



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:23 PM UTC

PDB ID : 2O8H / pdb_00002o8h
Title : Crystal structure of the catalytic domain of rat phosphodiesterase 10A
Authors : Pandit, J.; Marr, E.S.
Deposited on : 2006-12-12
Resolution : 1.80 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

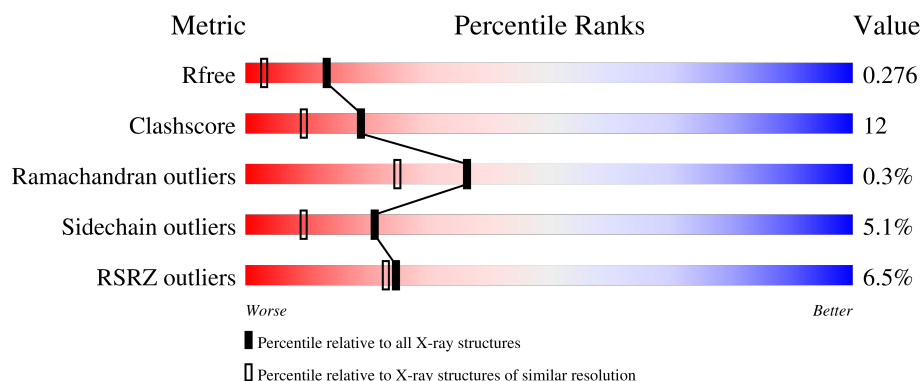
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

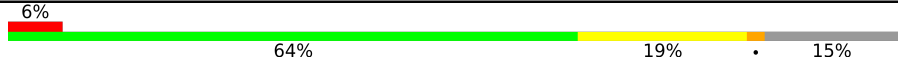
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	362	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2839 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 Phosphodiesterase-10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2491	1588	430	451	22			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	MET	-	initiating methionine	UNP Q9QYJ6
A	424	HIS	-	expression tag	UNP Q9QYJ6
A	425	HIS	-	expression tag	UNP Q9QYJ6
A	426	HIS	-	expression tag	UNP Q9QYJ6
A	427	HIS	-	expression tag	UNP Q9QYJ6
A	428	HIS	-	expression tag	UNP Q9QYJ6
A	429	HIS	-	expression tag	UNP Q9QYJ6
A	430	SER	-	cloning artifact	UNP Q9QYJ6
A	431	SER	-	cloning artifact	UNP Q9QYJ6
A	432	GLY	-	cloning artifact	UNP Q9QYJ6
A	433	LEU	-	cloning artifact	UNP Q9QYJ6
A	434	VAL	-	cloning artifact	UNP Q9QYJ6
A	435	PRO	-	cloning artifact	UNP Q9QYJ6
A	436	ARG	-	cloning artifact	UNP Q9QYJ6
A	437	GLY	-	cloning artifact	UNP Q9QYJ6
A	438	SER	-	cloning artifact	UNP Q9QYJ6
A	439	ALA	-	cloning artifact	UNP Q9QYJ6
A	440	MET	-	cloning artifact	UNP Q9QYJ6
A	441	GLY	-	cloning artifact	UNP Q9QYJ6

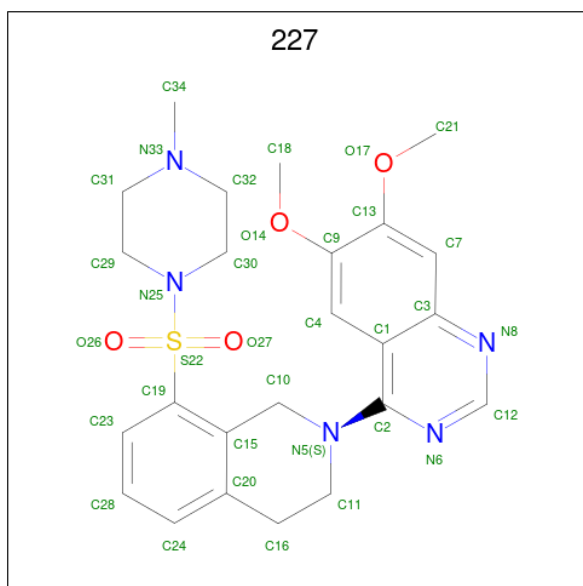
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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		

- Molecule 4 is 6,7-DIMETHOXY-4-{8-[(4-METHYLPYPERAZIN-1-YL)SULFONYL]-3,4-DIHYDROISOQUINOLIN-2(1H)-YL}QUINAZOLINE (CCD ID: 227) (formula: C₂₄H₂₉N₅O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	24	5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	312	Total	O	0	0
			312	312		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	120.62Å 120.62Å 82.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-1.80) 91.5 (30.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.273 0.228 , 0.276	Depositor DCC
R_{free} test set	2905 reflections (7.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2839	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: ZN, 227, 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	0.97	3/2552 (0.1%)	1.03	2/3455 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	659	MET	SD-CE	-13.76	1.45	1.79
1	A	725	ILE	CA-CB	11.60	1.60	1.54
1	A	483	MET	SD-CE	-6.00	1.64	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ILE	CB-CA-C	-6.96	99.88	111.29
1	A	736	PRO	N-CA-C	6.58	118.73	110.70

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	2491	0	2455	59	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	34	0	29	0	0
5	A	312	0	0	24	0
All	All	2839	0	2484	59	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 12.

All (59) 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:656:ILE:HA	1:A:659:MET:HE3	1.23	1.12
1:A:655:VAL:HG12	1:A:659:MET:HE2	1.39	1.02
1:A:656:ILE:CA	1:A:659:MET:HE3	2.01	0.91
1:A:530:ILE:O	1:A:530:ILE:HG22	1.69	0.90
1:A:539:THR:HB	5:A:17:HOH:O	1.79	0.82
1:A:497:LYS:HB3	5:A:151:HOH:O	1.80	0.81
1:A:508:ASN:HB3	5:A:306:HOH:O	1.86	0.75
1:A:588:GLN:OE1	5:A:306:HOH:O	2.03	0.75
1:A:530:ILE:C	5:A:292:HOH:O	2.33	0.70
1:A:655:VAL:HG12	1:A:659:MET:CE	2.23	0.64
1:A:714:GLN:NE2	1:A:756:ILE:HG12	2.13	0.64
1:A:467:PHE:HB3	1:A:525:HIS:CE1	2.33	0.63
1:A:746:ARG:NE	5:A:310:HOH:O	2.30	0.63
1:A:760:GLU:C	5:A:131:HOH:O	2.42	0.61
1:A:595:LEU:HD13	5:A:282:HOH:O	2.00	0.60
1:A:494:GLU:HB2	5:A:234:HOH:O	2.02	0.58
1:A:531:LEU:N	5:A:292:HOH:O	2.35	0.57
1:A:699:GLN:HG2	5:A:133:HOH:O	2.03	0.57
1:A:595:LEU:HB3	1:A:598:HIS:ND1	2.20	0.56
1:A:750:ASN:ND2	1:A:754:LYS:HE3	2.21	0.55
1:A:608:GLU:HG2	5:A:213:HOH:O	2.07	0.54
1:A:490:THR:HG22	5:A:117:HOH:O	2.09	0.53
1:A:454:LEU:O	1:A:455:PRO:C	2.52	0.52
1:A:750:ASN:HD21	1:A:754:LYS:HE3	1.75	0.52
1:A:617:ARG:O	1:A:621:ILE:HG12	2.10	0.51
1:A:565:LEU:HD22	1:A:570:HIS:CG	2.44	0.51
1:A:509:TYR:CE1	1:A:555:LEU:HD13	2.47	0.50
1:A:555:LEU:O	1:A:585:HIS:ND1	2.42	0.49
1:A:485:HIS:HA	1:A:489:GLY:O	2.12	0.49
1:A:497:LYS:CD	5:A:151:HOH:O	2.60	0.49
1:A:604:LEU:HG	1:A:608:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASP:OD1	1:A:543:ARG:NH2	2.45	0.48
1:A:699:GLN:CG	5:A:133:HOH:O	2.59	0.48
1:A:655:VAL:C	1:A:659:MET:CE	2.87	0.48
1:A:536:GLY:HA2	5:A:184:HOH:O	2.14	0.47
1:A:665:LEU:O	1:A:668:VAL:HG22	2.15	0.46
1:A:656:ILE:HG13	1:A:659:MET:HE1	1.98	0.46
1:A:690:GLY:HA3	1:A:704:MET:O	2.15	0.46
1:A:567:LYS:NZ	5:A:284:HOH:O	2.49	0.45
1:A:639:TYR:HB2	5:A:171:HOH:O	2.16	0.45
1:A:548:ILE:HD13	1:A:600:ILE:CD1	2.47	0.45
1:A:617:ARG:HD3	5:A:98:HOH:O	2.17	0.45
1:A:655:VAL:C	1:A:659:MET:HE2	2.42	0.44
1:A:537:LEU:HD11	5:A:254:HOH:O	2.17	0.44
1:A:548:ILE:HD13	1:A:600:ILE:HD11	1.99	0.44
1:A:670:LYS:NZ	5:A:172:HOH:O	2.51	0.44
1:A:604:LEU:HG	1:A:608:GLU:CB	2.48	0.43
1:A:618:LYS:HE2	1:A:653:ASP:OD2	2.18	0.43
1:A:746:ARG:NH2	5:A:310:HOH:O	2.51	0.43
1:A:484:ILE:HG22	1:A:485:HIS:N	2.33	0.43
1:A:501:PHE:O	1:A:505:VAL:HG23	2.19	0.42
1:A:549:ALA:O	1:A:553:HIS:HB3	2.20	0.42
1:A:629:PHE:HB3	5:A:281:HOH:O	2.19	0.42
1:A:530:ILE:O	1:A:530:ILE:CG2	2.39	0.41
1:A:565:LEU:HD11	1:A:581:MET:SD	2.60	0.41
1:A:497:LYS:HD2	5:A:151:HOH:O	2.21	0.41
1:A:472:PHE:HB2	1:A:475:MET:HG3	2.03	0.41
1:A:602:SER:C	1:A:604:LEU:H	2.29	0.41
1:A:541:LEU:HD12	1:A:611:GLN:NE2	2.36	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	305/362 (84%)	296 (97%)	8 (3%)	1 (0%)	36 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	ILE

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	275/322 (85%)	261 (95%)	14 (5%)	21 9

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	LEU
1	A	460	ARG
1	A	484	ILE
1	A	486	ARG
1	A	503	MET
1	A	531	LEU
1	A	541	LEU
1	A	555	LEU
1	A	558	ARG
1	A	603	THR
1	A	632	ARG
1	A	709	ARG
1	A	717	LEU
1	A	757	ARG

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	474	ASN

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Mol	Chain	Res	Type
1	A	485	HIS
1	A	566	GLN
1	A	584	HIS
1	A	611	GLN
1	A	634	GLN
1	A	648	ASN
1	A	750	ASN
1	A	751	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	227	A	999	-	38,38,38	1.89	5 (13%)	52,56,56	2.71	22 (42%)

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
4	227	A	999	-	-	0/20/39/39	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	227	S22-N25	6.94	1.73	1.63
4	A	999	227	C19-S22	5.70	1.85	1.78
4	A	999	227	O27-S22	-4.00	1.39	1.43
4	A	999	227	C3-N8	-2.74	1.32	1.37
4	A	999	227	C7-C13	2.29	1.40	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	227	O27-S22-N25	8.02	114.23	106.69
4	A	999	227	O27-S22-O26	-6.26	109.82	119.59
4	A	999	227	C2-C1-C3	5.72	119.27	115.47
4	A	999	227	O26-S22-C19	5.02	117.08	107.35
4	A	999	227	N8-C12-N6	-4.71	122.28	128.67
4	A	999	227	O14-C9-C4	-4.20	119.84	125.16
4	A	999	227	C12-N8-C3	3.80	119.75	115.43
4	A	999	227	C18-O14-C9	3.69	122.92	117.51
4	A	999	227	C1-C3-N8	-3.62	118.98	122.82
4	A	999	227	C31-N33-C32	3.41	114.97	109.54
4	A	999	227	C21-O17-C13	3.36	122.44	117.51
4	A	999	227	C30-N25-S22	-3.28	110.95	117.06
4	A	999	227	C12-N6-C2	3.20	119.98	116.84
4	A	999	227	C32-C30-N25	-3.13	105.64	108.97
4	A	999	227	C29-N25-S22	-3.04	111.41	117.06
4	A	999	227	O14-C9-C13	2.96	119.42	115.40
4	A	999	227	C1-C2-N5	2.79	125.97	121.18
4	A	999	227	C15-C10-N5	2.68	116.46	111.71
4	A	999	227	O27-S22-C19	-2.61	102.29	107.35
4	A	999	227	C7-C3-C1	2.43	122.29	119.58
4	A	999	227	C23-C19-S22	-2.30	114.35	117.48
4	A	999	227	C1-C2-N6	-2.13	117.39	122.11

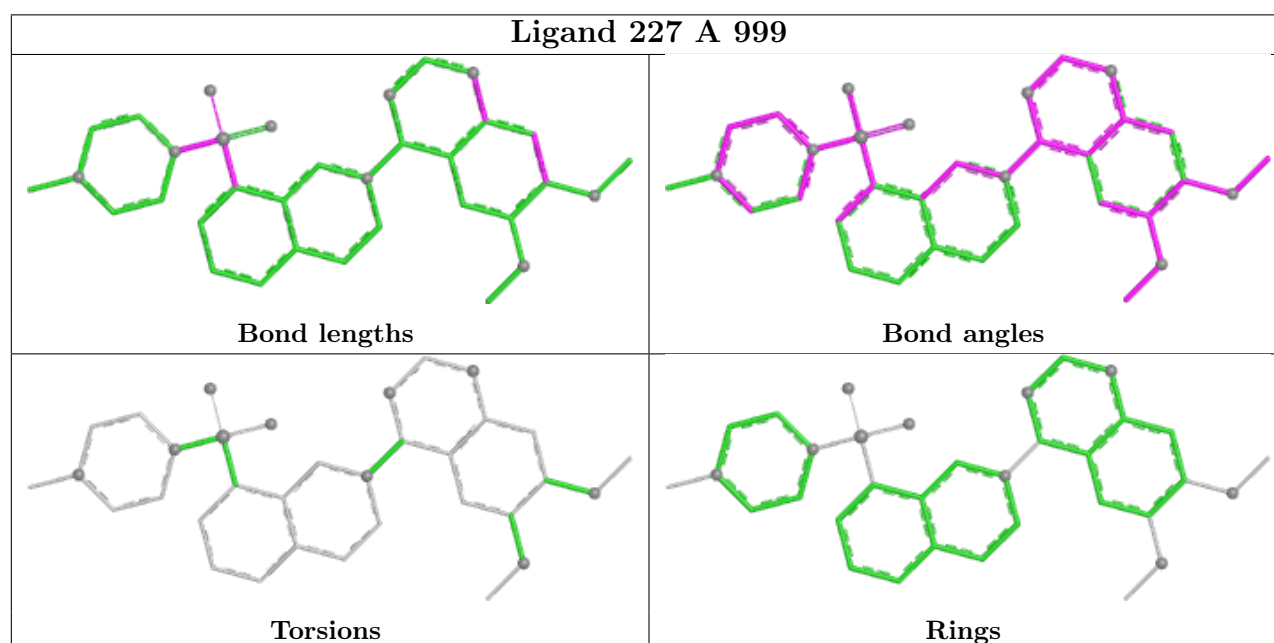
There are no chirality outliers.

There are no torsion outliers.

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 [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, 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	307/362 (84%)	0.75	20 (6%)	25 23	28, 38, 55, 69	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	LEU	4.7
1	A	492	CYS	3.5
1	A	699	GLN	3.4
1	A	593	LEU	3.4
1	A	595	LEU	3.3
1	A	604	LEU	3.3
1	A	491	SER	3.3
1	A	459	CYS	3.1
1	A	530	ILE	3.0
1	A	496	GLU	3.0
1	A	493	PHE	2.9
1	A	487	SER	2.8
1	A	489	GLY	2.6
1	A	598	HIS	2.4
1	A	460	ARG	2.3
1	A	488	CYS	2.3
1	A	758	GLY	2.3
1	A	566	GLN	2.2
1	A	548	ILE	2.1
1	A	474	ASN	2.1

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](#)

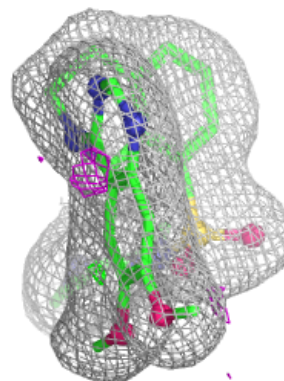
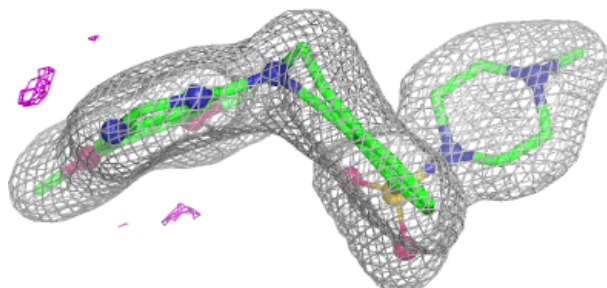
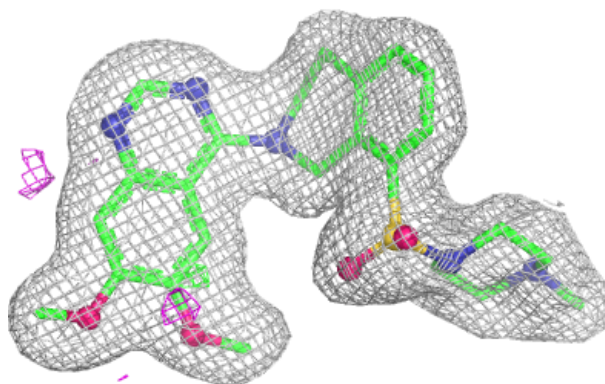
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	227	A	999	34/34	0.96	0.08	28,35,37,39	0
3	MG	A	1002	1/1	0.98	0.06	38,38,38,38	0
2	ZN	A	1001	1/1	1.00	0.01	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 227 A 999:

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.