



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:23 PM UTC

PDB ID : 3SNI / pdb_00003sni
Title : Highly Potent, Selective, and Orally Active Phosphodiesterase 10A Inhibitors
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Deposited on : 2011-06-29
Resolution : 1.90 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](#) ①) 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

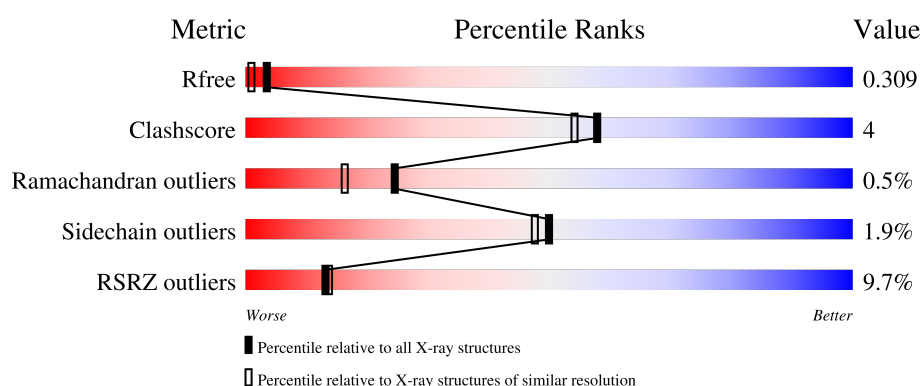
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	345	10% 79% 13% 7%
1	B	345	8% 78% 12% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5468 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 and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	2	0
			2623	1676	445	477	25			
1	B	310	Total	C	N	O	S	0	2	0
			2530	1611	431	463	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	GLY	-	expression tag	UNP Q9Y233
A	436	SER	-	expression tag	UNP Q9Y233
A	437	HIS	-	expression tag	UNP Q9Y233
A	438	MET	-	expression tag	UNP Q9Y233
B	435	GLY	-	expression tag	UNP Q9Y233
B	436	SER	-	expression tag	UNP Q9Y233
B	437	HIS	-	expression tag	UNP Q9Y233
B	438	MET	-	expression tag	UNP Q9Y233

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

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

- 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		

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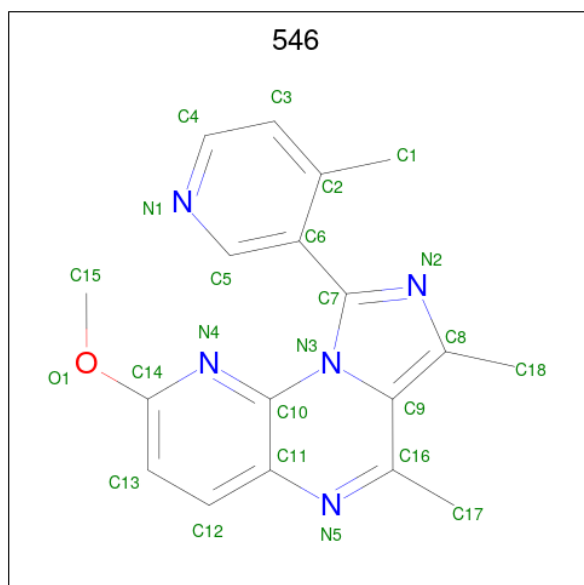
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is 2-methoxy-6,7-dimethyl-9-(4-methylpyridin-3-yl)imidazo[1,5-a]pyrido[3,2-e]pyrazine (CCD ID: 546) (formula: C₁₈H₁₇N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			24	18	5	1		
5	B	1	Total	C	N	O	0	0
			24	18	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	150	Total	O	0	0
			150	150		

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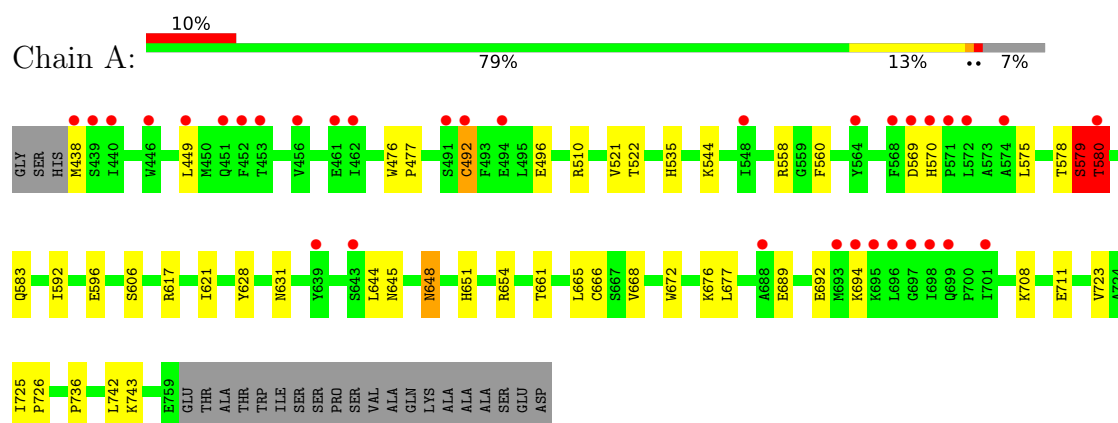
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	111	Total 111	O 111	0	0

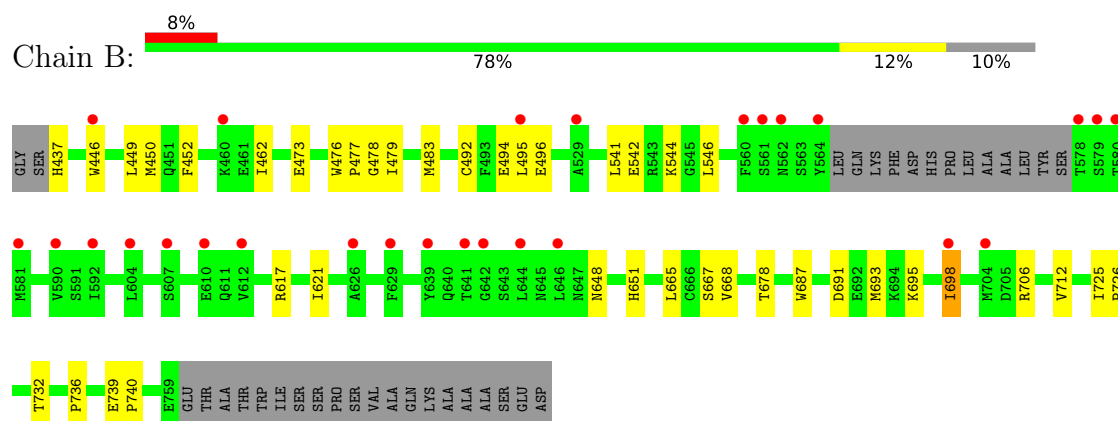
3 Residue-property plots

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 and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.24Å 81.34Å 157.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 1.90 48.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	59.8 (48.74-1.90) 60.1 (48.74-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.319 0.240 , 0.309	Depositor DCC
R_{free} test set	1589 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.1	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	0.93	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: 546, MG, ZN, CL

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	0.48	1/2687 (0.0%)	0.90	5/3638 (0.1%)
1	B	0.47	1/2590 (0.0%)	0.83	1/3504 (0.0%)
All	All	0.48	2/5277 (0.0%)	0.86	6/7142 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	ILE	CA-CB	6.05	1.57	1.54
1	B	712	VAL	CA-CB	5.42	1.57	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	SER	CA-C-N	7.11	134.50	121.70
1	A	579	SER	C-N-CA	7.11	134.50	121.70
1	A	579	SER	N-CA-C	6.40	119.91	111.28
1	B	736	PRO	N-CA-C	5.79	117.76	110.70
1	A	736	PRO	N-CA-C	5.57	117.50	110.70
1	A	580	THR	N-CA-C	-5.35	96.01	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	SER	Peptide

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	2623	0	2586	25	0
1	B	2530	0	2487	21	0
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	1	0	0	0	0
4	B	1	0	0	0	1
5	A	24	0	17	0	0
5	B	24	0	17	0	0
6	A	150	0	0	4	1
6	B	111	0	0	1	0
All	All	5468	0	5107	46	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 4.

All (46) 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:606:SER:HB2	6:A:215:HOH:O	1.95	0.67
1:B:473:GLU:HA	1:B:476:TRP:CE2	2.38	0.58
1:B:691:ASP:O	1:B:695:LYS:HG2	2.03	0.58
1:A:665:LEU:O	1:A:668:VAL:HG22	2.04	0.58
1:B:648:ASN:HB3	1:B:651:HIS:HD2	1.69	0.56
1:B:725:ILE:HB	1:B:726:PRO:HD3	1.88	0.55
1:A:672:TRP:CZ2	1:A:676:LYS:HD3	2.42	0.55
1:B:693:MET:HB3	1:B:698:ILE:HB	1.88	0.55
1:A:694:LYS:HA	6:A:73:HOH:O	2.08	0.53
1:B:617:ARG:O	1:B:621:ILE:HG12	2.09	0.52
1:A:579:SER:N	1:A:580:THR:OG1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ARG:HH11	1:A:558:ARG:HG3	1.74	0.51
1:A:492:CYS:SG	1:A:544:LYS:HE2	2.51	0.51
1:A:648:ASN:HD22	1:A:648:ASN:C	2.18	0.51
1:A:438:MET:HE2	1:A:592:ILE:HG13	1.93	0.50
1:B:687:TRP:HB3	1:B:706:ARG:HB3	1.94	0.50
1:B:450:MET:HG2	1:B:495:LEU:HG	1.95	0.49
1:B:541:LEU:HD23	1:B:544:LYS:HE3	1.94	0.49
1:A:522:THR:HG22	1:A:666:CYS:SG	2.53	0.49
1:A:560:PHE:HD2	1:A:689:GLU:HG3	1.78	0.49
1:B:542:GLU:O	1:B:546:LEU:HG	2.12	0.48
1:A:578:THR:O	1:A:583:GLN:NE2	2.47	0.48
1:A:449:LEU:HD13	1:A:477:PRO:HB2	1.96	0.48
1:A:692:GLU:HG2	6:A:120:HOH:O	2.13	0.48
1:B:667:SER:HB3	1:B:678:THR:HG21	1.95	0.47
1:B:449:LEU:HD13	1:B:477:PRO:HB2	1.96	0.47
1:B:732:THR:HG21	1:B:739:GLU:HG2	1.98	0.45
1:A:631:ASN:HD22	1:A:654:ARG:HH11	1.64	0.45
1:B:450:MET:HE3	1:B:495:LEU:HD23	1.99	0.45
1:A:617:ARG:O	1:A:621:ILE:HG12	2.17	0.45
1:B:437:HIS:N	6:B:56:HOH:O	2.49	0.45
1:A:535:HIS:HD2	6:A:34:HOH:O	1.98	0.44
1:B:452:PHE:CD2	1:B:478:GLY:HA3	2.53	0.44
1:A:496[B]:GLU:H	1:A:496[B]:GLU:CD	2.25	0.44
1:B:665:LEU:O	1:B:668:VAL:HG22	2.18	0.43
1:A:723:VAL:C	1:A:726:PRO:HD2	2.43	0.43
1:A:645:ASN:H	1:A:651:HIS:CD2	2.36	0.43
1:A:645:ASN:H	1:A:651:HIS:HD2	1.64	0.43
1:B:462:ILE:HD11	1:B:479:ILE:HG23	2.01	0.42
1:A:628:TYR:CD1	1:A:661:THR:HG21	2.54	0.42
1:A:708:LYS:HD3	1:A:711:GLU:OE2	2.19	0.42
1:A:644:LEU:HA	1:A:651:HIS:HD2	1.84	0.42
1:B:446:TRP:CZ3	1:B:496:GLU:HG3	2.54	0.42
1:B:739:GLU:N	1:B:740:PRO:CD	2.83	0.42
1:B:479:ILE:HG22	1:B:483:MET:HE2	2.01	0.42
1:A:476:TRP:HB3	1:A:521:VAL:HG21	2.03	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)
4:B:1:CL:CL	6:A:215:HOH:O[1_545]	1.92	0.28

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	322/345 (93%)	310 (96%)	9 (3%)	3 (1%)	14	6
1	B	308/345 (89%)	300 (97%)	8 (3%)	0	100	100
All	All	630/690 (91%)	610 (97%)	17 (3%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	THR
1	A	569	ASP
1	A	570	HIS

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	292/308 (95%)	284 (97%)	8 (3%)	39	34
1	B	283/308 (92%)	280 (99%)	3 (1%)	65	67
All	All	575/616 (93%)	564 (98%)	11 (2%)	50	47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	CYS
1	A	575	LEU
1	A	580	THR

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Mol	Chain	Res	Type
1	A	596	GLU
1	A	648	ASN
1	A	677	LEU
1	A	742	LEU
1	A	743	LYS
1	B	492	CYS
1	B	494	GLU
1	B	698	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	535	HIS
1	A	611	GLN
1	A	631	ASN
1	A	640	GLN
1	A	645	ASN
1	A	648	ASN
1	A	649	GLN
1	A	651	HIS
1	A	680	ASN
1	B	437	HIS
1	B	451	GLN
1	B	680	ASN
1	B	748	ASN
1	B	751	GLN

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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	546	A	782	-	26,27,27	0.91	1 (3%)	31,40,40	1.52	2 (6%)
5	546	B	782	-	26,27,27	0.92	1 (3%)	31,40,40	1.55	2 (6%)

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	546	A	782	-	-	2/6/6/6	0/4/4/4
5	546	B	782	-	-	2/6/6/6	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	782	546	O1-C14	2.59	1.39	1.35
5	B	782	546	O1-C14	2.57	1.39	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	782	546	N4-C10-N3	7.12	120.53	117.02
5	B	782	546	N4-C10-N3	6.77	120.36	117.02
5	B	782	546	C17-C16-N5	-3.31	116.34	119.62
5	A	782	546	C17-C16-N5	-2.11	117.53	119.62

There are no chirality outliers.

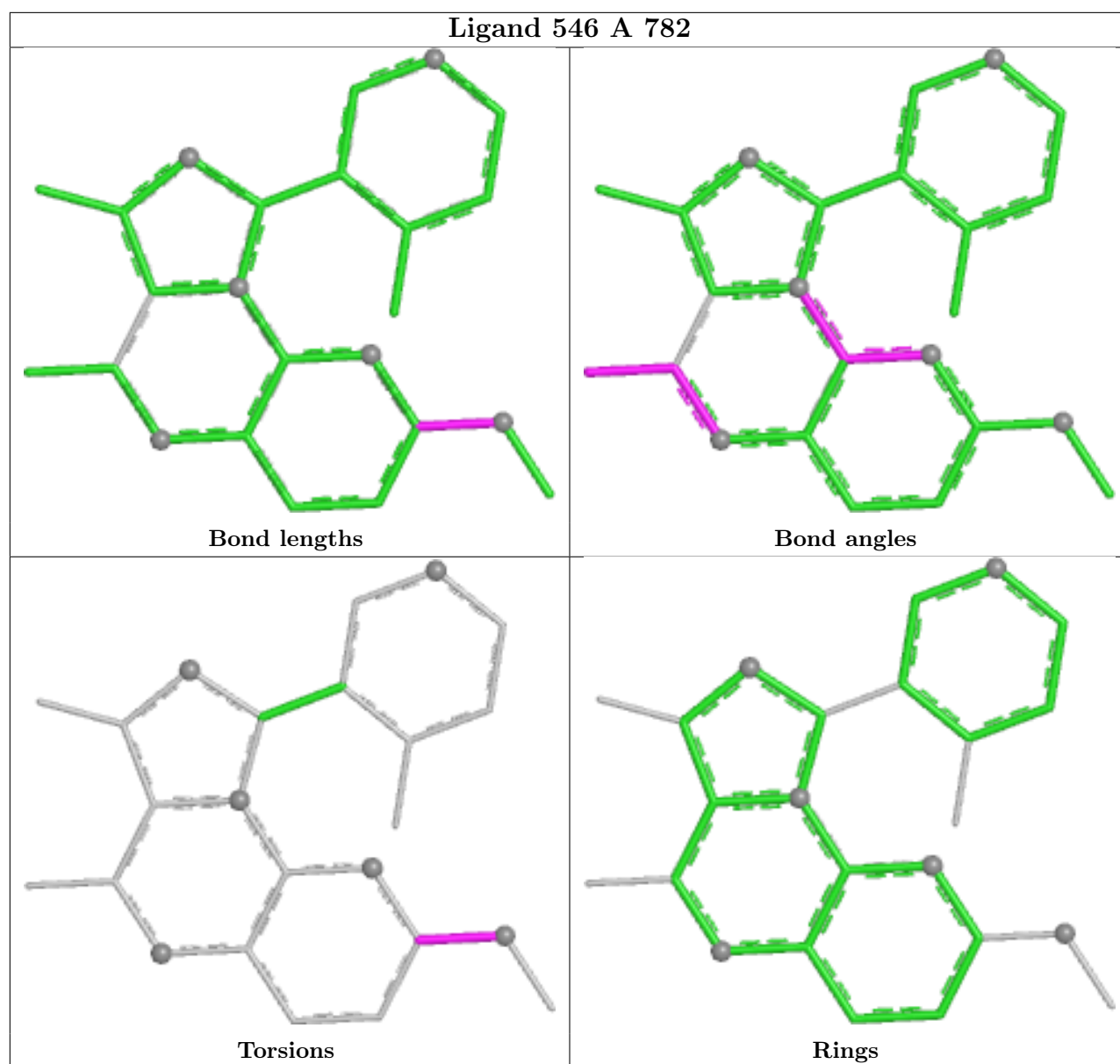
All (4) torsion outliers are listed below:

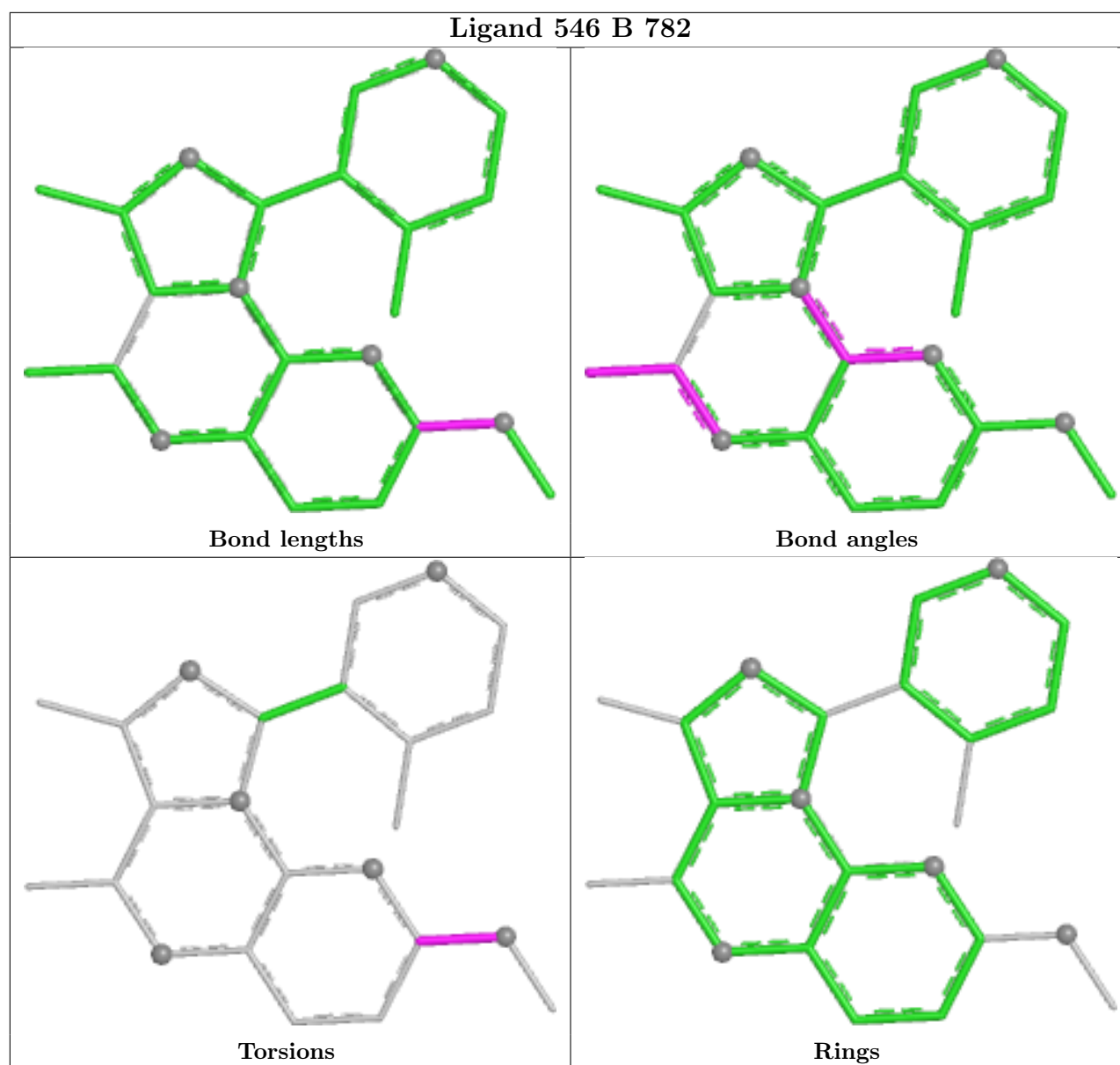
Mol	Chain	Res	Type	Atoms
5	B	782	546	N4-C14-O1-C15
5	B	782	546	C13-C14-O1-C15
5	A	782	546	C13-C14-O1-C15
5	A	782	546	N4-C14-O1-C15

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	322/345 (93%)	0.75	34 (10%)	11 12	14, 32, 51, 54	2 (0%)
1	B	310/345 (89%)	0.97	27 (8%)	16 17	19, 38, 59, 65	2 (0%)
All	All	632/690 (91%)	0.86	61 (9%)	13 14	14, 34, 56, 65	4 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	646	LEU	5.1
1	A	696	LEU	5.0
1	A	698	ILE	4.7
1	A	568	PHE	4.4
1	A	580	THR	4.2
1	A	569	ASP	3.9
1	B	644	LEU	3.7
1	B	562	ASN	3.6
1	B	564	TYR	3.5
1	B	580	THR	3.4
1	B	578	THR	3.4
1	B	641	THR	3.4
1	B	579	SER	3.3
1	B	581	MET	3.1
1	A	572	LEU	3.0
1	B	604	LEU	3.0
1	A	697	GLY	3.0
1	B	626	ALA	2.9
1	B	704	MET	2.8
1	A	571	PRO	2.8
1	A	564	TYR	2.7
1	B	642	GLY	2.7
1	B	560	PHE	2.7
1	A	693	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	446	TRP	2.6
1	A	451	GLN	2.6
1	A	461	GLU	2.6
1	B	592	ILE	2.6
1	A	570	HIS	2.6
1	A	701	ILE	2.6
1	B	590	VAL	2.6
1	A	491	SER	2.5
1	B	610	GLU	2.5
1	A	639	TYR	2.5
1	B	629	PHE	2.5
1	A	440	ILE	2.5
1	A	439	SER	2.5
1	A	438	MET	2.5
1	B	529	ALA	2.5
1	A	452	PHE	2.4
1	B	495	LEU	2.4
1	B	460	LYS	2.4
1	A	699	GLN	2.4
1	A	548	ILE	2.4
1	A	449	LEU	2.3
1	A	688	ALA	2.3
1	B	607	SER	2.2
1	B	446	TRP	2.2
1	B	612	VAL	2.2
1	A	574	ALA	2.2
1	A	462	ILE	2.2
1	A	695	LYS	2.2
1	B	639	TYR	2.1
1	A	453	THR	2.1
1	A	494	GLU	2.1
1	A	492	CYS	2.1
1	B	561	SER	2.1
1	A	694	LYS	2.1
1	A	643	SER	2.0
1	B	698	ILE	2.0
1	A	456	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

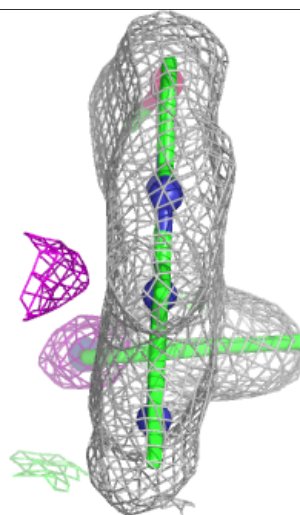
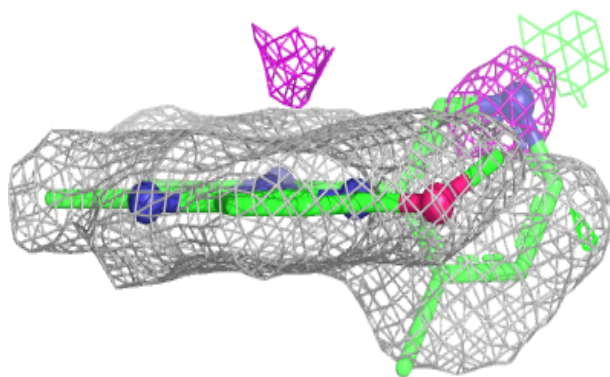
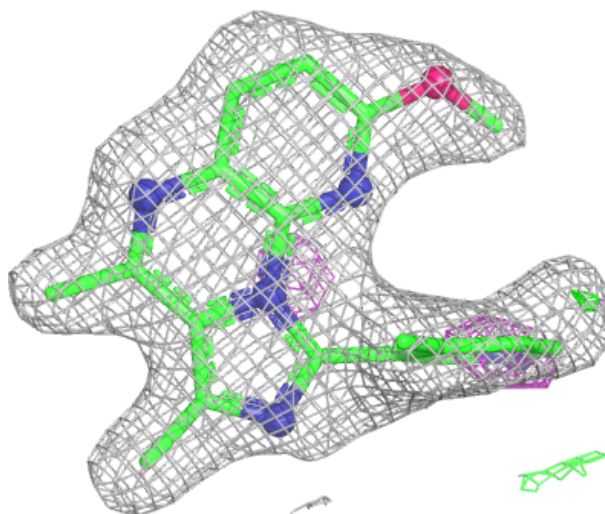
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	546	B	782	24/24	0.82	0.13	43,44,45,46	0
5	546	A	782	24/24	0.88	0.10	30,30,32,32	0
3	MG	B	781	1/1	0.95	0.07	32,32,32,32	0
4	CL	A	1	1/1	0.97	0.17	34,34,34,34	0
3	MG	A	781	1/1	0.98	0.06	14,14,14,14	0
4	CL	B	1	1/1	0.99	0.16	10,10,10,10	0
2	ZN	B	780	1/1	0.99	0.02	34,34,34,34	0
2	ZN	A	780	1/1	0.99	0.06	34,34,34,34	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.

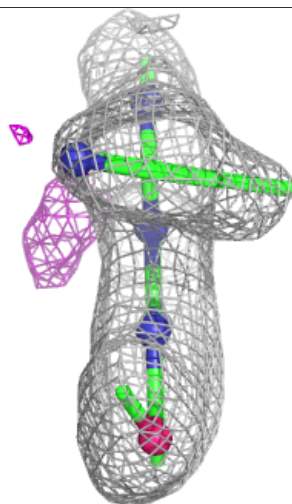
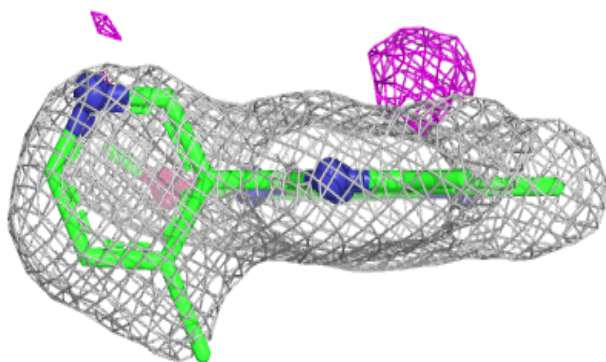
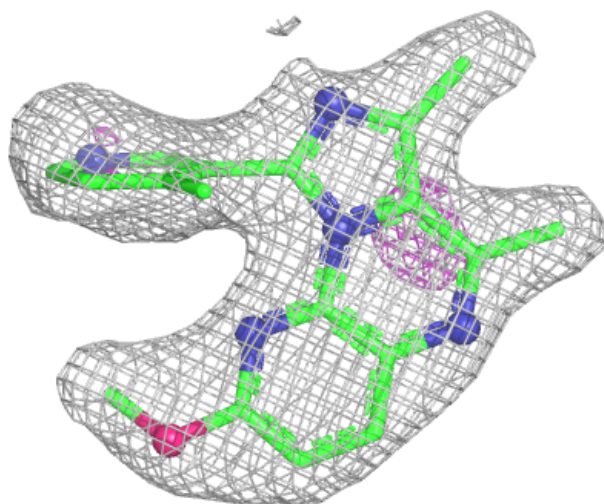
Electron density around 546 B 782:

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



Electron density around 546 A 782:

$2mF_o-DF_c$ (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.