



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:30 PM UTC

PDB ID : 8W4Q / pdb_00008w4q
Title : Crystal structure of PDE4D complexed with CX-4945
Authors : Liu, J.Y.; Li, M.J.; Xu, Y.C.
Deposited on : 2023-08-24
Resolution : 1.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

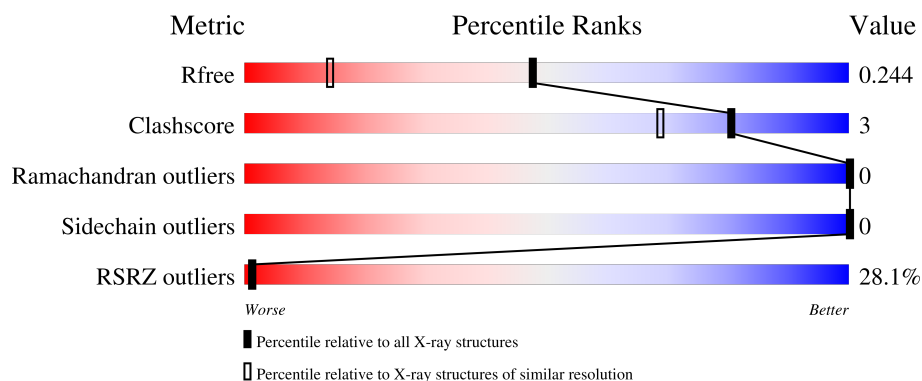
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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 ≥ 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	10% 89% 7%
1	B	349	42% 84% 9% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5299 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	324	Total	C	N	O	S	0	0	0
			2585	1640	440	491	14			
1	B	324	Total	C	N	O	S	0	0	0
			2527	1603	431	480	13			

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

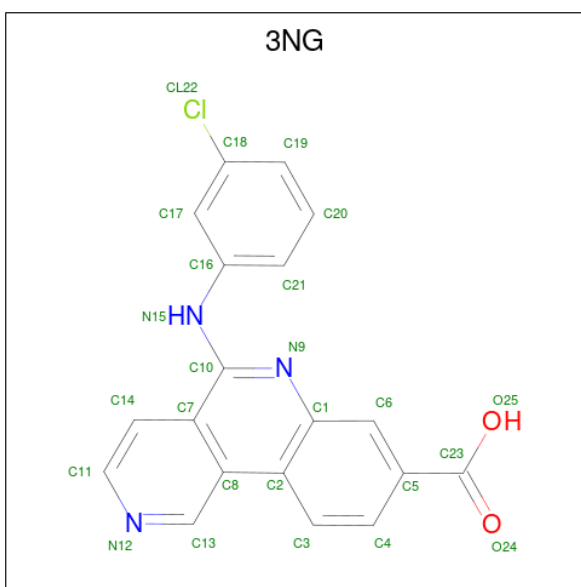
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

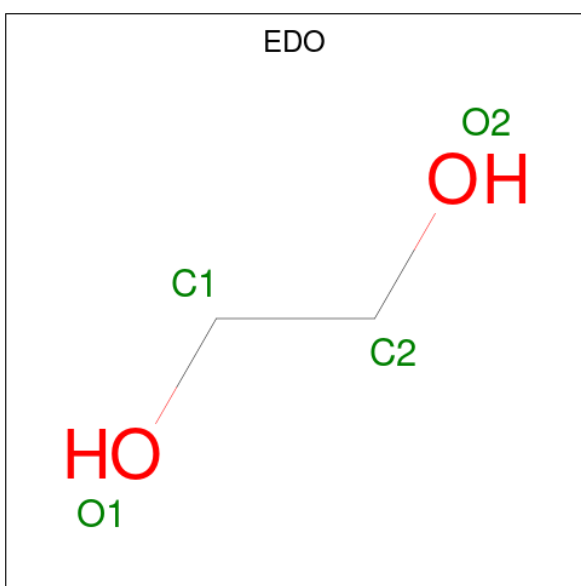
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is 5-[(3-chlorophenyl)amino]benzo[c][2,6]naphthyridine-8-carboxylic acid (CCD ID: 3NG) (formula: C₁₉H₁₂ClN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 25	C 19	Cl 1	N 3	O 2	0	0
4	B	1	Total 25	C 19	Cl 1	N 3	O 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

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

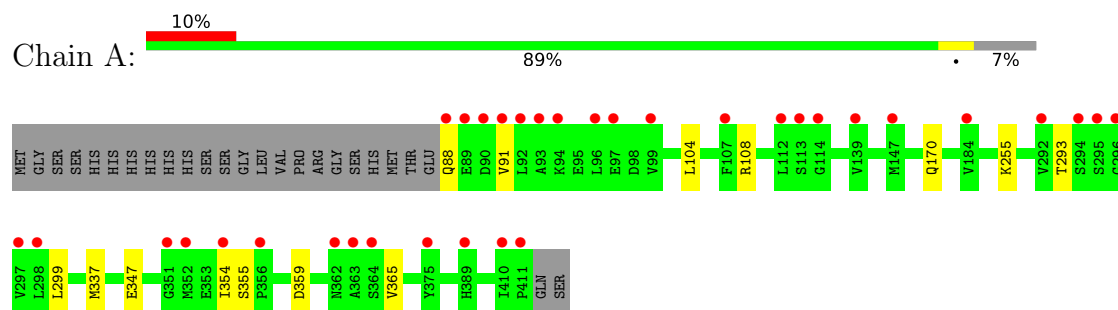
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total 64	O 64	0	0
6	B	45	Total 45	O 45	0	0

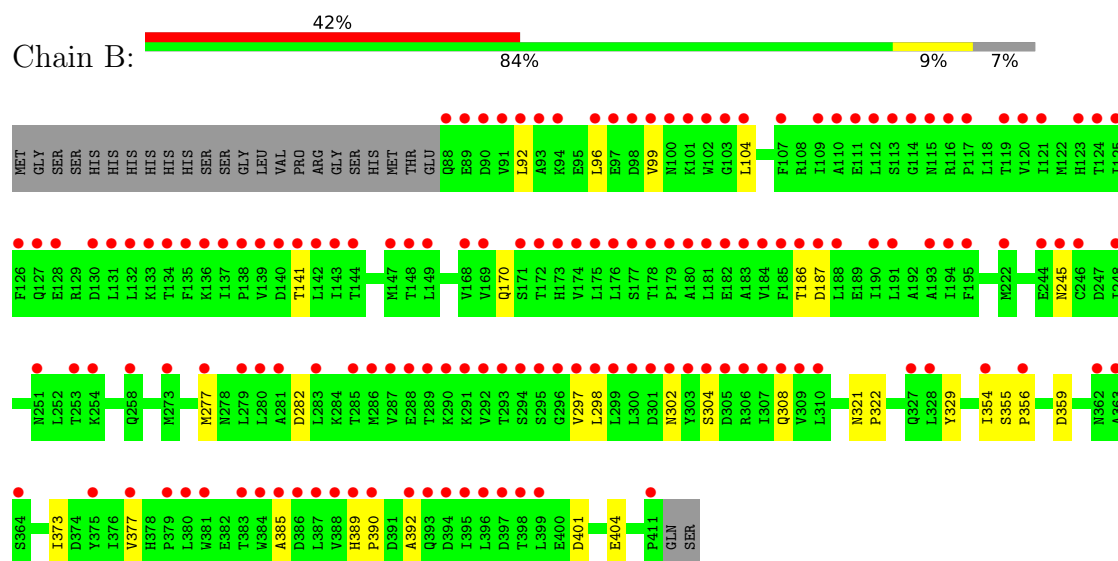
3 Residue-property plots [i](#)

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: 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	57.51Å 79.99Å 162.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.32 – 1.55 28.32 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.7 (28.32-1.55) 95.7 (28.32-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.226 , 0.240 0.228 , 0.244	Depositor DCC
R_{free} test set	5232 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.2	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	0.95	EDS
Total number of atoms	5299	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: MG, EDO, ZN, 3NG

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	0.23	0/2639	0.43	0/3592
1	B	0.20	0/2581	0.41	0/3526
All	All	0.22	0/5220	0.42	0/7118

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 [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	2585	0	2520	7	1
1	B	2527	0	2404	18	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	25	0	11	0	0
4	B	25	0	11	1	0
5	A	12	0	18	0	0
5	B	12	0	18	3	0
6	A	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	45	0	0	0	0
All	All	5299	0	4982	26	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 (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:B:92:LEU:O	1:B:96:LEU:HG	2.01	0.60
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.86	0.57
4:B:503:3NG:N9	4:B:503:3NG:H21	2.22	0.55
1:B:186:THR:HG22	1:B:187:ASP:H	1.75	0.52
1:A:293:THR:HG22	1:A:299:LEU:HG	1.92	0.51
1:B:302:ASN:HD22	1:B:304:SER:HB3	1.76	0.51
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.92	0.50
1:B:277:MET:HE2	1:B:277:MET:HA	1.94	0.48
1:B:355:SER:HB3	5:B:504:EDO:H12	1.96	0.47
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.97	0.47
1:A:337:MET:HE2	1:A:365:VAL:HG22	1.97	0.47
1:B:282:ASP:HB3	1:B:308:GLN:HE21	1.80	0.46
1:B:401:ASP:O	1:B:404:GLU:HB3	2.15	0.46
1:B:297:VAL:HG12	1:B:298:LEU:O	2.16	0.46
1:B:385:ALA:HA	1:B:392:ALA:HB3	1.97	0.45
1:B:356:PRO:O	5:B:504:EDO:H11	2.17	0.45
1:A:354:ILE:HG21	1:A:359:ASP:HB2	1.99	0.44
1:A:347:GLU:OE2	1:A:355:SER:OG	2.32	0.43
1:B:389:HIS:HA	1:B:390:PRO:HA	1.66	0.43
1:B:96:LEU:O	1:B:99:VAL:HG13	2.19	0.43
1:B:354:ILE:HG21	1:B:359:ASP:HB2	1.99	0.43
1:B:329:TYR:HE1	5:B:505:EDO:H12	1.84	0.43
1:B:373:ILE:HA	1:B:377:VAL:HB	2.02	0.42
1:B:141:THR:OG1	1:B:245:ASN:OD1	2.30	0.42
1:A:255:LYS:HA	1:A:255:LYS:HD2	1.76	0.41
1:A:88:GLN:HA	1:A:91:VAL:HG22	2.02	0.41

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:108:ARG:NH2	1:B:401:ASP:OD1[2_574]	2.09	0.11

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%)	317 (98%)	5 (2%)	0	100	100
1	B	322/349 (92%)	315 (98%)	7 (2%)	0	100	100
All	All	644/698 (92%)	632 (98%)	12 (2%)	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%)	287 (100%)	0	100	100
1	B	272/318 (86%)	272 (100%)	0	100	100
All	All	559/636 (88%)	559 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN

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Mol	Chain	Res	Type
1	A	369	GLN
1	B	210	GLN
1	B	251	ASN
1	B	308	GLN
1	B	362	ASN
1	B	378	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	506	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	A	506	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.51	0
4	3NG	B	503	-	28,28,28	0.67	0	39,40,40	0.80	1 (2%)
5	EDO	B	504	-	3,3,3	0.38	0	2,2,2	0.44	0
5	EDO	A	504	-	3,3,3	0.41	0	2,2,2	0.49	0
4	3NG	A	503	-	28,28,28	0.63	0	39,40,40	0.82	1 (2%)
5	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.46	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	506	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	505	-	-	0/1/1/1	-
4	3NG	B	503	-	-	0/8/8/8	0/4/4/4
5	EDO	B	504	-	-	1/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
4	3NG	A	503	-	-	0/8/8/8	0/4/4/4
5	EDO	A	505	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	3NG	C10-N9-C1	2.13	121.11	116.81
4	A	503	3NG	C10-N9-C1	2.03	120.90	116.81

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	EDO	O1-C1-C2-O2

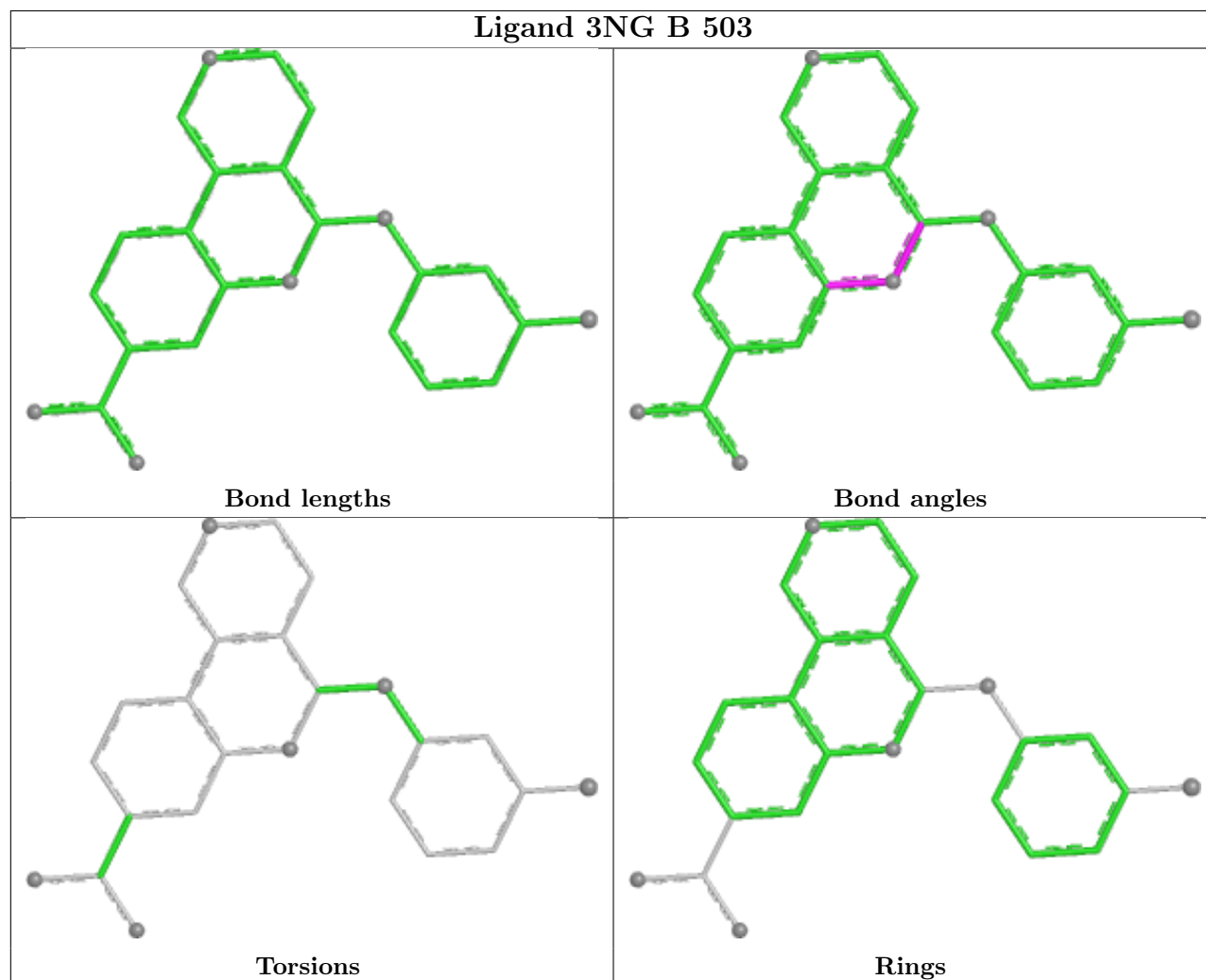
There are no ring outliers.

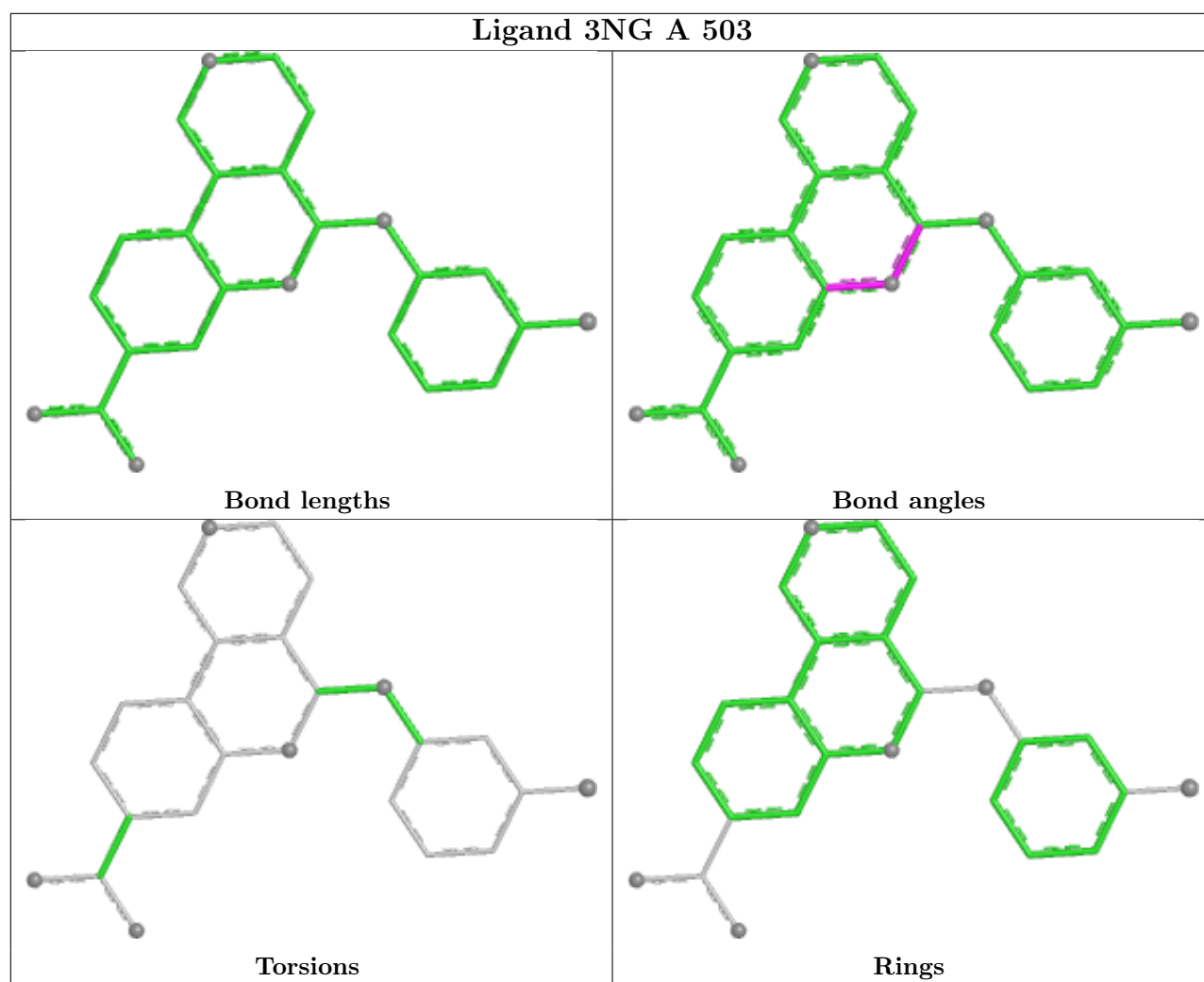
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	EDO	1	0
4	B	503	3NG	1	0
5	B	504	EDO	2	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	324/349 (92%)	0.78	34 (10%)	11 13	19, 33, 55, 73	0
1	B	324/349 (92%)	2.08	148 (45%)	0 0	21, 52, 87, 115	0
All	All	648/698 (92%)	1.43	182 (28%)	1 1	19, 41, 81, 115	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	6.9
1	B	393	GLN	6.1
1	B	135	PHE	6.1
1	B	292	VAL	5.9
1	B	125	ILE	5.7
1	B	186	THR	5.7
1	B	179	PRO	5.6
1	B	133	LYS	5.6
1	B	302	ASN	5.6
1	B	90	ASP	5.3
1	B	184	VAL	5.3
1	B	296	GLY	5.2
1	B	301	ASP	5.2
1	B	112	LEU	5.1
1	B	137	ILE	5.1
1	B	299	LEU	5.1
1	B	297	VAL	5.0
1	B	300	LEU	5.0
1	B	388	VAL	5.0
1	B	178	THR	5.0
1	B	180	ALA	5.0
1	B	134	THR	4.9
1	B	176	LEU	4.9
1	B	93	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	99	VAL	4.7
1	B	139	VAL	4.6
1	B	294	SER	4.4
1	B	182	GLU	4.3
1	B	174	VAL	4.3
1	B	140	ASP	4.3
1	B	188	LEU	4.2
1	B	387	LEU	4.2
1	B	287	VAL	4.2
1	B	175	LEU	4.2
1	B	185	PHE	4.2
1	B	91	VAL	4.2
1	B	298	LEU	4.2
1	B	390	PRO	4.1
1	B	288	GLU	4.1
1	B	395	ILE	4.1
1	B	279	LEU	4.1
1	B	384	TRP	4.0
1	B	190	ILE	4.0
1	A	411	PRO	4.0
1	B	94	LYS	3.9
1	B	92	LEU	3.9
1	B	132	LEU	3.9
1	B	307	ILE	3.9
1	B	281	ALA	3.9
1	B	138	PRO	3.8
1	B	181	LEU	3.8
1	A	89	GLU	3.8
1	B	89	GLU	3.8
1	B	375	TYR	3.8
1	B	385	ALA	3.8
1	B	309	VAL	3.7
1	B	389	HIS	3.7
1	B	289	THR	3.7
1	B	285	THR	3.6
1	B	109	ILE	3.6
1	B	191	LEU	3.6
1	B	120	VAL	3.6
1	B	392	ALA	3.6
1	B	303	TYR	3.6
1	B	104	LEU	3.6
1	B	143	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	3.5
1	A	362	ASN	3.5
1	B	411	PRO	3.5
1	B	144	THR	3.5
1	B	96	LEU	3.5
1	B	141	THR	3.5
1	B	148	THR	3.5
1	B	88	GLN	3.4
1	B	142	LEU	3.4
1	B	396	LEU	3.4
1	B	394	ASP	3.4
1	B	295	SER	3.4
1	B	131	LEU	3.4
1	A	90	ASP	3.4
1	B	102	TRP	3.3
1	A	114	GLY	3.3
1	B	136	LYS	3.3
1	B	187	ASP	3.2
1	B	103	GLY	3.2
1	B	253	THR	3.2
1	B	121	ILE	3.2
1	B	354	ILE	3.2
1	A	184	VAL	3.2
1	A	292	VAL	3.2
1	A	375	TYR	3.2
1	A	91	VAL	3.1
1	B	97	GLU	3.1
1	B	308	GLN	3.1
1	A	96	LEU	3.1
1	A	93	ALA	3.1
1	B	124	THR	3.1
1	B	126	PHE	3.1
1	B	115	ASN	3.0
1	B	119	THR	3.0
1	B	383	THR	3.0
1	A	294	SER	3.0
1	B	169	VAL	3.0
1	B	168	VAL	3.0
1	A	112	LEU	3.0
1	A	295	SER	3.0
1	B	293	THR	3.0
1	A	364	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	101	LYS	3.0
1	B	110	ALA	2.9
1	B	364	SER	2.9
1	A	88	GLN	2.9
1	A	410	ILE	2.9
1	B	177	SER	2.9
1	B	114	GLY	2.9
1	B	280	LEU	2.9
1	B	397	ASP	2.8
1	B	386	ASP	2.8
1	B	100	ASN	2.8
1	B	291	LYS	2.8
1	A	297	VAL	2.7
1	B	286	MET	2.7
1	A	356	PRO	2.7
1	B	113	SER	2.7
1	B	290	LYS	2.7
1	B	123	HIS	2.7
1	B	194	ILE	2.7
1	B	107	PHE	2.7
1	B	193	ALA	2.6
1	B	147	MET	2.6
1	A	363	ALA	2.6
1	B	327	GLN	2.6
1	A	147	MET	2.6
1	B	363	ALA	2.6
1	A	94	LYS	2.6
1	A	99	VAL	2.6
1	B	127	GLN	2.6
1	A	351	GLY	2.6
1	B	117	PRO	2.5
1	A	113	SER	2.5
1	A	296	GLY	2.5
1	B	244	GLU	2.5
1	B	381	TRP	2.5
1	B	246	CYS	2.4
1	B	149	LEU	2.4
1	B	98	ASP	2.4
1	B	130	ASP	2.4
1	B	305	ASP	2.4
1	B	173	HIS	2.4
1	B	362	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	111	GLU	2.4
1	A	107	PHE	2.4
1	B	254	LYS	2.4
1	B	128	GLU	2.4
1	B	399	LEU	2.3
1	B	245	ASN	2.3
1	B	116	ARG	2.3
1	B	306	ARG	2.3
1	B	195	PHE	2.3
1	A	389	HIS	2.3
1	B	304	SER	2.3
1	B	172	THR	2.2
1	B	398	THR	2.2
1	A	139	VAL	2.2
1	A	354	ILE	2.2
1	B	377	VAL	2.2
1	B	251	ASN	2.2
1	B	273	MET	2.2
1	B	171	SER	2.2
1	B	379	PRO	2.1
1	A	298	LEU	2.1
1	B	283	LEU	2.1
1	B	277	MET	2.1
1	B	380	LEU	2.1
1	B	248	ILE	2.1
1	A	92	LEU	2.0
1	B	258	GLN	2.0
1	A	97	GLU	2.0
1	B	356	PRO	2.0
1	A	352	MET	2.0
1	B	222	MET	2.0
1	B	328	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

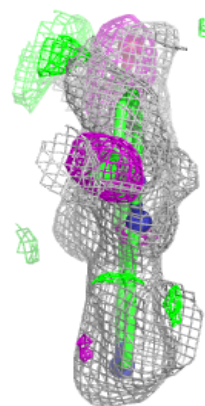
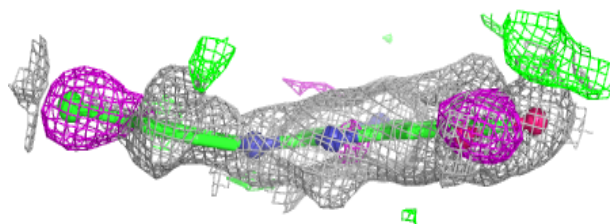
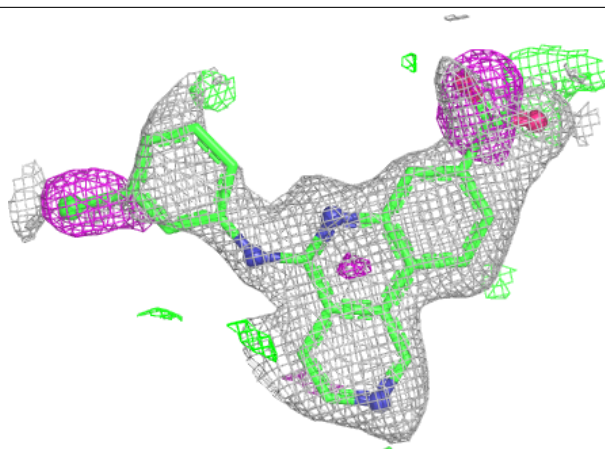
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

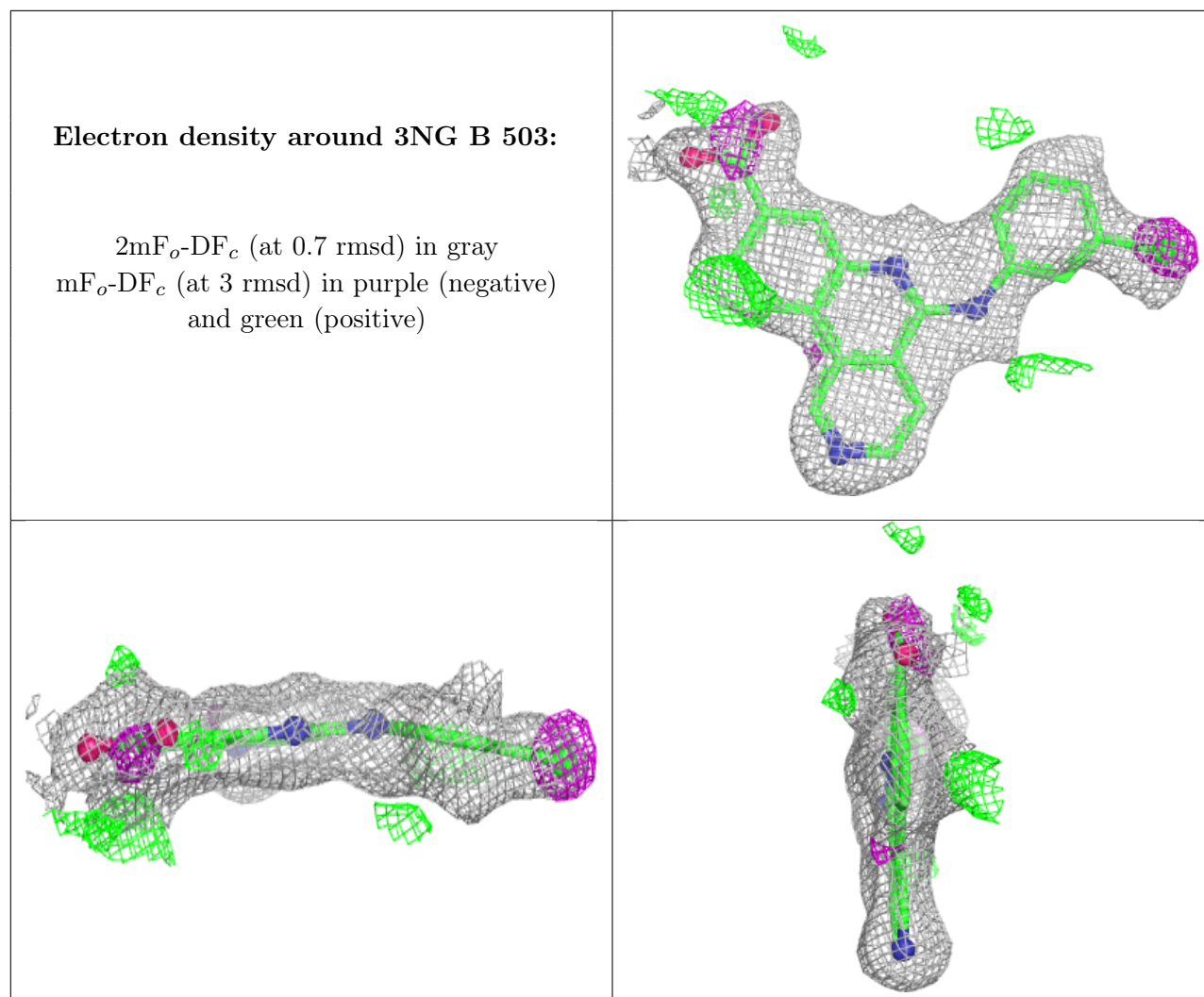
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	3NG	A	503	25/25	0.76	0.16	39,42,67,75	0
4	3NG	B	503	25/25	0.77	0.14	42,45,66,71	0
5	EDO	A	504	4/4	0.77	0.22	50,50,50,51	0
5	EDO	B	505	4/4	0.79	0.20	53,53,53,54	0
5	EDO	B	506	4/4	0.85	0.15	44,45,45,45	0
5	EDO	B	504	4/4	0.87	0.11	42,42,43,43	0
5	EDO	A	506	4/4	0.88	0.11	34,34,34,35	0
5	EDO	A	505	4/4	0.91	0.10	43,44,44,44	0
2	MG	A	501	1/1	0.97	0.05	19,19,19,19	0
3	ZN	B	502	1/1	0.97	0.09	27,27,27,27	0
2	MG	B	501	1/1	0.98	0.05	23,23,23,23	0
3	ZN	A	502	1/1	0.99	0.05	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 3NG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.