE	2.5
1	B	254	LYS	2.5
1	B	138	PRO	2.5
1	B	134	THR	2.5
1	B	396	LEU	2.5
1	B	103	GLY	2.5
1	B	251	ASN	2.5
1	A	90	ASP	2.4
1	B	389	HIS	2.4
1	B	362	ASN	2.4
1	A	354	ILE	2.4
1	B	384	TRP	2.4
1	A	356	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	282	ASP	2.4
1	B	273	MET	2.4
1	B	290	LYS	2.4
1	B	110	ALA	2.3
1	B	300	LEU	2.3
1	A	291	LYS	2.3
1	B	185	PHE	2.3
1	B	252	LEU	2.3
1	B	95	GLU	2.3
1	A	184	VAL	2.3
1	B	309	VAL	2.3
1	A	411	PRO	2.3
1	B	306	ARG	2.3
1	B	121	ILE	2.2
1	B	101	LYS	2.2
1	B	291	LYS	2.2
1	B	144	THR	2.2
1	B	187	ASP	2.2
1	B	345	ASP	2.2
1	A	389	HIS	2.2
1	B	175	LEU	2.2
1	B	191	LEU	2.2
1	B	348	ARG	2.2
1	B	303	TYR	2.2
1	B	394	ASP	2.2
1	B	279	LEU	2.1
1	B	299	LEU	2.1
1	A	177	SER	2.1
1	A	353	GLU	2.1
1	B	111	GLU	2.1
1	B	174	VAL	2.1
1	A	349	GLU	2.1
1	B	359	ASP	2.1
1	A	341	PHE	2.1
1	B	126	PHE	2.1
1	B	100	ASN	2.0
1	B	119	THR	2.0
1	A	89	GLU	2.0
1	B	310	LEU	2.0
1	B	247	ASP	2.0
1	B	173	HIS	2.0
1	B	114	GLY	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 [i](#)

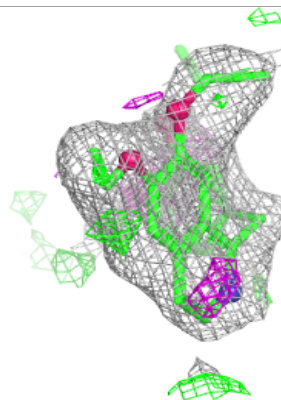
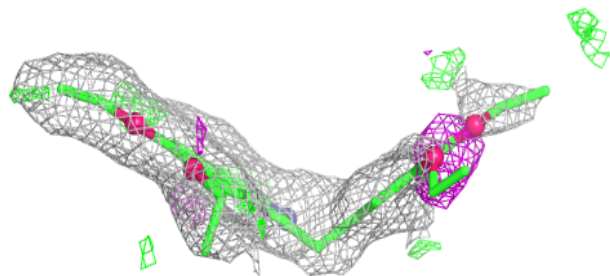
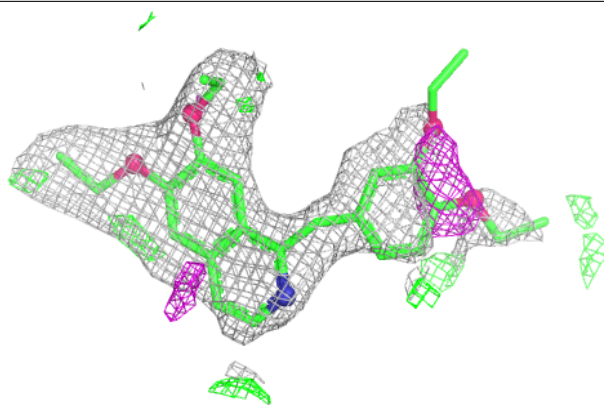
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VIC	A	701	29/29	0.72	0.20	37,44,55,56	0
2	VIC	B	501	29/29	0.78	0.19	37,49,61,62	0
5	EDO	A	704	4/4	0.85	0.15	37,37,38,38	0
3	MG	B	502	1/1	0.96	0.06	23,23,23,23	0
3	MG	A	702	1/1	0.96	0.03	19,19,19,19	0
4	ZN	B	503	1/1	1.00	0.03	31,31,31,31	0
4	ZN	A	703	1/1	1.00	0.02	20,20,20,20	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.

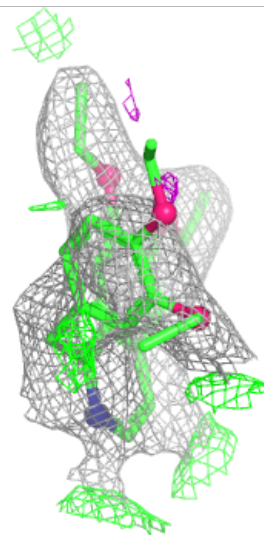
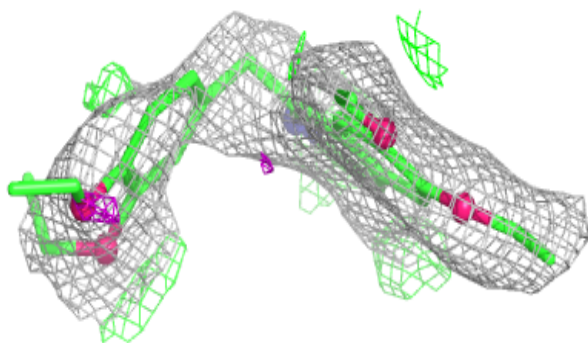
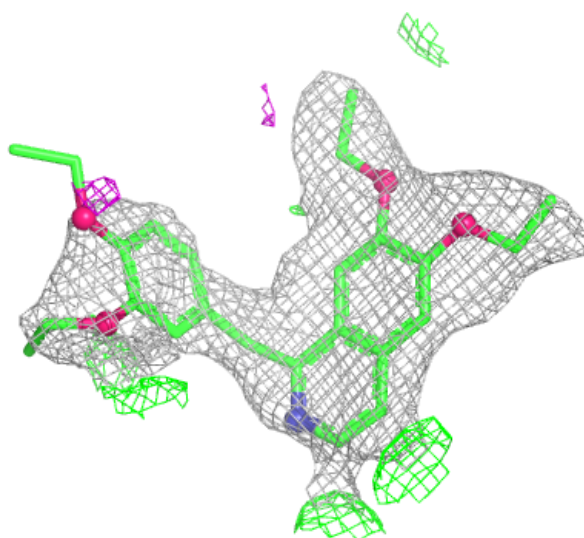
Electron density around VIC A 701:

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



Electron density around VIC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.