



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:24 PM UTC

PDB ID : 2PW3 / pdb_00002pw3
Title : Structure of the PDE4D-cAMP complex
Authors : Wang, H.; Robinson, H.; Ke, H.
Deposited on : 2007-05-10
Resolution : 1.56 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

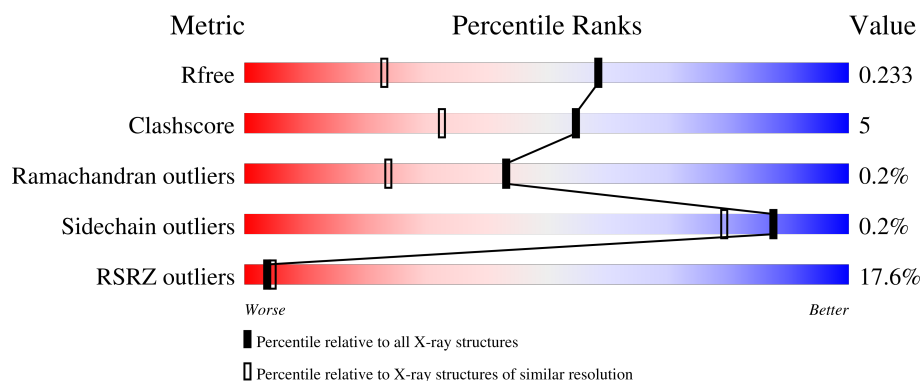
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	327	7% 89% 11%
1	B	327	28% 85% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5854 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	327	Total	C	N	O	S	0	0	0
			2648	1673	453	508	14			
1	B	325	Total	C	N	O	S	0	0	0
			2632	1664	451	503	14			

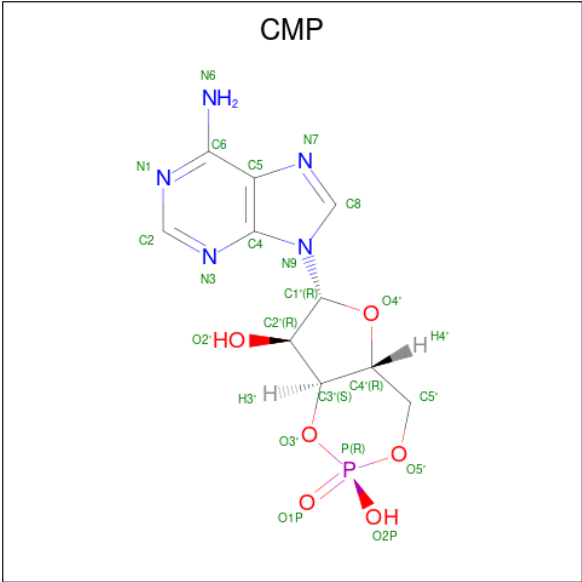
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	ASN	ASP	engineered mutation	UNP Q08499
B	201	ASN	ASP	engineered mutation	UNP Q08499

- 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 ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: C₁₀H₁₂N₅O₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

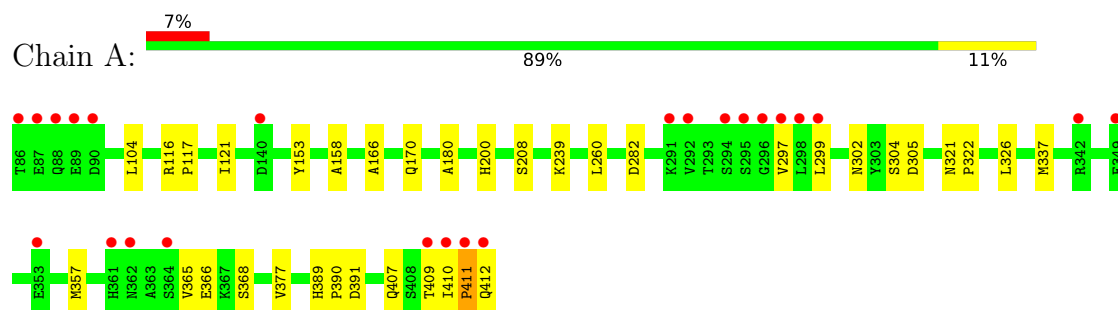
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	323	Total	O	0	0
			323	323		
4	B	205	Total	O	0	0
			205	205		

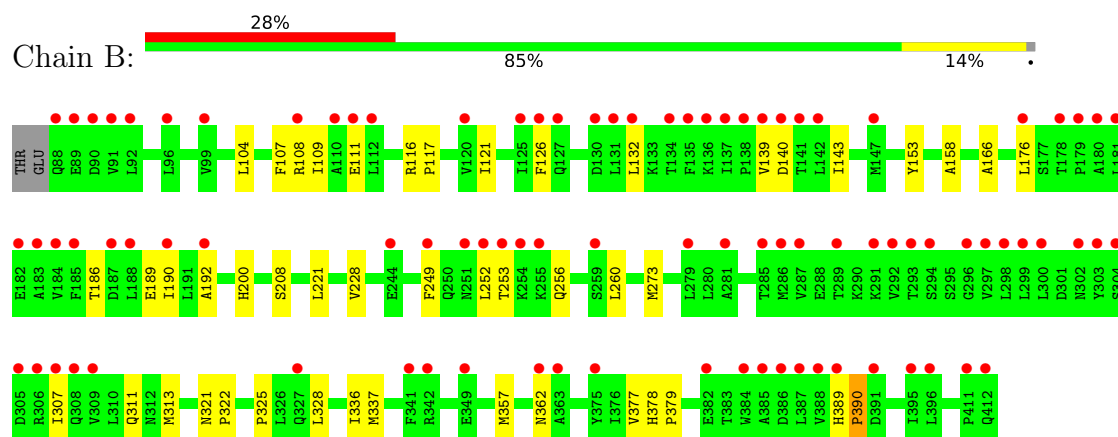
3 Residue-property plots

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-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	57.85Å 81.00Å 163.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.56 30.00 – 1.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.56) 94.7 (30.00-1.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.56Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.231 0.215 , 0.233	Depositor DCC
R_{free} test set	10867 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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, CMP

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	0.34	0/2702	0.82	7/3670 (0.2%)
1	B	0.32	0/2686	0.79	6/3648 (0.2%)
All	All	0.33	0/5388	0.81	13/7318 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ALA	N-CA-C	7.22	119.15	111.28
1	B	377	VAL	N-CA-C	7.05	117.18	110.42
1	B	158	ALA	N-CA-C	7.03	118.94	111.28
1	A	377	VAL	N-CA-C	6.69	116.82	110.53
1	A	153	TYR	N-CA-C	-6.26	100.36	110.32
1	B	200	HIS	N-CA-C	6.25	120.47	112.34
1	A	200	HIS	N-CA-C	6.18	120.38	112.34
1	A	391	ASP	N-CA-C	5.69	118.21	111.33
1	A	326	LEU	N-CA-C	5.63	118.15	111.33
1	B	153	TYR	N-CA-C	-5.37	100.95	109.96
1	B	228	VAL	N-CA-C	5.21	115.65	110.23
1	B	208	SER	N-CA-C	5.03	117.02	110.53
1	A	208	SER	N-CA-C	5.01	116.99	110.53

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	2648	0	2601	20	0
1	B	2632	0	2588	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	11	2	0
3	B	22	0	11	2	0
4	A	323	0	0	1	0
4	B	205	0	0	2	0
All	All	5854	0	5211	50	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 5.

All (50) 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)
3:A:1:CMP:H2	3:A:1:CMP:C2	0.97	1.48
3:B:1:CMP:H2	3:B:1:CMP:C2	0.97	1.48
1:A:337:MET:HE2	1:A:365:VAL:HG22	1.46	0.93
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.75	0.69
1:A:407:GLN:O	1:A:411:PRO:HD3	1.95	0.66
1:A:302:ASN:ND2	1:A:305:ASP:H	1.95	0.64
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.82	0.59
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.84	0.59
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.84	0.58
1:B:253:THR:OG1	1:B:256:GLN:HG3	2.04	0.58
1:B:362:ASN:HB2	4:B:674:HOH:O	2.06	0.55
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.90	0.54
1:B:126:PHE:HB3	1:B:132:LEU:HD11	1.91	0.52
1:A:410:ILE:O	1:A:412:GLN:HG3	2.10	0.52
1:A:180:ALA:O	1:A:297:VAL:HG13	2.09	0.51
1:B:325:PRO:HD2	1:B:328:LEU:HD12	1.93	0.50
1:B:357:MET:HE1	4:B:548:HOH:O	2.12	0.50
1:B:249:PHE:CE1	1:B:260:LEU:HD21	2.47	0.49
1:B:132:LEU:H	1:B:132:LEU:HD12	1.78	0.48
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.49	0.48
1:A:357:MET:HE3	1:A:368:SER:HB3	1.96	0.47
1:B:107:PHE:O	1:B:111:GLU:HG3	2.15	0.46
1:B:336:ILE:HG23	1:B:337:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:C	1:A:260:LEU:HD13	2.41	0.45
1:B:132:LEU:HD12	1:B:132:LEU:N	2.31	0.45
1:A:104:LEU:HD22	1:A:170:GLN:HG3	1.98	0.45
1:A:116:ARG:N	1:A:117:PRO:CD	2.79	0.45
1:B:139:VAL:O	1:B:143:ILE:HG12	2.16	0.45
1:B:126:PHE:HB3	1:B:132:LEU:CD1	2.46	0.45
1:B:307:ILE:O	1:B:311:GLN:HG3	2.17	0.44
1:B:249:PHE:CZ	1:B:260:LEU:HD21	2.52	0.44
1:B:186:THR:OG1	1:B:189:GLU:HG3	2.18	0.44
1:A:282:ASP:HB2	4:A:665:HOH:O	2.18	0.44
1:A:410:ILE:O	1:A:412:GLN:N	2.51	0.44
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.18	0.43
1:B:139:VAL:HG13	1:B:140:ASP:N	2.32	0.43
1:B:104:LEU:HD11	1:B:109:ILE:HD11	2.00	0.43
1:B:116:ARG:N	1:B:117:PRO:CD	2.82	0.43
1:B:378:HIS:HB3	1:B:379:PRO:HD3	2.00	0.43
1:A:121:ILE:HD12	1:A:166:ALA:HB1	2.01	0.42
1:A:239:LYS:HD3	1:B:221:LEU:HD21	1.99	0.42
1:A:302:ASN:ND2	1:A:304:SER:HB3	2.34	0.42
1:A:357:MET:HE1	3:A:1:CMP:H2	2.02	0.41
1:B:273:MET:HG3	3:B:1:CMP:H4'	2.02	0.41
1:B:176:LEU:HD23	1:B:313:MET:HE1	2.02	0.41
1:A:299:LEU:C	1:A:299:LEU:HD23	2.45	0.41
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.85	0.41
1:B:176:LEU:HD13	1:B:190:ILE:HG23	2.04	0.40
1:A:410:ILE:HB	1:A:411:PRO:HD3	2.03	0.40
1:B:389:HIS:CE1	1:B:390:PRO:HB3	2.56	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	325/327 (99%)	316 (97%)	8 (2%)	1 (0%)	36	18
1	B	323/327 (99%)	312 (97%)	11 (3%)	0	100	100
All	All	648/654 (99%)	628 (97%)	19 (3%)	1 (0%)	43	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	PRO

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	299/299 (100%)	299 (100%)	0	100	100
1	B	297/299 (99%)	296 (100%)	1 (0%)	86	77
All	All	596/598 (100%)	595 (100%)	1 (0%)	87	79

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	127	GLN
1	A	210	GLN
1	A	242	GLN
1	A	245	ASN
1	A	250	GLN
1	A	302	ASN
1	A	369	GLN
1	A	389	HIS

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	412	GLN
1	B	88	GLN
1	B	127	GLN
1	B	242	GLN
1	B	245	ASN
1	B	258	GLN
1	B	278	ASN
1	B	362	ASN
1	B	369	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 4 ligands modelled in this entry, 2 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	$\# Z > 2$
3	CMP	B	1	-	25,25,25	0.94	3 (12%)	37,39,39	1.56	3 (8%)
3	CMP	A	1	-	25,25,25	0.96	3 (12%)	37,39,39	1.54	3 (8%)

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
3	CMP	B	1	-	-	0/4/31/31	0/4/4/4
3	CMP	A	1	-	-	0/4/31/31	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	CMP	P-O5'	2.70	1.60	1.57
3	A	1	CMP	P-O5'	2.68	1.60	1.57
3	B	1	CMP	O3'-C3'	-2.22	1.41	1.44
3	A	1	CMP	O3'-C3'	-2.19	1.41	1.44
3	A	1	CMP	P-O3'	2.08	1.61	1.57
3	B	1	CMP	P-O3'	2.06	1.61	1.57

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	CMP	O3'-C3'-C4'	-7.60	104.98	110.71
3	B	1	CMP	O3'-C3'-C4'	-7.55	105.01	110.71
3	A	1	CMP	O2P-P-O1P	3.63	119.71	108.56
3	B	1	CMP	O2P-P-O1P	3.60	119.63	108.56
3	B	1	CMP	O3'-C3'-C2'	3.25	118.79	115.61
3	A	1	CMP	O3'-C3'-C2'	2.66	118.22	115.61

There are no chirality outliers.

There are no torsion outliers.

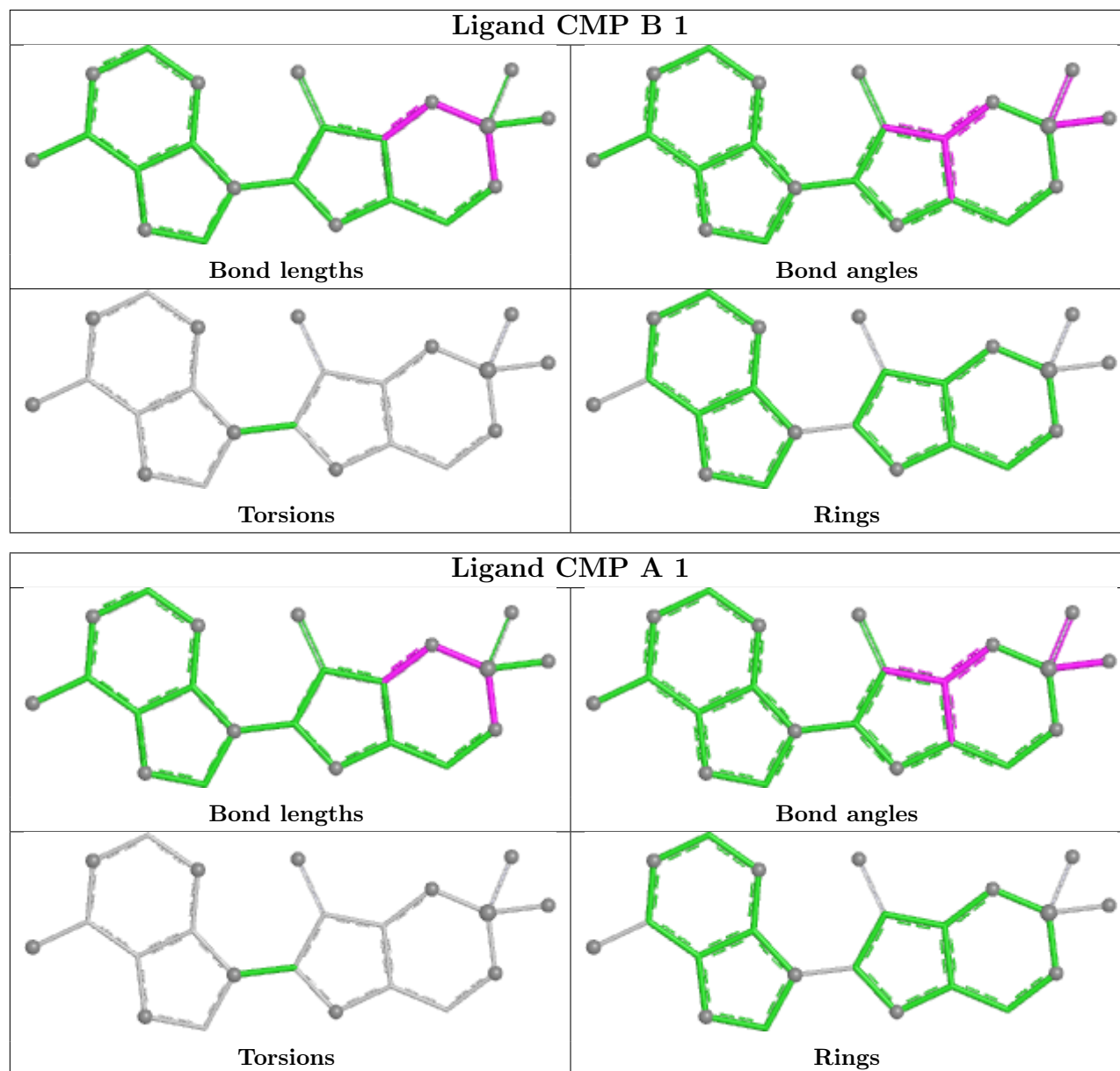
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	CMP	2	0
3	A	1	CMP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	327/327 (100%)	0.33	24 (7%) 21 24	11, 17, 31, 52	0
1	B	325/327 (99%)	1.22	91 (28%) 1 1	12, 24, 42, 57	0
All	All	652/654 (99%)	0.77	115 (17%) 4 5	11, 20, 41, 57	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	6.4
1	A	295	SER	5.8
1	A	410	ILE	5.2
1	A	411	PRO	4.8
1	B	130	ASP	4.6
1	B	303	TYR	4.3
1	B	292	VAL	4.3
1	B	297	VAL	4.3
1	B	300	LEU	4.1
1	B	412	GLN	4.1
1	B	91	VAL	4.0
1	B	294	SER	3.9
1	A	412	GLN	3.9
1	B	299	LEU	3.8
1	B	140	ASP	3.8
1	B	181	LEU	3.7
1	B	178	THR	3.7
1	B	287	VAL	3.7
1	B	135	PHE	3.6
1	B	252	LEU	3.6
1	B	386	ASP	3.6
1	B	131	LEU	3.5
1	B	139	VAL	3.5
1	B	298	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	294	SER	3.4
1	B	92	LEU	3.3
1	A	362	ASN	3.3
1	B	362	ASN	3.2
1	B	134	THR	3.2
1	B	289	THR	3.2
1	B	90	ASP	3.2
1	B	132	LEU	3.1
1	B	138	PRO	3.1
1	B	88	GLN	3.1
1	B	125	ILE	3.0
1	B	137	ILE	3.0
1	A	409	THR	3.0
1	B	291	LYS	3.0
1	B	388	VAL	2.9
1	B	183	ALA	2.8
1	B	363	ALA	2.8
1	B	176	LEU	2.8
1	B	108	ARG	2.8
1	B	349	GLU	2.8
1	B	302	ASN	2.8
1	B	126	PHE	2.8
1	A	87	GLU	2.8
1	B	179	PRO	2.7
1	A	296	GLY	2.7
1	B	309	VAL	2.7
1	B	285	THR	2.7
1	A	90	ASP	2.7
1	B	308	GLN	2.7
1	B	251	ASN	2.6
1	B	89	GLU	2.6
1	B	254	LYS	2.6
1	A	353	GLU	2.6
1	B	327	GLN	2.6
1	B	304	SER	2.6
1	B	182	GLU	2.5
1	B	110	ALA	2.5
1	B	187	ASP	2.5
1	B	375	TYR	2.5
1	B	99	VAL	2.5
1	B	253	THR	2.5
1	A	89	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	GLN	2.4
1	B	112	LEU	2.4
1	B	249	PHE	2.4
1	B	184	VAL	2.4
1	A	342	ARG	2.4
1	B	391	ASP	2.4
1	A	299	LEU	2.4
1	B	96	LEU	2.4
1	B	341	PHE	2.4
1	B	281	ALA	2.4
1	B	120	VAL	2.4
1	B	389	HIS	2.4
1	B	395	ILE	2.4
1	B	255	LYS	2.4
1	A	292	VAL	2.3
1	B	136	LYS	2.3
1	B	188	LEU	2.3
1	A	140	ASP	2.3
1	A	88	GLN	2.3
1	B	306	ARG	2.3
1	B	384	TRP	2.3
1	B	180	ALA	2.3
1	B	141	THR	2.3
1	B	147	MET	2.3
1	A	298	LEU	2.3
1	B	111	GLU	2.3
1	B	307	ILE	2.3
1	B	342	ARG	2.2
1	A	349	GLU	2.2
1	B	259	SER	2.2
1	B	142	LEU	2.2
1	B	244	GLU	2.2
1	B	305	ASP	2.2
1	B	387	LEU	2.2
1	B	190	ILE	2.2
1	B	192	ALA	2.2
1	B	385	ALA	2.2
1	B	296	GLY	2.1
1	A	364	SER	2.1
1	B	286	MET	2.1
1	B	396	LEU	2.1
1	A	361	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	2.1
1	B	411	PRO	2.1
1	B	293	THR	2.1
1	A	291	LYS	2.1
1	B	382	GLU	2.0
1	B	185	PHE	2.0
1	B	279	LEU	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](#)

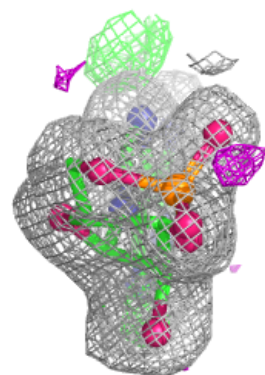
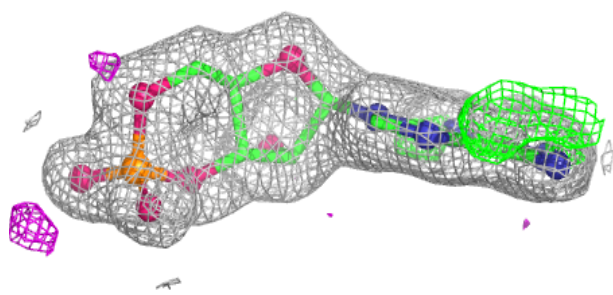
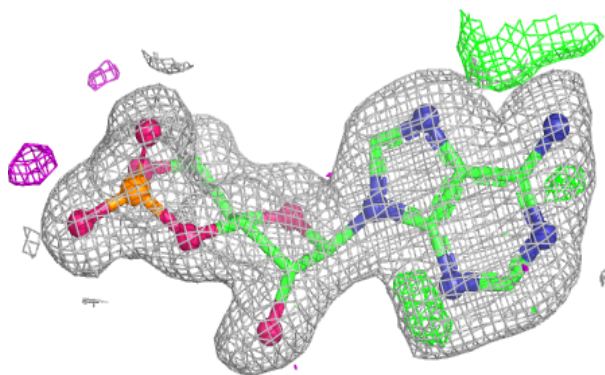
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CMP	A	1	22/22	0.95	0.08	19,22,24,27	0
3	CMP	B	1	22/22	0.95	0.08	20,23,26,27	0
2	ZN	A	501	1/1	0.99	0.11	20,20,20,20	0
2	ZN	B	501	1/1	0.99	0.13	22,22,22,22	0

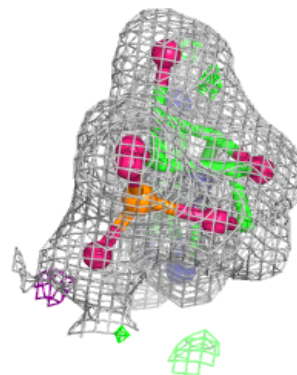
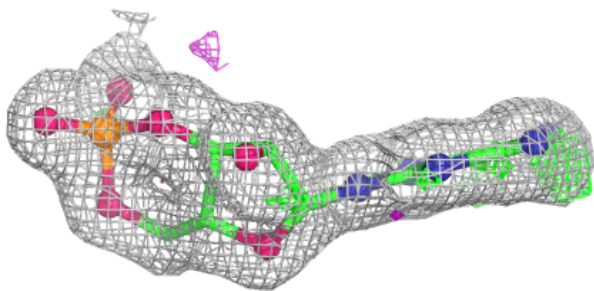
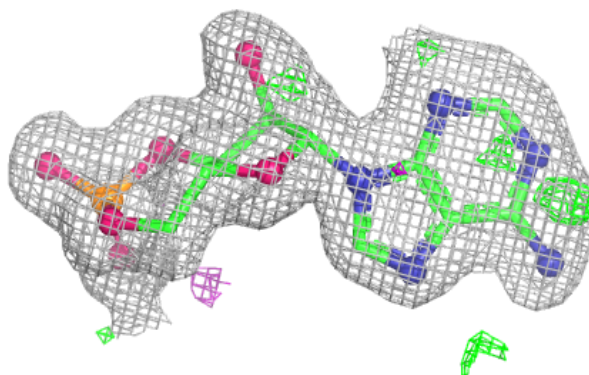
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CMP A 1:

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

**Electron density around CMP B 1:**

$2mF_o-DF_c$ (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.