



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 7Y3V / pdb_00007y3v
Title : Crystal structure of CdpNPT in complex with harmane
Authors : Nakashima, Y.; Morita, H.
Deposited on : 2022-06-13
Resolution : 2.43 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

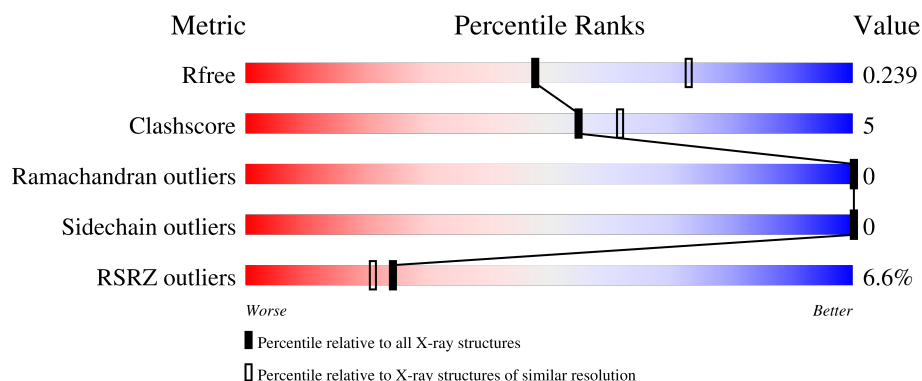
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

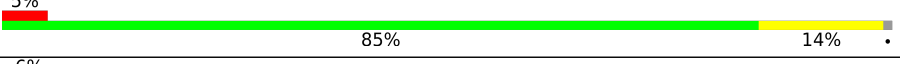
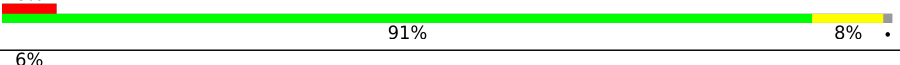
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	404	
1	B	404	
1	C	404	
1	D	404	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	501	-	-	X	-
2	PO4	D	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12965 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 Cyclic dipeptide N-prenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3014	1945	513	539	17			
1	B	399	Total	C	N	O	S	0	0	0
			3150	2030	530	573	17			
1	C	399	Total	C	N	O	S	0	0	0
			3140	2025	528	569	18			
1	D	404	Total	C	N	O	S	0	0	0
			3195	2060	537	581	17			

There are 4 discrepancies between the modelled and reference sequences:

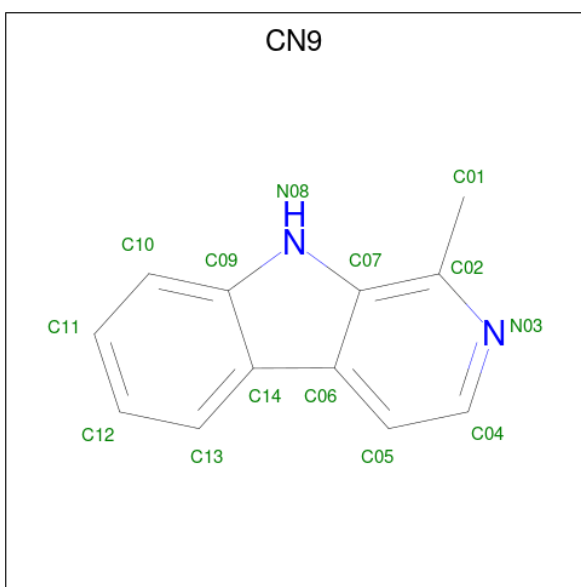
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP D1D8L6
B	37	MET	-	initiating methionine	UNP D1D8L6
C	37	MET	-	initiating methionine	UNP D1D8L6
D	37	MET	-	initiating methionine	UNP D1D8L6

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is 1-methyl-9H-pyrido[3,4-b]indole (CCD ID: CN9) (formula: C₁₂H₁₀N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			14	12	2		

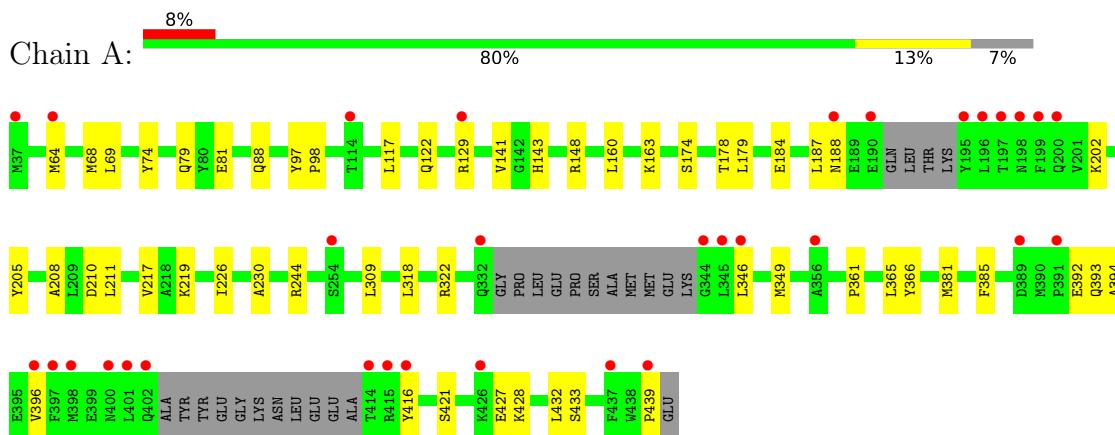
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	78	Total	O	0	0
			78	78		
4	B	120	Total	O	0	0
			120	120		
4	C	118	Total	O	0	0
			118	118		
4	D	96	Total	O	0	0
			96	96		

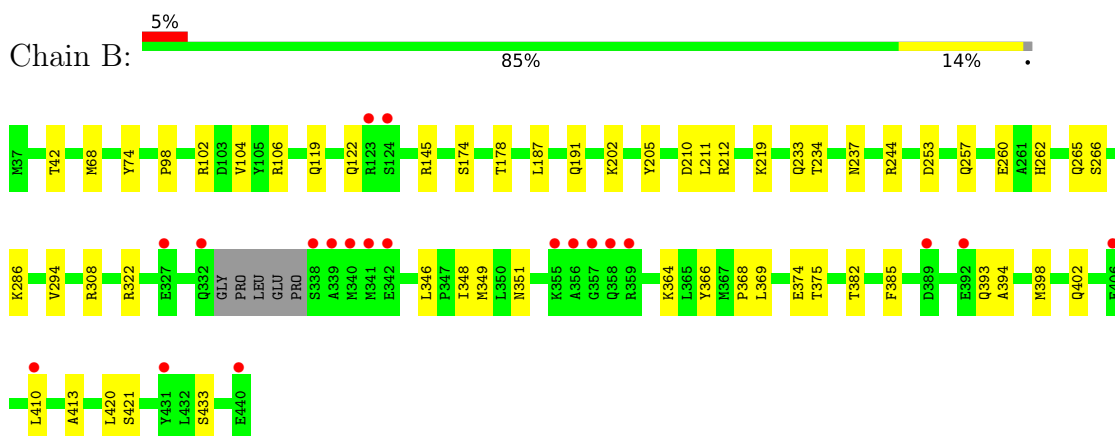
3 Residue-property plots [i](#)

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.

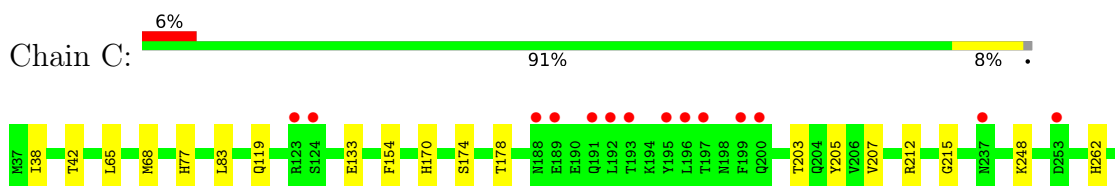
- Molecule 1: Cyclic dipeptide N-prenyltransferase

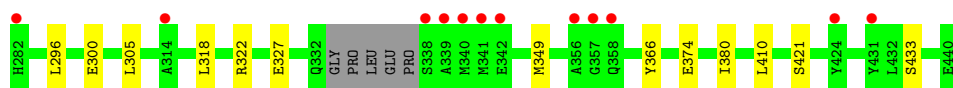


- Molecule 1: Cyclic dipeptide N-prenyltransferase

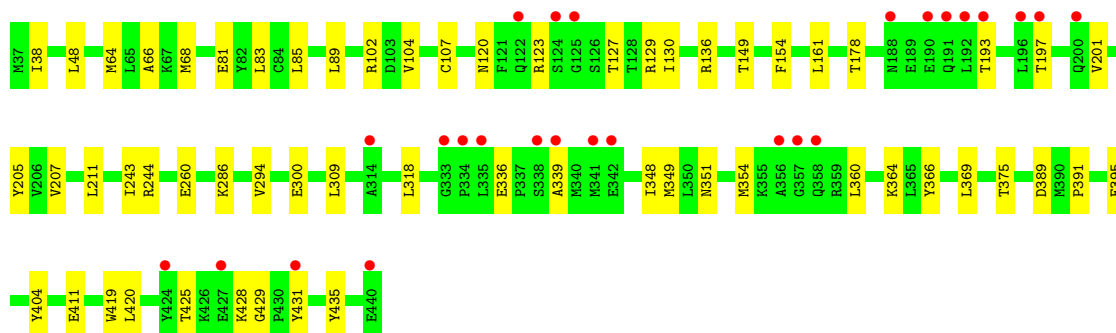
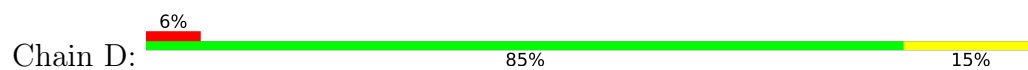


- Molecule 1: Cyclic dipeptide N-prenyltransferase





- Molecule 1: Cyclic dipeptide N-prenyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.66Å 157.24Å 161.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.94 – 2.43 46.94 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.94-2.43) 99.9 (46.94-2.43)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.217 , 0.236 0.220 , 0.239	Depositor DCC
R_{free} test set	4250 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12965	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: PO4, CN9

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	0.11	0/3090	0.31	0/4192
1	B	0.11	0/3230	0.31	0/4392
1	C	0.10	0/3219	0.29	0/4376
1	D	0.11	0/3278	0.31	0/4457
All	All	0.11	0/12817	0.30	0/17417

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	3014	0	2973	33	0
1	B	3150	0	3054	34	0
1	C	3140	0	3045	18	0
1	D	3195	0	3112	36	0
2	A	10	0	0	1	0
2	B	10	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	2	0
3	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	78	0	0	2	0
4	B	120	0	0	2	0
4	C	118	0	0	0	0
4	D	96	0	0	0	0
All	All	12965	0	12184	118	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 (118) 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:D:300:GLU:HG2	1:D:318:LEU:HD11	1.59	0.84
1:A:174:SER:OG	1:A:205:TYR:OH	2.09	0.70
1:A:219:LYS:NZ	2:A:501:PO4:O1	2.23	0.70
1:B:234:THR:HG23	1:B:237:ASN:H	1.58	0.68
1:D:123:ARG:NH1	1:D:389:ASP:O	2.27	0.67
1:D:286:LYS:NZ	2:D:501:PO4:O4	2.32	0.62
1:B:174:SER:OG	1:B:205:TYR:OH	2.16	0.61
1:C:300:GLU:HG2	1:C:318:LEU:HD11	1.83	0.60
1:B:286:LYS:NZ	2:B:501:PO4:O3	2.35	0.60
1:D:243:ILE:HD13	1:D:354:MET:HE1	1.82	0.59
1:B:174:SER:O	1:B:178:THR:OG1	2.19	0.58
1:D:85:LEU:HG	1:D:89:LEU:HD22	1.85	0.58
1:B:262:HIS:O	1:B:266:SER:OG	2.20	0.58
1:B:234:THR:HG22	1:B:237:ASN:HB2	1.85	0.57
1:B:68:MET:HE3	1:B:119:GLN:HB2	1.87	0.57
1:D:136:ARG:HH21	1:D:149:THR:HG22	1.69	0.57
1:D:244:ARG:NH2	1:D:260:GLU:OE1	2.37	0.57
1:B:219:LYS:NZ	2:B:501:PO4:O2	2.38	0.57
1:D:336:GLU:H	1:D:336:GLU:CD	2.13	0.56
1:C:349:MET:HB2	1:C:366:TYR:HB2	1.88	0.56
1:B:265:GLN:OE1	1:B:308:ARG:NH2	2.36	0.56
1:B:385:PHE:HB2	1:B:394:ALA:HB2	1.87	0.56
1:D:64:MET:HE3	1:D:404:TYR:HB3	1.87	0.55
1:A:385:PHE:HB2	1:A:394:ALA:HB2	1.89	0.55
1:A:174:SER:O	1:A:178:THR:OG1	2.22	0.54
1:D:129:ARG:NH1	2:D:501:PO4:O1	2.41	0.53
1:A:129:ARG:HD2	1:A:208:ALA:HB1	1.90	0.53
1:A:427:GLU:HG2	1:A:428:LYS:HG2	1.91	0.53
1:D:369:LEU:HD11	1:D:420:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:MET:HB2	1:D:366:TYR:HB2	1.90	0.52
1:C:38:ILE:O	1:C:42:THR:OG1	2.26	0.52
1:D:294:VAL:HG22	1:D:348:ILE:HG23	1.92	0.52
1:D:375:THR:HG21	1:D:411:GLU:HG2	1.91	0.52
1:C:296:LEU:HD21	1:C:322:ARG:HG2	1.92	0.51
1:A:148:ARG:NH2	1:A:184:GLU:OE1	2.37	0.51
1:A:309:LEU:HD21	1:A:361:PRO:HG2	1.92	0.51
1:B:122:GLN:O	1:B:393:GLN:NE2	2.35	0.51
1:A:381:MET:HE1	1:A:432:LEU:HD22	1.92	0.50
1:A:416:TYR:HE1	1:A:439:PRO:HG3	1.76	0.50
1:D:120:ASN:HB3	1:D:431:TYR:CE1	2.47	0.49
1:D:178:THR:HG21	1:D:205:TYR:CZ	2.47	0.49
1:B:244:ARG:NH2	1:B:260:GLU:OE1	2.39	0.49
1:C:154:PHE:HE2	1:C:207:VAL:HG11	1.78	0.48
1:D:391:PRO:O	1:D:395:GLU:HG3	2.13	0.48
1:C:327:GLU:HB3	1:C:380:ILE:HD12	1.94	0.48
1:B:294:VAL:HG22	1:B:348:ILE:HG23	1.96	0.48
1:C:133:GLU:OE1	1:C:203:THR:OG1	2.28	0.48
1:B:364:LYS:NZ	2:B:501:PO4:O4	2.46	0.47
1:D:351:ASN:HD21	1:D:364:LYS:HD2	1.79	0.47
1:B:349:MET:HB2	1:B:366:TYR:HB2	1.95	0.47
1:D:154:PHE:HE2	1:D:207:VAL:HG11	1.78	0.47
1:A:188:ASN:OD1	1:A:188:ASN:N	2.34	0.47
1:A:81:GLU:HB2	1:B:42:THR:HG23	1.96	0.47
1:B:351:ASN:HD21	1:B:364:LYS:HD2	1.80	0.47
1:B:382:THR:HG23	1:B:394:ALA:HB1	1.97	0.47
1:D:64:MET:HG2	1:D:68:MET:HE2	1.96	0.47
1:D:120:ASN:HB2	1:D:127:THR:HB	1.95	0.47
1:A:141:VAL:HG23	1:A:143:HIS:HD2	1.80	0.46
1:B:102:ARG:HG2	1:B:104:VAL:HG13	1.98	0.46
1:D:193:THR:O	1:D:197:THR:HG23	2.15	0.46
1:D:425:THR:OG1	1:D:428:LYS:HB2	2.15	0.46
1:B:369:LEU:HD11	1:B:420:LEU:HB2	1.97	0.46
1:D:89:LEU:HD11	1:D:161:LEU:HD12	1.97	0.45
1:B:322:ARG:NH1	4:B:614:HOH:O	2.48	0.45
1:C:68:MET:HE2	1:C:119:GLN:HB3	1.98	0.45
1:C:212:ARG:HB2	1:C:215:GLY:O	2.17	0.45
1:B:253:ASP:O	1:B:257:GLN:HG3	2.17	0.45
1:A:202:LYS:HA	1:A:226:ILE:HD11	1.99	0.45
1:C:77:HIS:CE1	1:D:38:ILE:HG12	2.52	0.45
1:A:68:MET:HE1	1:A:117:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:HE2	1:C:248:LYS:HB2	1.88	0.44
1:A:148:ARG:NH1	1:A:179:LEU:O	2.50	0.44
1:C:374:GLU:HB2	1:C:410:LEU:HB3	2.00	0.44
1:C:178:THR:HG21	1:C:205:TYR:CZ	2.52	0.44
1:A:244:ARG:NH1	4:A:616:HOH:O	2.50	0.43
1:C:421:SER:OG	1:C:433:SER:HB2	2.18	0.43
1:C:42:THR:HG22	1:D:81:GLU:HB2	1.99	0.43
1:D:419:TRP:HB2	1:D:435:TYR:HB2	2.00	0.43
1:A:210:ASP:HB3	1:A:217:VAL:HG23	2.00	0.43
1:B:210:ASP:OD2	1:B:212:ARG:NE	2.46	0.43
1:D:425:THR:O	1:D:429:GLY:N	2.50	0.43
1:D:130:ILE:HD11	1:D:211:LEU:HD11	2.00	0.43
1:A:74:TYR:OH	1:A:211:LEU:O	2.23	0.43
1:B:402:GLN:HA	1:B:410:LEU:HD11	2.01	0.43
1:C:65:LEU:HD23	1:C:83:LEU:HD23	2.01	0.43
1:B:187:LEU:HA	1:B:191:GLN:OE1	2.19	0.42
1:B:74:TYR:OH	1:B:211:LEU:O	2.33	0.42
1:D:336:GLU:HB2	1:D:339:ALA:HB3	2.01	0.42
1:D:66:ALA:HB2	1:D:83:LEU:HD11	2.00	0.42
1:B:374:GLU:HG2	1:B:413:ALA:O	2.19	0.42
1:A:88:GLN:NE2	4:A:610:HOH:O	2.42	0.42
1:A:349:MET:HB2	1:A:366:TYR:HB2	2.01	0.42
1:B:233:GLN:HG2	1:B:237:ASN:HB3	2.02	0.42
1:C:170:HIS:O	1:C:174:SER:HB2	2.20	0.42
1:A:97:TYR:HA	1:A:98:PRO:HD3	1.90	0.41
1:B:421:SER:HB3	1:B:433:SER:HB2	2.02	0.41
1:A:68:MET:HE1	1:A:117:LEU:HD13	2.01	0.41
1:A:122:GLN:O	1:A:393:GLN:NE2	2.53	0.41
1:A:69:LEU:HD13	1:A:79:GLN:HA	2.02	0.41
1:A:318:LEU:O	1:A:322:ARG:HG3	2.20	0.41
1:B:234:THR:HG21	4:B:712:HOH:O	2.20	0.41
1:D:107:CYS:HA	1:D:201:VAL:HG11	2.02	0.41
1:A:421:SER:OG	1:A:433:SER:HB2	2.21	0.41
1:C:262:HIS:CD2	1:C:305:LEU:HD23	2.56	0.41
1:A:365:LEU:O	1:A:421:SER:HA	2.21	0.41
1:D:309:LEU:HD23	1:D:360:LEU:HD13	2.02	0.41
1:A:64:MET:HE3	1:A:64:MET:HB2	1.98	0.41
1:B:145:ARG:O	1:B:202:LYS:NZ	2.47	0.41
1:D:154:PHE:CE2	1:D:207:VAL:HG11	2.55	0.41
1:B:346:LEU:HB2	1:B:368:PRO:HB3	2.03	0.40
1:D:48:LEU:HD23	1:D:48:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ARG:HG2	1:D:104:VAL:HG13	2.02	0.40
1:B:375:THR:HG22	1:B:398:MET:HE1	2.02	0.40
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.95	0.40
1:A:392:GLU:O	1:A:396:VAL:HG23	2.21	0.40
1:B:98:PRO:HB2	1:B:106:ARG:NH1	2.36	0.40
1:A:160:LEU:O	1:A:163:LYS:NZ	2.54	0.40
1:A:187:LEU:HD13	1:A:230:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

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	369/404 (91%)	358 (97%)	11 (3%)	0	100	100
1	B	395/404 (98%)	382 (97%)	13 (3%)	0	100	100
1	C	395/404 (98%)	378 (96%)	17 (4%)	0	100	100
1	D	402/404 (100%)	392 (98%)	10 (2%)	0	100	100
All	All	1561/1616 (97%)	1510 (97%)	51 (3%)	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	319/346 (92%)	319 (100%)	0	100	100
1	B	326/346 (94%)	326 (100%)	0	100	100
1	C	323/346 (93%)	323 (100%)	0	100	100
1	D	332/346 (96%)	332 (100%)	0	100	100
All	All	1300/1384 (94%)	1300 (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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	176	HIS
1	B	157	GLN
1	B	171	HIS
1	B	351	ASN
1	C	122	GLN
1	C	176	HIS
1	C	358	GLN
1	C	393	GLN
1	C	402	GLN
1	D	57	HIS
1	D	171	HIS
1	D	176	HIS
1	D	351	ASN
1	D	358	GLN
1	D	417	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

9 ligands are modelled in this entry.

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
2	PO4	A	501	-	4,4,4	0.95	0	6,6,6	0.51	0
2	PO4	A	502	-	4,4,4	0.95	0	6,6,6	0.45	0
2	PO4	C	501	-	4,4,4	0.96	0	6,6,6	0.46	0
2	PO4	D	502	-	4,4,4	0.96	0	6,6,6	0.47	0
2	PO4	B	502	-	4,4,4	0.95	0	6,6,6	0.48	0
2	PO4	D	501	-	4,4,4	0.96	0	6,6,6	0.48	0
3	CN9	A	503	-	15,16,16	1.32	2 (13%)	19,23,23	1.30	3 (15%)
2	PO4	B	501	-	4,4,4	0.95	0	6,6,6	0.45	0
2	PO4	C	502	-	4,4,4	0.95	0	6,6,6	0.47	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
3	CN9	A	503	-	-	-	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	CN9	C06-C07	-2.45	1.38	1.41
3	A	503	CN9	C14-C09	-2.26	1.38	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	CN9	C05-C04-N03	-2.53	120.88	123.97
3	A	503	CN9	C05-C06-C07	-2.22	116.98	120.02
3	A	503	CN9	C04-N03-C02	2.17	120.82	118.35

There are no chirality outliers.

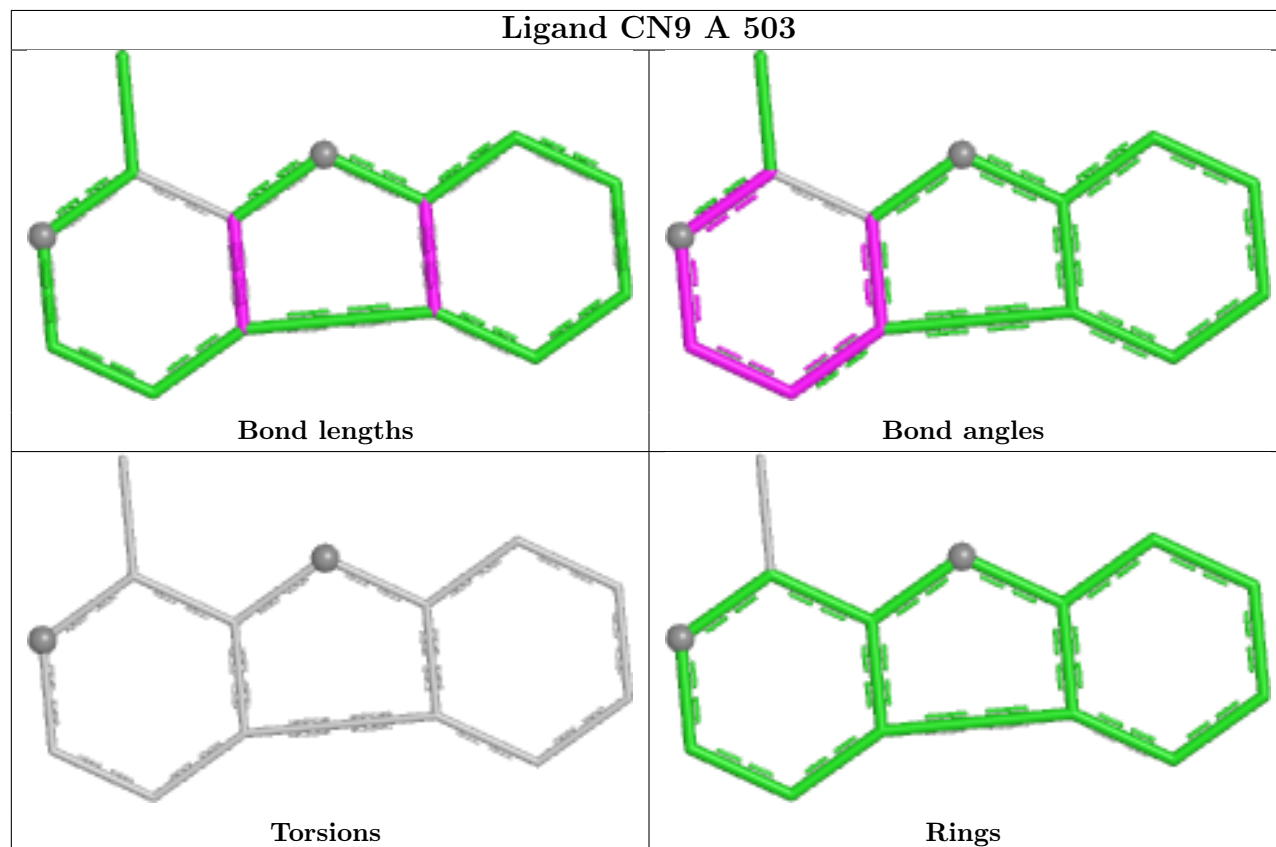
There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PO4	1	0
2	D	501	PO4	2	0
2	B	501	PO4	3	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	377/404 (93%)	0.47	32 (8%)	16	14	21, 38, 70, 94	0
1	B	399/404 (98%)	0.33	20 (5%)	34	31	21, 37, 62, 88	0
1	C	399/404 (98%)	0.40	26 (6%)	25	21	20, 40, 68, 102	0
1	D	404/404 (100%)	0.44	26 (6%)	25	22	20, 40, 68, 92	0
All	All	1579/1616 (97%)	0.41	104 (6%)	24	21	20, 39, 68, 102	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	TYR	7.4
1	B	338	SER	7.0
1	B	339	ALA	6.5
1	C	338	SER	6.0
1	C	339	ALA	6.0
1	D	124	SER	4.9
1	A	416	TYR	4.6
1	B	341	MET	4.6
1	B	355	LYS	4.4
1	A	401	LEU	4.3
1	C	341	MET	4.0
1	B	356	ALA	4.0
1	A	414	THR	4.0
1	A	344	GLY	3.9
1	C	199	PHE	3.8
1	A	439	PRO	3.8
1	C	191	GLN	3.7
1	C	340	MET	3.6
1	A	415	ARG	3.5
1	A	197	THR	3.5
1	A	402	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	357	GLY	3.5
1	A	190	GLU	3.4
1	D	197	THR	3.4
1	D	440	GLU	3.3
1	B	358	GLN	3.3
1	A	188	ASN	3.3
1	A	398	MET	3.2
1	D	125	GLY	3.2
1	A	391	PRO	3.2
1	B	340	MET	3.2
1	C	314	ALA	3.2
1	A	199	PHE	3.2
1	A	332	GLN	3.1
1	D	193	THR	3.1
1	C	188	ASN	3.1
1	D	335	LEU	3.0
1	B	410	LEU	2.9
1	C	192	LEU	2.9
1	B	406	GLU	2.9
1	D	341	MET	2.9
1	B	392	GLU	2.9
1	A	195	TYR	2.8
1	C	124	SER	2.8
1	D	357	GLY	2.7
1	A	345	LEU	2.7
1	D	192	LEU	2.7
1	D	338	SER	2.7
1	D	190	GLU	2.6
1	B	332	GLN	2.6
1	C	358	GLN	2.6
1	A	389	ASP	2.6
1	D	427	GLU	2.6
1	D	339	ALA	2.6
1	B	359	ARG	2.5
1	B	342	GLU	2.5
1	C	200	GLN	2.5
1	D	191	GLN	2.5
1	C	197	THR	2.5
1	B	431	TYR	2.4
1	A	356	ALA	2.4
1	D	200	GLN	2.4
1	C	357	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	253	ASP	2.4
1	D	358	GLN	2.4
1	A	129	ARG	2.4
1	C	356	ALA	2.4
1	A	114	THR	2.4
1	D	356	ALA	2.4
1	C	123	ARG	2.3
1	D	333	GLY	2.3
1	D	122	GLN	2.3
1	A	198	ASN	2.3
1	D	314	ALA	2.3
1	A	254	SER	2.3
1	D	342	GLU	2.3
1	D	196	LEU	2.3
1	C	196	LEU	2.2
1	A	437	PHE	2.2
1	C	424	TYR	2.2
1	A	37	MET	2.2
1	B	124	SER	2.2
1	C	342	GLU	2.2
1	A	400	ASN	2.2
1	C	282	HIS	2.2
1	C	237	ASN	2.1
1	A	346	LEU	2.1
1	A	64	MET	2.1
1	C	189	GLU	2.1
1	C	195	TYR	2.1
1	D	334	PRO	2.1
1	B	440	GLU	2.1
1	A	196	LEU	2.1
1	B	327	GLU	2.1
1	C	193	THR	2.1
1	A	426	LYS	2.1
1	C	431	TYR	2.1
1	A	396	VAL	2.0
1	A	397	PHE	2.0
1	D	424	TYR	2.0
1	A	200	GLN	2.0
1	B	123	ARG	2.0
1	D	188	ASN	2.0
1	B	389	ASP	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 ⓘ

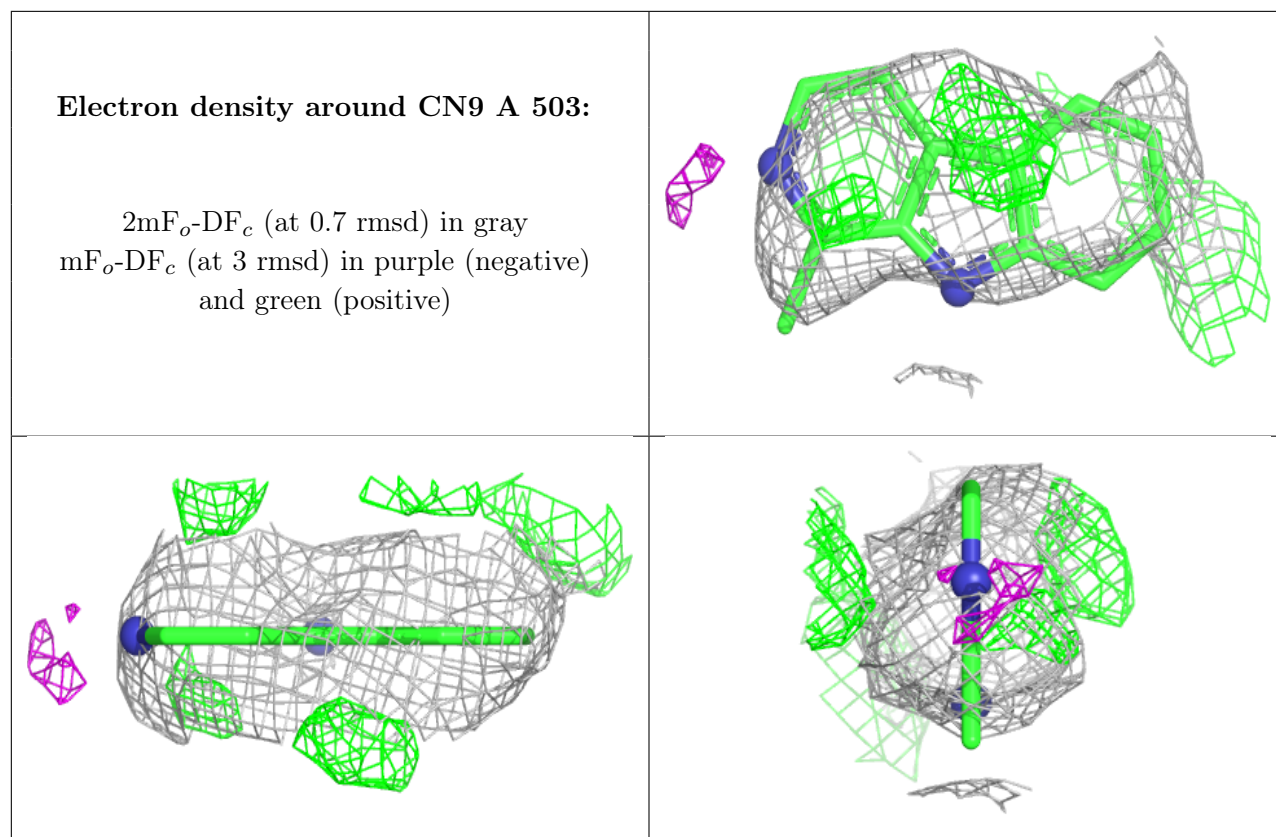
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	PO4	D	502	5/5	0.70	0.19	94,94,94,95	0
2	PO4	B	501	5/5	0.72	0.20	93,93,93,94	0
2	PO4	A	502	5/5	0.75	0.17	79,80,80,81	0
2	PO4	B	502	5/5	0.82	0.14	70,71,72,73	0
2	PO4	D	501	5/5	0.83	0.19	90,90,91,91	0
3	CN9	A	503	14/14	0.83	0.34	104,104,105,105	0
2	PO4	C	502	5/5	0.84	0.14	78,79,79,79	0
2	PO4	A	501	5/5	0.84	0.14	74,75,75,75	0
2	PO4	C	501	5/5	0.89	0.15	85,85,85,86	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.