



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:42 PM UTC

PDB ID : 3ZU0 / pdb_00003zu0
Title : Structure of Haemophilus influenzae NAD nucleotidase (NadN)
Authors : Garavaglia, S.; Bruzzone, S.; Cassani, C.; Canella, L.; Allegrone, G.; Sturla, L.; Mannino, E.; Millo, E.; De Flora, A.; Rizzi, M.
Deposited on : 2011-07-13
Resolution : 2.00 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

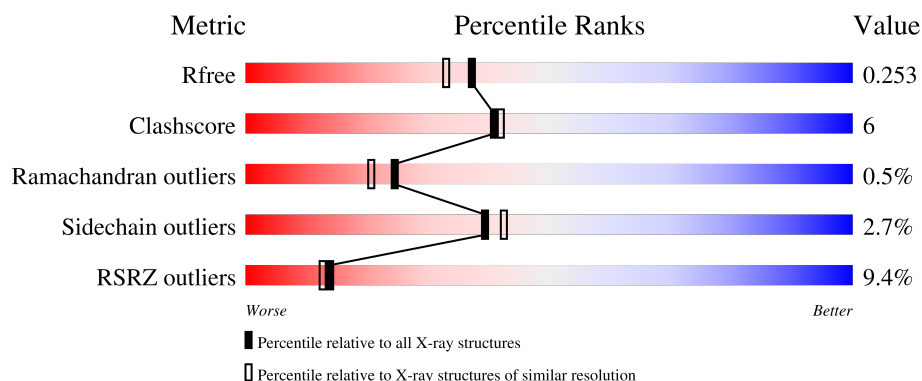
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	579	5% 83% 12% • •
1	B	579	12% 72% 15% • 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8813 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.

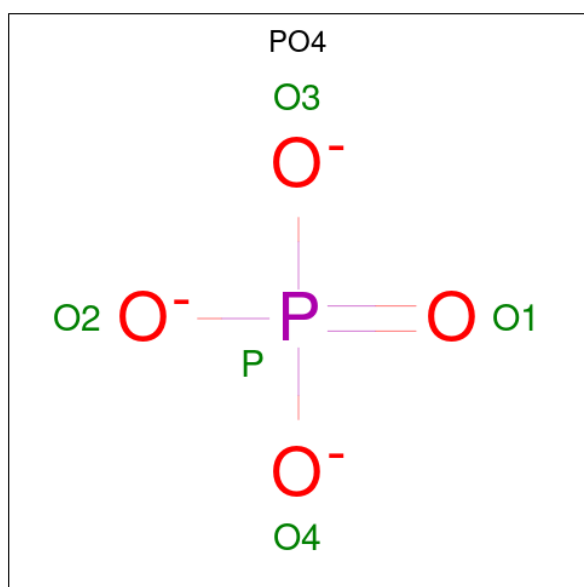
- Molecule 1 is a protein called NAD NUCLEOTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4373	2790	734	839	10			
1	B	505	Total	C	N	O	S	8	0	0
			3971	2549	657	756	9			

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

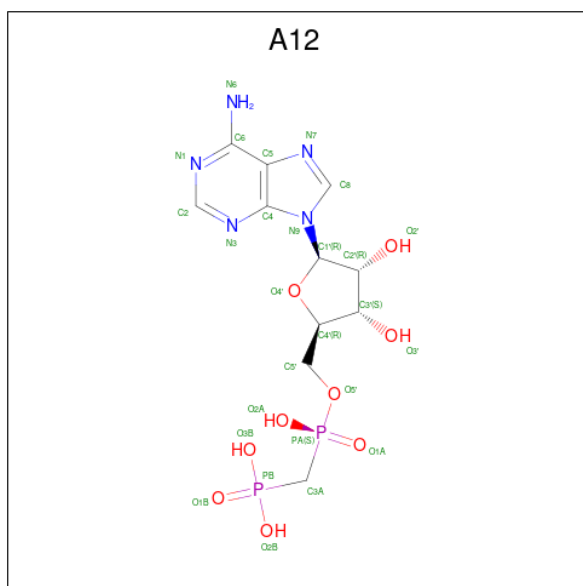
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: A12) (formula: $C_{11}H_{17}N_5O_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	11	5	9	2		
4	B	1	Total	C	N	O	P	0	0
			27	11	5	9	2		

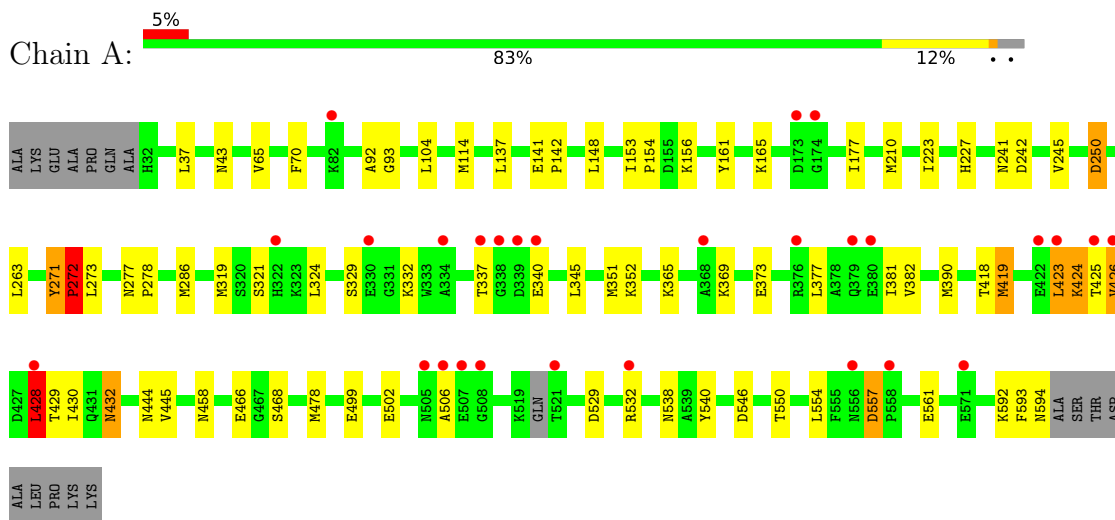
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total	O	0	0
			237	237		
5	B	169	Total	O	0	0
			169	169		

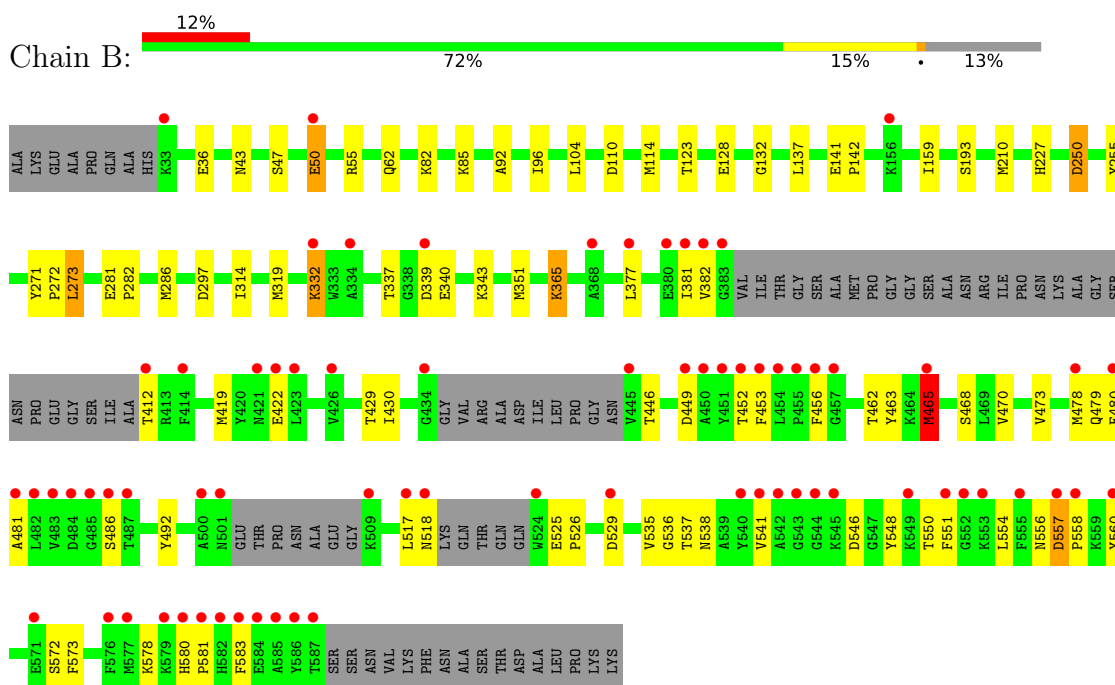
3 Residue-property plots [i](#)

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: NAD NUCLEOTIDASE



• Molecule 1: NAD NUCLEOTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.63Å 104.05Å 119.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.71 – 2.00 47.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.5 (47.71-2.00) 96.6 (47.71-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.215 , 0.247 0.214 , 0.253	Depositor DCC
R_{free} test set	390 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8813	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, PO4, A12

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	0.58	8/4466 (0.2%)	1.19	9/6043 (0.1%)
1	B	0.62	11/4054 (0.3%)	0.78	2/5479 (0.0%)
All	All	0.60	19/8520 (0.2%)	1.02	11/11522 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	GLU	CD-OE2	-7.70	1.10	1.25
1	A	319	MET	SD-CE	7.09	1.97	1.79
1	B	351	MET	SD-CE	6.76	1.96	1.79
1	A	114	MET	SD-CE	6.07	1.94	1.79
1	B	478	MET	SD-CE	5.97	1.94	1.79
1	A	390	MET	SD-CE	5.96	1.94	1.79
1	B	419	MET	SD-CE	5.96	1.94	1.79
1	B	210	MET	SD-CE	5.88	1.94	1.79
1	B	319	MET	SD-CE	5.85	1.94	1.79
1	B	419	MET	CG-SD	5.80	1.95	1.80
1	A	286	MET	SD-CE	5.78	1.94	1.79
1	A	210	MET	CG-SD	5.62	1.94	1.80
1	B	478	MET	CG-SD	5.59	1.94	1.80
1	A	419	MET	SD-CE	5.53	1.93	1.79
1	B	286	MET	SD-CE	5.50	1.93	1.79
1	B	114	MET	SD-CE	5.48	1.93	1.79
1	B	465	MET	CG-SD	5.35	1.94	1.80
1	A	286	MET	CG-SD	5.22	1.93	1.80
1	A	114	MET	CG-SD	5.03	1.93	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	TYR	CA-C-N	48.08	179.94	119.84
1	A	271	TYR	C-N-CA	48.08	179.94	119.84
1	A	271	TYR	C-N-CD	-12.38	74.26	125.00
1	A	93	GLY	N-CA-C	6.91	119.09	112.04
1	B	557	ASP	CA-C-N	6.89	128.46	119.84
1	B	557	ASP	C-N-CA	6.89	128.46	119.84
1	A	557	ASP	CA-C-N	6.48	127.94	119.84
1	A	557	ASP	C-N-CA	6.48	127.94	119.84
1	A	272	PRO	N-CA-C	-5.88	100.37	112.47
1	A	428	LEU	CA-CB-CG	5.69	136.21	116.30
1	A	424	LYS	N-CA-C	5.23	121.95	110.80

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	4373	0	4351	42	0
1	B	3971	0	3956	66	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	5	0	0	0	0
4	A	27	0	14	1	0
4	B	27	0	14	2	0
5	A	237	0	0	0	0
5	B	169	0	0	4	0
All	All	8813	0	8335	108	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 6.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:HIS:HB3	1:B:583:PHE:HB2	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:THR:HG22	1:B:538:ASN:H	1.38	0.87
1:B:463:TYR:HB2	1:B:465:MET:HE3	1.57	0.87
1:B:465:MET:HE1	1:B:551:PHE:CE1	2.11	0.85
1:B:465:MET:HE1	1:B:551:PHE:HE1	1.45	0.82
1:A:321:SER:HB2	1:A:345:LEU:HD21	1.65	0.77
1:B:449:ASP:C	5:B:2157:HOH:O	2.29	0.75
1:A:432:ASN:HD22	1:A:432:ASN:H	1.34	0.74
1:A:429:THR:O	1:A:430:ILE:HD13	1.86	0.74
1:B:337:THR:O	1:B:340:GLU:HG2	1.87	0.74
1:B:453:PHE:HD2	1:B:573:PHE:HE2	1.36	0.71
1:B:430:ILE:O	1:B:537:THR:HG23	1.90	0.71
1:A:458:ASN:HD21	4:A:1598:A12:HN62	1.36	0.69
1:A:502:GLU:HG2	1:A:593:PHE:CZ	2.26	0.69
1:A:227:HIS:CD2	1:A:250:ASP:HB2	2.28	0.69
1:B:537:THR:HG22	1:B:538:ASN:N	2.07	0.68
1:A:141:GLU:HB2	1:A:142:PRO:HD3	1.75	0.68
1:B:465:MET:HE2	1:B:554:LEU:HD12	1.76	0.66
1:A:381:ILE:HD12	1:A:444:ASN:HB3	1.78	0.65
1:B:452:THR:HB	5:B:2157:HOH:O	1.97	0.64
1:A:592:LYS:HE2	1:A:594:ASN:OD1	1.98	0.64
1:A:137:LEU:O	1:A:141:GLU:HG2	2.01	0.61
1:B:465:MET:HE2	1:B:554:LEU:CD1	2.31	0.60
1:B:96:ILE:HD11	1:B:128:GLU:HA	1.83	0.60
1:B:480:PHE:CE2	1:B:486:SER:HB3	2.37	0.59
1:B:50:GLU:H	1:B:50:GLU:CD	2.11	0.59
1:B:550:THR:O	1:B:554:LEU:HG	2.02	0.59
1:B:422:GLU:HG3	1:B:572:SER:OG	2.02	0.59
1:A:426:VAL:CG1	1:A:428:LEU:H	2.16	0.58
1:A:141:GLU:HB2	1:A:142:PRO:CD	2.33	0.58
1:B:468:SER:HB3	1:B:529:ASP:HB3	1.85	0.57
1:B:446:THR:O	1:B:449:ASP:HB2	2.03	0.56
1:B:452:THR:N	5:B:2157:HOH:O	2.37	0.56
1:B:43:ASN:HB3	1:B:92:ALA:HB3	1.87	0.56
1:A:263:LEU:HD21	1:A:351:MET:HE1	1.88	0.56
1:A:468:SER:HB3	1:A:529:ASP:HB3	1.89	0.55
1:B:453:PHE:HD2	1:B:573:PHE:CE2	2.21	0.55
1:B:50:GLU:OE1	1:B:50:GLU:N	2.28	0.54
1:B:541:VAL:HG12	1:B:551:PHE:CD2	2.43	0.54
1:A:423:LEU:O	1:A:425:THR:N	2.41	0.54
1:B:104:LEU:HB3	1:B:377:LEU:HD11	1.92	0.52
1:A:426:VAL:HG13	1:A:428:LEU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HD12	1:B:518:ASN:H	1.74	0.52
1:A:499:GLU:HG3	1:A:592:LYS:HG3	1.92	0.51
1:A:429:THR:C	1:A:430:ILE:HD13	2.35	0.51
1:B:578:LYS:O	1:B:581:PRO:HD3	2.10	0.51
1:B:463:TYR:HB2	1:B:465:MET:CE	2.35	0.51
1:A:550:THR:O	1:A:554:LEU:HD13	2.11	0.50
1:B:55:ARG:HD2	1:B:62:GLN:HG3	1.93	0.50
1:B:137:LEU:O	1:B:141:GLU:HG2	2.11	0.50
1:B:227:HIS:CD2	1:B:250:ASP:HB2	2.47	0.50
1:B:47:SER:HA	1:B:110:ASP:OD1	2.11	0.50
1:A:432:ASN:H	1:A:432:ASN:ND2	2.09	0.48
1:A:223:ILE:HD12	1:A:245:VAL:HB	1.95	0.48
1:A:466:GLU:HG3	1:A:532:ARG:HD2	1.95	0.48
1:B:104:LEU:HD22	1:B:377:LEU:CD1	2.43	0.48
1:B:481:ALA:HA	1:B:486:SER:O	2.13	0.48
1:B:297:ASP:HB3	1:B:314:ILE:O	2.14	0.47
1:B:339:ASP:OD2	1:B:343:LYS:HE2	2.14	0.47
1:B:573:PHE:C	1:B:573:PHE:CD1	2.92	0.47
1:B:412:THR:HG22	1:B:492:TYR:HB2	1.95	0.47
1:B:456:PHE:CE2	4:B:1590:A12:C4	2.98	0.47
1:B:255:TYR:CE2	1:B:273:LEU:HD22	2.50	0.47
1:A:104:LEU:HD13	1:A:377:LEU:HD12	1.97	0.46
1:B:453:PHE:CD2	1:B:573:PHE:HE2	2.24	0.46
1:B:541:VAL:HG13	1:B:548:TYR:CG	2.49	0.46
1:B:573:PHE:C	1:B:573:PHE:HD1	2.23	0.46
1:B:470:VAL:O	1:B:473:VAL:HG12	2.16	0.46
1:B:541:VAL:HG12	1:B:551:PHE:CE2	2.50	0.45
1:B:554:LEU:HD22	1:B:560:TYR:CE2	2.52	0.45
1:B:36:GLU:HB3	1:B:85:LYS:HD2	1.99	0.44
1:A:65:VAL:HG12	1:A:324:LEU:HD23	2.00	0.44
1:A:43:ASN:HB3	1:A:92:ALA:HB3	2.00	0.44
1:A:177:ILE:HD12	1:A:177:ILE:N	2.33	0.44
1:B:557:ASP:HA	1:B:558:PRO:HD2	1.84	0.44
1:A:277:ASN:HB2	1:A:278:PRO:CD	2.47	0.44
1:A:419:MET:O	1:A:423:LEU:HB2	2.17	0.44
1:B:580:HIS:O	1:B:581:PRO:C	2.60	0.43
1:B:517:LEU:HD12	1:B:518:ASN:N	2.32	0.43
1:A:241:ASN:O	1:A:242:ASP:HB2	2.18	0.43
1:A:369:LYS:O	1:A:373:GLU:HG3	2.18	0.43
1:B:541:VAL:HG13	1:B:548:TYR:CD2	2.53	0.43
1:B:546:ASP:CG	4:B:1590:A12:HO2'	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ASN:OD1	1:A:540:TYR:HB3	2.19	0.43
1:B:159:ILE:HG12	5:B:2065:HOH:O	2.18	0.43
1:A:499:GLU:HA	1:A:592:LYS:O	2.19	0.42
1:B:255:TYR:HE2	1:B:273:LEU:HD22	1.84	0.42
1:B:141:GLU:HB2	1:B:142:PRO:HD3	2.02	0.42
1:B:365:LYS:NZ	1:B:365:LYS:HB2	2.34	0.42
1:B:525:GLU:O	1:B:526:PRO:C	2.61	0.42
1:A:271:TYR:CD2	1:A:272:PRO:HD3	2.54	0.42
1:B:332:LYS:NZ	1:B:332:LYS:CB	2.82	0.42
1:A:369:LYS:HE3	1:A:369:LYS:HB2	1.56	0.42
1:B:132:GLY:HA2	1:B:193:SER:O	2.20	0.42
1:A:156:LYS:HA	1:A:161:TYR:CD1	2.54	0.42
1:A:557:ASP:C	1:A:557:ASP:OD1	2.63	0.42
1:B:281:GLU:HA	1:B:282:PRO:HD3	1.94	0.41
1:B:554:LEU:HD22	1:B:560:TYR:CD2	2.55	0.41
1:A:148:LEU:HA	1:A:165:LYS:O	2.21	0.41
1:A:382:VAL:HG22	1:A:445:VAL:O	2.20	0.41
1:A:478:MET:HE2	1:A:478:MET:HB3	1.94	0.41
1:B:429:THR:HA	1:B:536:GLY:O	2.20	0.41
1:A:153:ILE:HA	1:A:154:PRO:HD3	1.93	0.40
1:B:573:PHE:HD1	1:B:573:PHE:O	2.04	0.40
1:A:337:THR:O	1:A:340:GLU:HG3	2.21	0.40
1:A:426:VAL:HG12	1:A:428:LEU:H	1.86	0.40
1:B:462:THR:HA	1:B:535:VAL:O	2.21	0.40
1:B:271:TYR:HA	1:B:272:PRO:HA	1.95	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	558/579 (96%)	531 (95%)	23 (4%)	4 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	495/579 (86%)	477 (96%)	17 (3%)	1 (0%)	43	42
All	All	1053/1158 (91%)	1008 (96%)	40 (4%)	5 (0%)	24	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	PRO
1	A	424	LYS
1	B	250	ASP
1	A	506	ALA
1	A	250	ASP

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	471/483 (98%)	457 (97%)	14 (3%)	36	38
1	B	428/483 (89%)	418 (98%)	10 (2%)	44	49
All	All	899/966 (93%)	875 (97%)	24 (3%)	39	42

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	70	PHE
1	A	273	LEU
1	A	329	SER
1	A	332	LYS
1	A	352	LYS
1	A	365	LYS
1	A	418	THR
1	A	423	LEU
1	A	426	VAL
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	432	ASN
1	A	546	ASP
1	A	561	GLU
1	B	82	LYS
1	B	123	THR
1	B	273	LEU
1	B	332	LYS
1	B	365	LYS
1	B	381	ILE
1	B	382	VAL
1	B	465	MET
1	B	479	GLN
1	B	556	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	432	ASN
1	A	458	ASN
1	A	582	HIS
1	B	238	GLN
1	B	472	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	PO4	A	1597	2	4,4,4	0.86	0	6,6,6	0.89	0
4	A12	A	1598	-	26,29,29	1.58	7 (26%)	40,45,45	2.14	14 (35%)
4	A12	B	1590	-	26,29,29	1.70	7 (26%)	40,45,45	2.42	17 (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	A12	A	1598	-	-	5/16/32/32	0/3/3/3
4	A12	B	1590	-	-	6/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1590	A12	PB-O3B	-3.91	1.46	1.55
4	A	1598	A12	PB-O1B	3.78	1.57	1.50
4	B	1590	A12	PB-O1B	3.67	1.57	1.50
4	A	1598	A12	PB-O3B	-2.94	1.48	1.55
4	B	1590	A12	C6-N6	2.50	1.40	1.34
4	A	1598	A12	C6-N6	2.46	1.40	1.34
4	B	1590	A12	O3'-C3'	-2.41	1.37	1.43
4	B	1590	A12	O2'-C2'	-2.33	1.37	1.43
4	A	1598	A12	C5'-C4'	-2.33	1.44	1.51
4	A	1598	A12	O3'-C3'	-2.31	1.37	1.43
4	B	1590	A12	C5'-C4'	-2.31	1.44	1.51
4	A	1598	A12	O2'-C2'	-2.28	1.37	1.43
4	B	1590	A12	PA-O1A	2.28	1.56	1.51
4	A	1598	A12	C3'-C4'	-2.28	1.47	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1590	A12	O1A-PA-C3A	-5.87	93.59	109.05
4	B	1590	A12	C5-C4-N3	-4.87	120.02	126.72
4	A	1598	A12	N9-C8-N7	-4.83	107.08	113.94
4	B	1590	A12	N3-C2-N1	-4.48	121.81	128.58
4	A	1598	A12	C5-C4-N3	-4.44	120.60	126.72
4	B	1590	A12	N9-C8-N7	-4.40	107.70	113.94
4	A	1598	A12	C4-N9-C8	4.37	110.33	105.74
4	A	1598	A12	N3-C2-N1	-4.15	122.30	128.58
4	A	1598	A12	C5-N7-C8	3.98	109.71	103.45
4	B	1590	A12	C4-N9-C8	3.95	109.89	105.74
4	B	1590	A12	N3-C4-N9	3.86	133.74	127.17
4	B	1590	A12	C5-N7-C8	3.82	109.45	103.45
4	A	1598	A12	N3-C4-N9	3.61	133.31	127.17
4	B	1590	A12	C4-C5-N7	-3.38	106.72	110.58
4	A	1598	A12	C4-C5-N7	-3.32	106.79	110.58
4	B	1590	A12	O5'-C5'-C4'	3.25	120.06	108.99
4	A	1598	A12	O2A-PA-C3A	3.24	120.14	106.73
4	B	1590	A12	C2-N3-C4	3.18	119.59	111.83
4	B	1590	A12	O2A-PA-C3A	3.04	119.31	106.73
4	A	1598	A12	C2-N3-C4	2.91	118.95	111.83
4	B	1590	A12	O2A-PA-O1A	2.87	119.29	109.95
4	B	1590	A12	O2B-PB-O1B	-2.61	105.64	112.39
4	A	1598	A12	O5'-C5'-C4'	2.54	117.66	108.99
4	B	1590	A12	O1B-PB-C3A	-2.27	106.43	111.37
4	A	1598	A12	O2B-PB-O1B	-2.26	106.54	112.39
4	B	1590	A12	O4'-C4'-C3'	-2.26	100.67	105.15
4	A	1598	A12	O1A-PA-C3A	-2.18	103.31	109.05
4	B	1590	A12	O2B-PB-C3A	2.15	111.61	106.40
4	A	1598	A12	O2A-PA-O1A	2.10	116.77	109.95
4	A	1598	A12	O4'-C4'-C3'	-2.07	101.04	105.15
4	B	1590	A12	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1598	A12	PB-C3A-PA-O1A
4	A	1598	A12	PB-C3A-PA-O2A
4	A	1598	A12	C5'-O5'-PA-O1A
4	A	1598	A12	C4'-C5'-O5'-PA
4	B	1590	A12	PB-C3A-PA-O1A
4	B	1590	A12	PB-C3A-PA-O2A
4	B	1590	A12	C5'-O5'-PA-O2A

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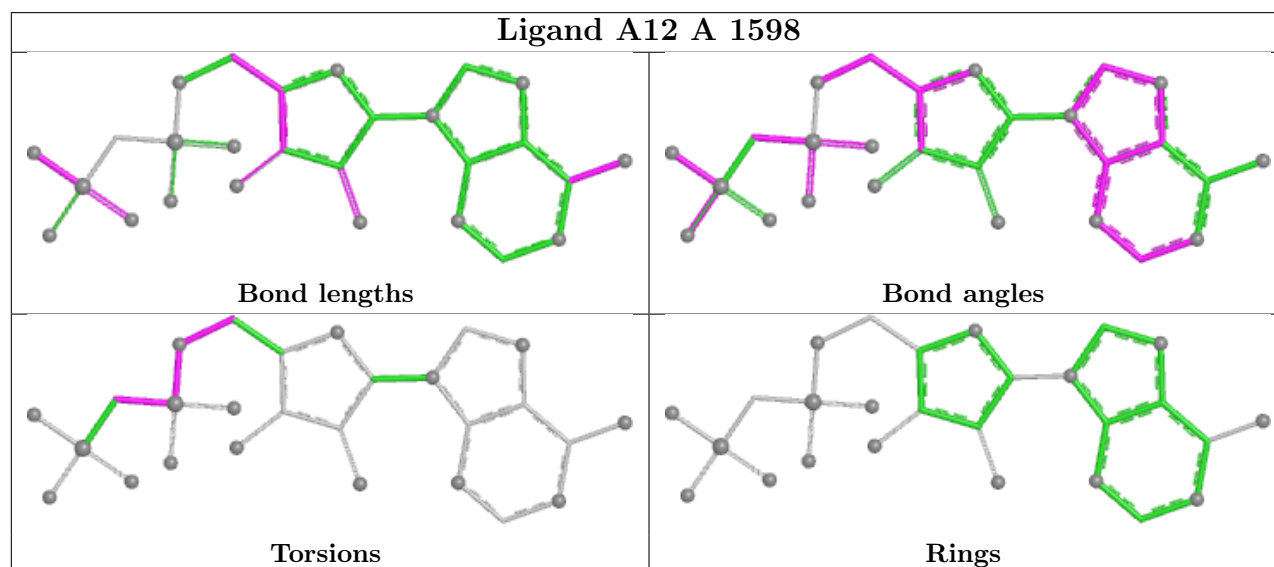
Mol	Chain	Res	Type	Atoms
4	B	1590	A12	C3'-C4'-C5'-O5'
4	B	1590	A12	O4'-C4'-C5'-O5'
4	A	1598	A12	C5'-O5'-PA-O2A
4	B	1590	A12	C5'-O5'-PA-C3A

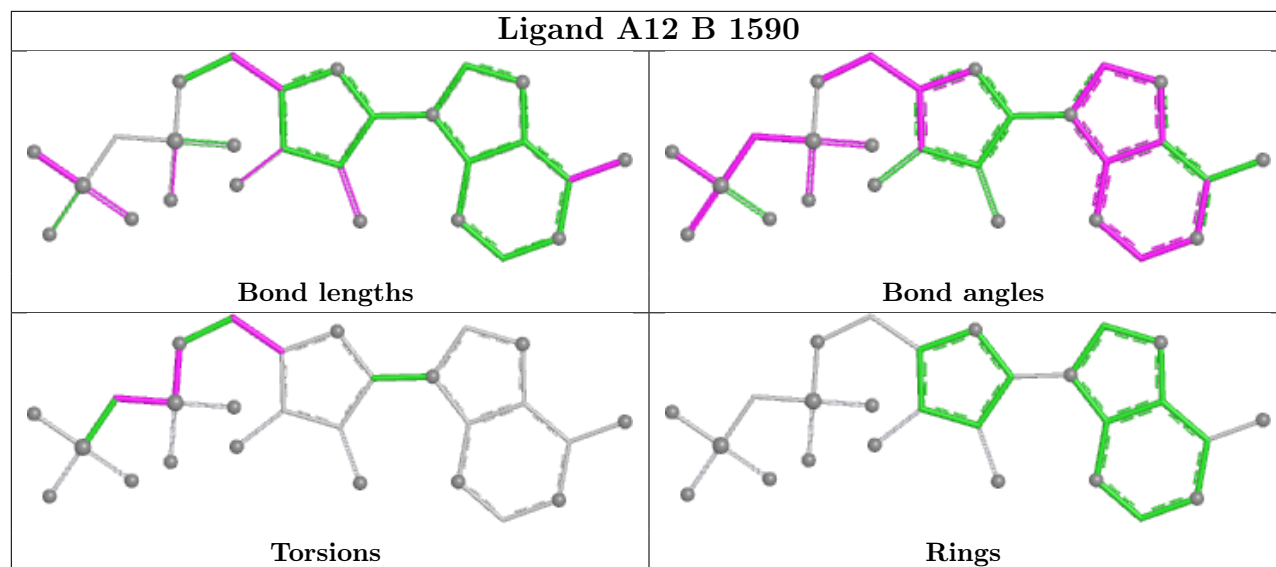
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1598	A12	1	0
4	B	1590	A12	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	562/579 (97%)	0.34	28 (4%) 34 33	23, 33, 51, 68	0
1	B	504/579 (87%)	0.83	72 (14%) 6 5	25, 36, 62, 85	0
All	All	1066/1158 (92%)	0.57	100 (9%) 14 13	23, 34, 57, 85	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	TYR	7.4
1	B	583	PHE	7.2
1	B	383	GLY	6.4
1	B	585	ALA	6.4
1	B	382	VAL	6.2
1	B	587	THR	6.1
1	B	517	LEU	6.0
1	B	555	PHE	5.5
1	B	501	ASN	5.4
1	B	453	PHE	5.4
1	A	506	ALA	5.3
1	B	485	GLY	5.2
1	B	381	ILE	4.9
1	B	581	PRO	4.7
1	B	449	ASP	4.6
1	B	377	LEU	4.5
1	B	445	VAL	4.5
1	B	580	HIS	4.4
1	B	518	ASN	4.4
1	A	508	GLY	4.2
1	B	434	GLY	4.1
1	A	521	THR	4.1
1	B	582	HIS	3.9
1	B	584	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	579	LYS	3.7
1	B	465	MET	3.7
1	B	484	ASP	3.6
1	B	451	TYR	3.6
1	B	549	LYS	3.6
1	B	422	GLU	3.6
1	B	553	LYS	3.4
1	B	450	ALA	3.4
1	A	380	GLU	3.3
1	B	33	LYS	3.3
1	B	481	ALA	3.2
1	B	412	THR	3.2
1	B	552	GLY	3.2
1	B	560	TYR	3.1
1	B	509	LYS	3.1
1	B	545	LYS	3.1
1	B	50	GLU	3.1
1	B	557	ASP	3.1
1	B	576	PHE	3.0
1	A	425	THR	3.0
1	A	334	ALA	3.0
1	A	423	LEU	2.9
1	B	423	LEU	2.9
1	B	544	GLY	2.8
1	A	337	THR	2.8
1	B	455	PRO	2.7
1	A	174	GLY	2.7
1	B	486	SER	2.6
1	B	541	VAL	2.6
1	B	551	PHE	2.6
1	B	478	MET	2.6
1	A	338	GLY	2.6
1	B	380	GLU	2.5
1	A	376	ARG	2.5
1	A	368	ALA	2.5
1	B	500	ALA	2.5
1	B	414	PHE	2.5
1	B	480	PHE	2.5
1	B	421	ASN	2.5
1	B	542	ALA	2.4
1	B	524	TRP	2.4
1	B	558	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	368	ALA	2.4
1	A	428	LEU	2.4
1	A	339	ASP	2.4
1	A	322	HIS	2.4
1	A	558	PRO	2.4
1	A	507	GLU	2.3
1	A	556	ASN	2.3
1	B	456	PHE	2.3
1	A	379	GLN	2.3
1	B	543	GLY	2.3
1	A	330	GLU	2.3
1	B	334	ALA	2.3
1	A	82	LYS	2.3
1	B	452	THR	2.3
1	A	532	ARG	2.3
1	B	577	MET	2.3
1	A	426	VAL	2.2
1	A	571	GLU	2.2
1	B	426	VAL	2.2
1	A	340	GLU	2.2
1	A	422	GLU	2.2
1	A	173	ASP	2.2
1	B	529	ASP	2.2
1	B	571	GLU	2.1
1	B	457	GLY	2.1
1	B	339	ASP	2.1
1	B	487	THR	2.1
1	B	156	LYS	2.1
1	A	505	ASN	2.1
1	B	483	VAL	2.1
1	B	454	LEU	2.0
1	B	482	LEU	2.0
1	B	332	LYS	2.0
1	B	540	TYR	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](#)

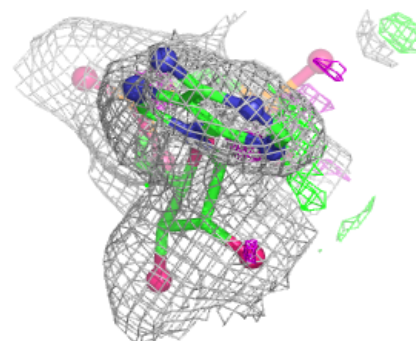
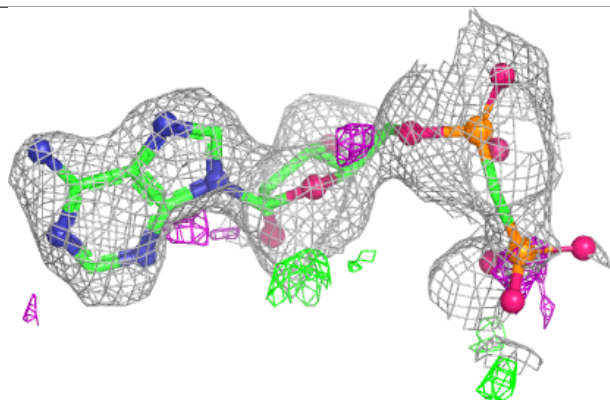
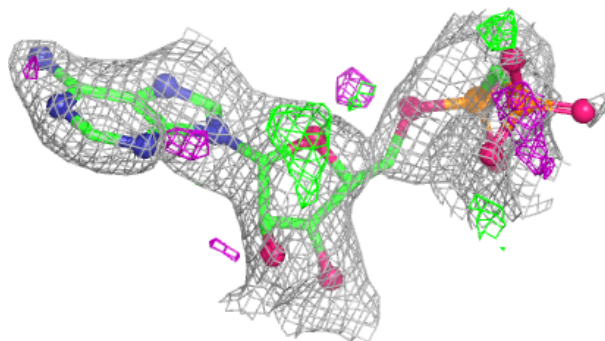
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	A12	B	1590	27/27	0.67	0.16	52,62,87,98	0
4	A12	A	1598	27/27	0.93	0.09	24,28,51,53	0
3	PO4	A	1597	5/5	0.96	0.10	31,33,44,45	0
2	ZN	B	1589	1/1	1.00	0.02	27,27,27,27	0
2	ZN	A	1595	1/1	1.00	0.01	28,28,28,28	0
2	ZN	A	1596	1/1	1.00	0.01	28,28,28,28	0
2	ZN	B	1588	1/1	1.00	0.02	27,27,27,27	0

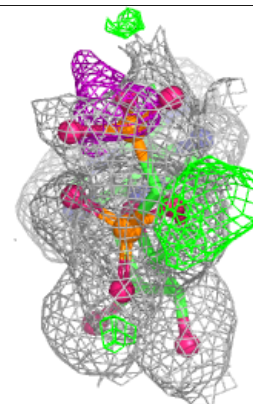
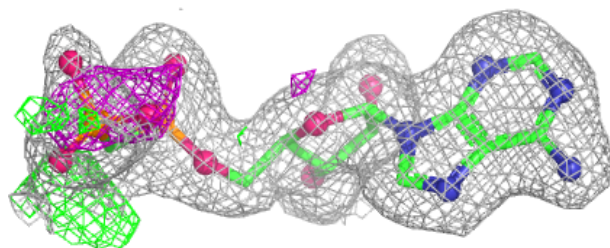
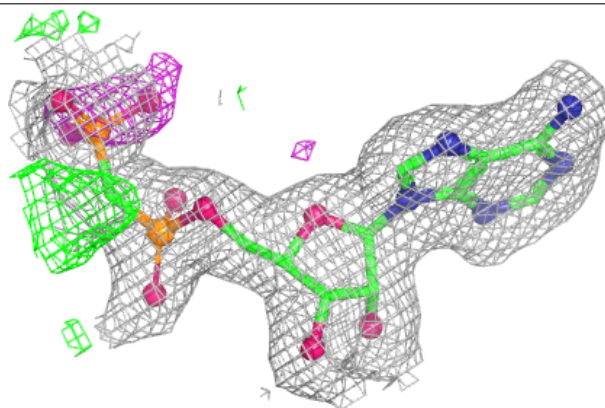
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A12 B 1590:

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

**Electron density around A12 A 1598:**

$2mF_o-DF_c$ (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.