



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:09 PM UTC

PDB ID : 2OD2 / pdb_00002od2
Title : Crystal Structure of yHst2 I117F mutant bound to carba-NAD⁺ and an acetylated H4 peptide
Authors : Sanders, B.D.
Deposited on : 2006-12-21
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

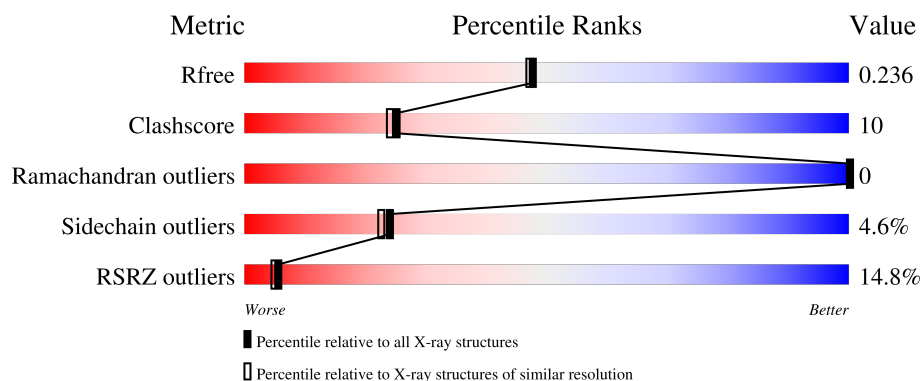
1 Overall quality at a glance

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	308	
2	B	14	

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
4	CNA	A	1001	X	-	-	-
5	GOL	A	1989	-	X	-	-
5	GOL	A	1990	-	X	-	-
5	GOL	A	1991	-	X	-	-
5	GOL	A	1992	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2602 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-dependent deacetylase HST2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2312	1494	380	426	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P53686
A	-12	ARG	-	cloning artifact	UNP P53686
A	-11	GLY	-	cloning artifact	UNP P53686
A	-10	SER	-	cloning artifact	UNP P53686
A	-9	HIS	-	expression tag	UNP P53686
A	-8	HIS	-	expression tag	UNP P53686
A	-7	HIS	-	expression tag	UNP P53686
A	-6	HIS	-	expression tag	UNP P53686
A	-5	HIS	-	expression tag	UNP P53686
A	-4	HIS	-	expression tag	UNP P53686
A	-3	GLY	-	cloning artifact	UNP P53686
A	-2	MET	-	cloning artifact	UNP P53686
A	-1	ALA	-	cloning artifact	UNP P53686
A	0	SER	-	cloning artifact	UNP P53686
A	117	PHE	ILE	engineered mutation	UNP P53686

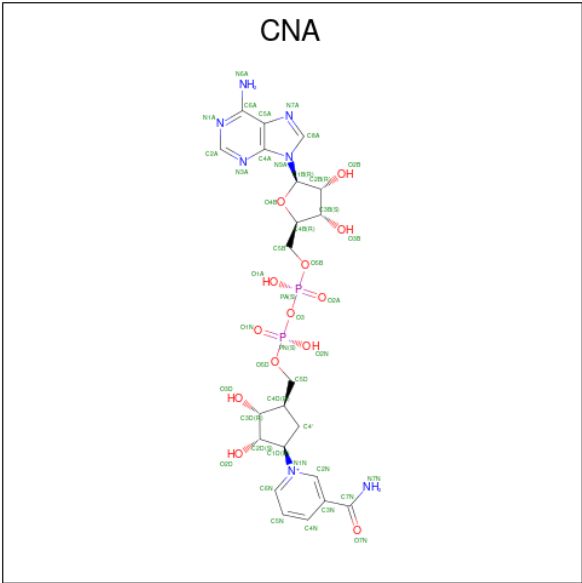
- Molecule 2 is a protein called Acetylated H4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			55	33	14	8			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

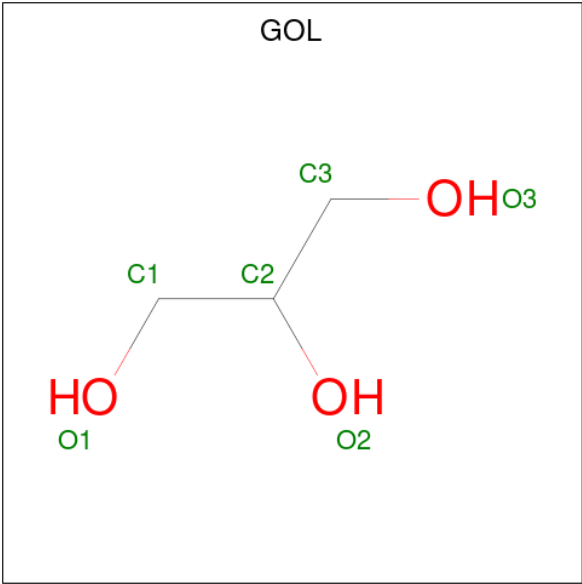
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CARBA-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: CNA) (formula: C₂₂H₃₀N₇O₁₃P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	22	7	13	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

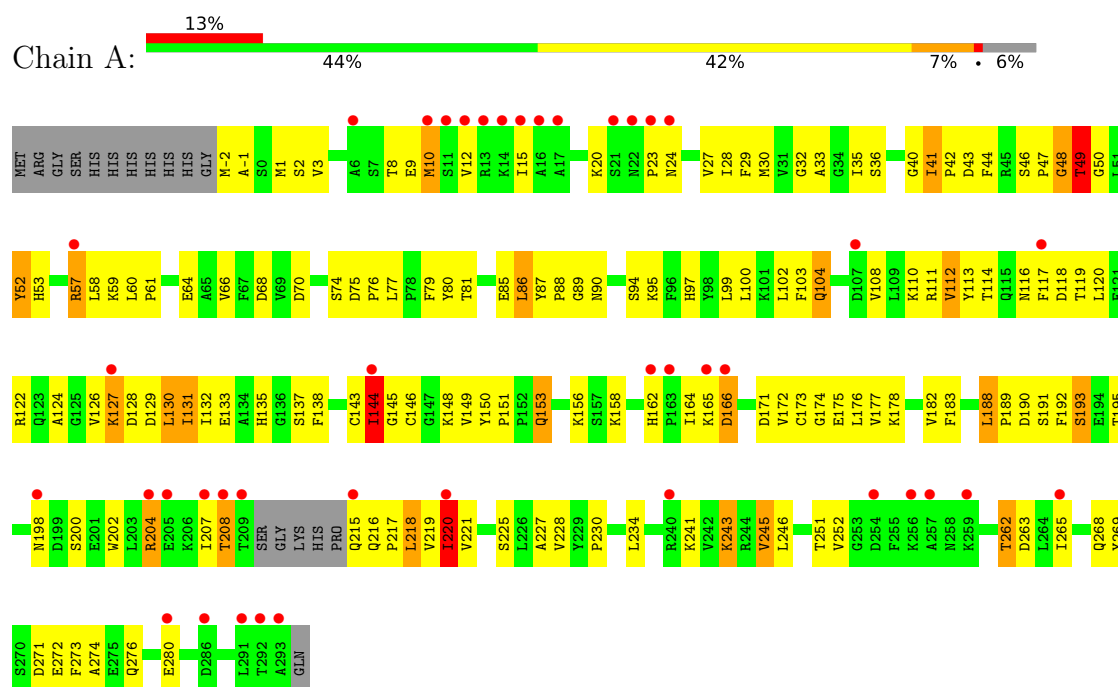
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	160	Total O 160 160	0	0
6	B	6	Total O 6 6	0	0

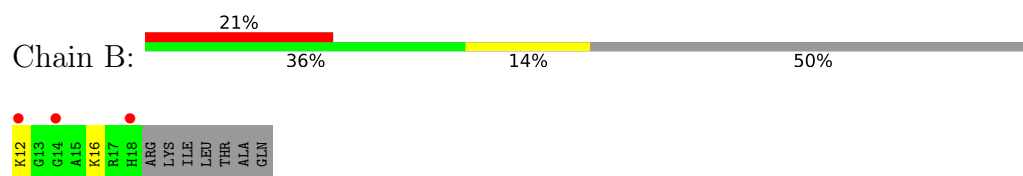
3 Residue-property plots [i](#)

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-dependent deacetylase HST2



• Molecule 2: Acetylated H4 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.64Å 106.64Å 67.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.89 – 2.00 41.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (41.89-2.00) 86.0 (41.89-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.233 0.240 , 0.236	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2602	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 4.21% 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, GOL, ALY, CNA

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	2.53	136/2372 (5.7%)	1.89	51/3215 (1.6%)
2	B	0.34	0/42	0.61	0/51
All	All	2.51	136/2414 (5.6%)	1.88	51/3266 (1.6%)

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

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

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ASP	N-CA	15.31	1.66	1.46
1	A	79	PHE	C-O	11.15	1.36	1.24
1	A	216	GLN	CA-C	10.45	1.64	1.52
1	A	193	SER	C-O	10.00	1.35	1.24
1	A	269	TYR	C-O	9.82	1.35	1.23
1	A	28	ILE	CA-CB	-9.72	1.42	1.54
1	A	10	MET	SD-CE	9.71	2.03	1.79
1	A	143	CYS	C-O	9.67	1.35	1.23
1	A	122	ARG	C-O	9.63	1.35	1.24
1	A	156	LYS	C-O	9.13	1.34	1.24
1	A	112	VAL	CA-CB	8.76	1.64	1.54
1	A	166	ASP	CA-C	8.43	1.61	1.53
1	A	88	PRO	CA-C	-8.30	1.42	1.52
1	A	64	GLU	CA-C	8.22	1.63	1.52
1	A	273	PHE	N-CA	8.15	1.56	1.46
1	A	221	VAL	CA-CB	-7.95	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	HIS	CA-C	7.91	1.63	1.52
1	A	131	ILE	CA-CB	7.87	1.64	1.54
1	A	262	THR	CA-C	7.78	1.63	1.52
1	A	144	ILE	CA-CB	7.70	1.64	1.54
1	A	208	THR	CA-C	7.65	1.63	1.53
1	A	119	THR	CA-CB	7.59	1.65	1.53
1	A	85	GLU	CA-C	7.42	1.62	1.52
1	A	191	SER	C-O	7.40	1.33	1.24
1	A	219	VAL	C-O	7.33	1.31	1.24
1	A	79	PHE	N-CA	7.30	1.55	1.46
1	A	156	LYS	CD-CE	7.21	1.74	1.52
1	A	120	LEU	C-O	7.19	1.33	1.24
1	A	116	ASN	CG-OD1	7.14	1.37	1.23
1	A	252	VAL	C-O	-7.14	1.16	1.23
1	A	245	VAL	CA-C	7.07	1.60	1.52
1	A	188	LEU	CA-C	7.05	1.62	1.53
1	A	80	TYR	CA-CB	7.02	1.64	1.53
1	A	189	PRO	CA-C	7.01	1.61	1.52
1	A	111	ARG	N-CA	6.92	1.54	1.46
1	A	30	MET	SD-CE	6.91	1.96	1.79
1	A	246	LEU	CA-C	-6.74	1.44	1.52
1	A	75	ASP	CA-C	6.71	1.61	1.52
1	A	-1	ALA	N-CA	6.62	1.54	1.46
1	A	192	PHE	C-O	6.59	1.32	1.24
1	A	86	LEU	CG-CD2	6.50	1.74	1.52
1	A	162	HIS	CA-C	6.47	1.61	1.52
1	A	119	THR	C-N	-6.42	1.25	1.33
1	A	48	GLY	N-CA	6.38	1.55	1.44
1	A	95	LYS	CG-CD	6.37	1.71	1.52
1	A	32	GLY	N-CA	6.35	1.54	1.45
1	A	24	ASN	N-CA	6.33	1.53	1.46
1	A	47	PRO	C-N	-6.32	1.23	1.33
1	A	124	ALA	C-O	6.32	1.32	1.24
1	A	165	LYS	CA-C	6.28	1.60	1.52
1	A	42	PRO	CA-CB	6.27	1.62	1.53
1	A	228	VAL	CA-CB	6.24	1.61	1.54
1	A	200	SER	C-O	6.20	1.31	1.24
1	A	124	ALA	CA-C	6.20	1.61	1.52
1	A	86	LEU	C-O	-6.15	1.15	1.24
1	A	228	VAL	N-CA	-6.13	1.39	1.46
1	A	90	ASN	CA-C	6.11	1.60	1.52
1	A	198	ASN	N-CA	6.07	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ASP	CB-CG	6.02	1.67	1.52
1	A	79	PHE	CB-CG	5.97	1.64	1.50
1	A	219	VAL	CA-C	5.96	1.60	1.52
1	A	228	VAL	C-O	5.95	1.30	1.24
1	A	133	GLU	CA-C	-5.93	1.45	1.52
1	A	132	ILE	CA-CB	5.93	1.62	1.54
1	A	119	THR	N-CA	5.89	1.55	1.46
1	A	198	ASN	CB-CG	5.89	1.66	1.52
1	A	193	SER	N-CA	5.89	1.53	1.46
1	A	143	CYS	CA-CB	5.88	1.62	1.53
1	A	114	THR	CA-C	5.88	1.59	1.52
1	A	40	GLY	CA-C	5.87	1.59	1.51
1	A	274	ALA	CA-CB	5.85	1.62	1.53
1	A	74	SER	C-O	5.83	1.31	1.24
1	A	43	ASP	CA-C	5.81	1.59	1.52
1	A	81	THR	CA-C	5.80	1.60	1.52
1	A	234	LEU	C-O	5.80	1.30	1.24
1	A	268	GLN	CD-OE1	5.77	1.34	1.23
1	A	24	ASN	CA-C	5.77	1.60	1.52
1	A	137	SER	CA-CB	5.76	1.62	1.53
1	A	75	ASP	CA-CB	5.74	1.62	1.53
1	A	272	GLU	CA-C	5.74	1.60	1.52
1	A	8	THR	CA-CB	5.72	1.62	1.53
1	A	41	ILE	CA-C	5.70	1.58	1.52
1	A	43	ASP	C-O	5.68	1.31	1.24
1	A	274	ALA	C-O	5.68	1.30	1.24
1	A	246	LEU	N-CA	5.67	1.52	1.46
1	A	227	ALA	CA-C	-5.66	1.45	1.52
1	A	149	VAL	N-CA	5.65	1.53	1.46
1	A	110	LYS	CG-CD	5.64	1.69	1.52
1	A	80	TYR	N-CA	5.60	1.53	1.46
1	A	48	GLY	CA-C	5.59	1.59	1.51
1	A	61	PRO	C-O	5.58	1.30	1.24
1	A	3	VAL	CA-CB	5.57	1.62	1.54
1	A	122	ARG	CG-CD	5.55	1.69	1.52
1	A	2	SER	C-N	-5.49	1.27	1.33
1	A	44	PHE	CA-C	5.49	1.60	1.52
1	A	20	LYS	CA-C	5.48	1.59	1.52
1	A	129	ASP	CA-CB	5.47	1.62	1.53
1	A	66	VAL	CA-CB	5.42	1.62	1.54
1	A	165	LYS	CG-CD	5.40	1.68	1.52
1	A	172	VAL	C-O	5.38	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ILE	CA-CB	5.38	1.60	1.54
1	A	174	GLY	N-CA	5.37	1.53	1.45
1	A	263	ASP	N-CA	5.32	1.53	1.46
1	A	195	THR	C-O	-5.29	1.17	1.24
1	A	68	ASP	N-CA	5.27	1.52	1.46
1	A	95	LYS	CA-C	5.27	1.59	1.52
1	A	80	TYR	CA-C	5.26	1.59	1.52
1	A	50	GLY	C-O	5.25	1.30	1.23
1	A	60	LEU	C-O	5.24	1.30	1.24
1	A	128	ASP	CA-CB	5.23	1.61	1.53
1	A	87	TYR	CA-C	5.20	1.58	1.53
1	A	271	ASP	CA-C	5.17	1.59	1.52
1	A	28	ILE	N-CA	5.16	1.52	1.46
1	A	2	SER	C-O	-5.15	1.17	1.23
1	A	200	SER	CA-C	5.15	1.59	1.52
1	A	76	PRO	C-O	5.15	1.30	1.24
1	A	29	PHE	CA-C	5.14	1.58	1.52
1	A	10	MET	N-CA	5.13	1.52	1.46
1	A	148	LYS	C-O	-5.12	1.17	1.23
1	A	94	SER	CA-C	5.11	1.60	1.53
1	A	99	LEU	N-CA	5.11	1.52	1.46
1	A	273	PHE	C-O	5.11	1.30	1.24
1	A	100	LEU	CA-CB	5.10	1.61	1.53
1	A	172	VAL	CA-C	5.09	1.60	1.53
1	A	135	HIS	N-CA	5.07	1.52	1.46
1	A	183	PHE	CA-C	5.06	1.60	1.53
1	A	263	ASP	CB-CG	-5.06	1.39	1.52
1	A	225	SER	CA-CB	5.05	1.62	1.53
1	A	102	LEU	N-CA	5.05	1.52	1.46
1	A	52	TYR	N-CA	-5.05	1.40	1.46
1	A	1	MET	CG-SD	5.03	1.93	1.80
1	A	12	VAL	CA-CB	5.02	1.61	1.54
1	A	81	THR	C-N	-5.01	1.27	1.33
1	A	113	TYR	N-CA	5.01	1.52	1.46
1	A	164	ILE	CA-C	5.00	1.58	1.52
1	A	177	VAL	CA-CB	-5.00	1.48	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	PRO	CA-C-N	-15.15	100.33	122.46
1	A	47	PRO	C-N-CA	-15.15	100.33	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	N-CA-C	11.41	135.10	110.80
1	A	151	PRO	O-C-N	9.29	125.58	121.31
1	A	46	SER	CA-C-O	8.55	125.65	119.32
1	A	146	CYS	N-CA-C	8.08	124.22	113.72
1	A	138	PHE	N-CA-C	7.77	122.43	113.19
1	A	158	LYS	N-CA-C	7.76	119.74	111.28
1	A	49	THR	N-CA-CB	-7.40	98.24	110.23
1	A	46	SER	N-CA-C	7.28	119.36	109.24
1	A	77	LEU	O-C-N	7.27	126.12	120.38
1	A	276	GLN	N-CA-C	-7.13	103.59	111.36
1	A	47	PRO	O-C-N	-7.07	114.09	122.86
1	A	8	THR	N-CA-C	-6.91	104.05	113.30
1	A	108	VAL	N-CA-C	6.67	118.71	111.77
1	A	48	GLY	N-CA-C	6.63	122.97	115.08
1	A	178	LYS	CA-C-N	6.58	126.60	119.89
1	A	178	LYS	C-N-CA	6.58	126.60	119.89
1	A	79	PHE	CA-C-O	6.54	127.68	120.82
1	A	35	ILE	N-CA-C	6.50	121.02	112.76
1	A	33	ALA	N-CA-C	6.48	120.29	112.38
1	A	89	GLY	CA-C-O	6.45	126.13	118.97
1	A	172	VAL	N-CA-C	-6.37	105.49	111.48
1	A	88	PRO	CA-C-O	6.35	128.58	121.34
1	A	183	PHE	O-C-N	-6.27	115.91	122.94
1	A	103	PHE	N-CA-C	-6.25	104.55	111.36
1	A	49	THR	CA-CB-OG1	6.12	118.78	109.60
1	A	143	CYS	CA-CB-SG	-6.05	100.48	114.40
1	A	79	PHE	O-C-N	-5.87	116.02	122.07
1	A	251	THR	OG1-CB-CG2	-5.86	97.59	109.30
1	A	23	PRO	N-CA-C	5.76	121.06	113.86
1	A	171	ASP	N-CA-C	5.74	120.03	113.19
1	A	122	ARG	N-CA-C	5.73	117.53	111.28
1	A	204	ARG	CG-CD-NE	-5.66	99.55	112.00
1	A	177	VAL	N-CA-C	-5.61	100.33	108.36
1	A	49	THR	CA-C-N	5.58	126.28	120.03
1	A	49	THR	C-N-CA	5.58	126.28	120.03
1	A	50	GLY	CA-C-O	-5.54	115.37	120.80
1	A	104	GLN	N-CA-C	5.50	116.95	111.07
1	A	220	ILE	N-CA-CB	-5.48	104.52	111.64
1	A	15	ILE	O-C-N	5.37	127.48	121.90
1	A	70	ASP	CB-CG-OD2	5.36	130.74	118.40
1	A	127	LYS	N-CA-C	5.34	117.97	110.23
1	A	81	THR	CA-C-O	-5.33	115.23	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	CB-CG-CD	5.28	123.44	111.30
1	A	130	LEU	N-CA-C	5.27	119.71	113.28
1	A	150	TYR	O-C-N	5.20	127.40	121.94
1	A	100	LEU	N-CA-C	-5.13	105.60	111.14
1	A	188	LEU	O-C-N	-5.13	116.16	121.60
1	A	173	CYS	N-CA-C	5.11	119.66	113.38
1	A	87	TYR	CA-C-O	-5.08	114.89	120.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2312	0	2290	45	0
2	B	55	0	57	5	0
3	A	1	0	0	0	0
4	A	44	0	26	0	0
5	A	24	0	16	2	0
6	A	160	0	0	1	0
6	B	6	0	0	1	0
All	All	2602	0	2389	47	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 10.

All (47) 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:10:MET:SD	1:A:10:MET:CE	2.03	1.46
1:A:9:GLU:OE2	1:A:280:GLU:OE2	1.85	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:HE22	1:A:127:LYS:H	1.17	0.88
1:A:48:GLY:H	1:A:53:HIS:HE1	1.19	0.86
5:A:1990:GOL:H11	6:A:2004:HOH:O	1.77	0.83
1:A:144:ILE:HD11	1:A:175:GLU:HB3	1.60	0.81
1:A:144:ILE:CD1	1:A:175:GLU:HB3	2.16	0.76
1:A:48:GLY:H	1:A:53:HIS:CE1	2.06	0.74
1:A:220:ILE:HD13	1:A:245:VAL:HB	1.69	0.73
1:A:220:ILE:HD13	1:A:245:VAL:CB	2.19	0.72
1:A:207:ILE:HD13	1:A:241:LYS:HB2	1.72	0.70
1:A:243:LYS:NZ	1:A:262:THR:O	2.28	0.66
1:A:207:ILE:HG22	1:A:207:ILE:O	1.94	0.66
1:A:53:HIS:O	1:A:57:ARG:HG3	1.96	0.65
1:A:49:THR:CG2	1:A:52:TYR:H	2.11	0.63
1:A:144:ILE:HD12	1:A:176:LEU:O	1.99	0.62
1:A:104:GLN:HE22	1:A:127:LYS:N	1.95	0.61
1:A:104:GLN:NE2	1:A:127:LYS:H	1.95	0.60
1:A:190:ASP:HA	2:B:12:LYS:HE2	1.84	0.58
1:A:144:ILE:HD13	1:A:145:GLY:N	2.18	0.58
1:A:36:SER:HB3	1:A:41:ILE:HD12	1.85	0.57
1:A:153:GLN:HE21	1:A:153:GLN:H	1.54	0.54
1:A:49:THR:HG22	1:A:52:TYR:HB3	1.88	0.54
1:A:265:ILE:N	1:A:265:ILE:HD12	2.25	0.52
1:A:202:TRP:HE1	5:A:1992:GOL:H12	1.74	0.51
1:A:41:ILE:HG23	1:A:86:LEU:HD22	1.93	0.51
1:A:49:THR:HG23	1:A:52:TYR:H	1.76	0.50
1:A:193:SER:HB2	2:B:12:LYS:HD2	1.94	0.50
1:A:49:THR:HG22	1:A:52:TYR:CB	2.42	0.50
1:A:104:GLN:HE21	1:A:130:LEU:HD12	1.76	0.49
1:A:58:LEU:O	1:A:59:LYS:HB2	2.13	0.49
1:A:126:VAL:HG12	1:A:131:ILE:HG13	1.94	0.49
1:A:144:ILE:HD12	1:A:144:ILE:H	1.76	0.49
1:A:207:ILE:O	1:A:207:ILE:CG2	2.63	0.47
1:A:153:GLN:H	1:A:153:GLN:NE2	2.13	0.45
1:A:27:VAL:HA	1:A:218:LEU:O	2.16	0.45
1:A:190:ASP:HA	2:B:12:LYS:CE	2.46	0.45
1:A:49:THR:HG22	1:A:52:TYR:H	1.82	0.45
1:A:144:ILE:HD13	1:A:144:ILE:C	2.42	0.45
2:B:12:LYS:HG3	6:B:49:HOH:O	2.17	0.45
1:A:204:ARG:HG2	1:A:204:ARG:NH1	2.33	0.44
1:A:193:SER:CB	2:B:12:LYS:HD2	2.49	0.42
1:A:188:LEU:HD22	1:A:230:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:O	1:A:59:LYS:CB	2.68	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.95	0.41
1:A:182:VAL:HG11	1:A:188:LEU:HD12	2.02	0.40
1:A:220:ILE:HD13	1:A:245:VAL:CG2	2.50	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	287/308 (93%)	276 (96%)	11 (4%)	0	100	100
2	B	4/14 (29%)	4 (100%)	0	0	100	100
All	All	291/322 (90%)	280 (96%)	11 (4%)	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	256/271 (94%)	244 (95%)	12 (5%)	23	22
2	B	3/9 (33%)	3 (100%)	0	100	100
All	All	259/280 (92%)	247 (95%)	12 (5%)	24	22

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	MET
1	A	49	THR
1	A	112	VAL
1	A	144	ILE
1	A	153	GLN
1	A	166	ASP
1	A	208	THR
1	A	215	GLN
1	A	217	PRO
1	A	218	LEU
1	A	220	ILE
1	A	243	LYS

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	18	HIS
1	A	53	HIS
1	A	73	GLN
1	A	104	GLN
1	A	123	GLN
1	A	153	GLN
1	A	162	HIS
1	A	215	GLN
1	A	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	ALY	B	16	2	10,11,12	1.53	2 (20%)	7,12,14	2.14	1 (14%)

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
2	ALY	B	16	2	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	ALY	OH-CH	3.13	1.30	1.23
2	B	16	ALY	CH-NZ	3.04	1.42	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	ALY	CE-NZ-CH	-5.37	114.63	122.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	1991	-	5,5,5	3.93	3 (60%)	5,5,5	5.63	4 (80%)
5	GOL	A	1990	-	5,5,5	4.00	3 (60%)	5,5,5	5.64	4 (80%)
4	CNA	A	1001	-	47,48,48	4.83	28 (59%)	65,73,73	2.77	26 (40%)
5	GOL	A	1992	-	5,5,5	4.06	3 (60%)	5,5,5	5.65	4 (80%)
5	GOL	A	1989	-	5,5,5	3.99	3 (60%)	5,5,5	5.58	4 (80%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1991	-	-	2/4/4/4	-
5	GOL	A	1990	-	-	2/4/4/4	-
4	CNA	A	1001	-	1/1/11/11	10/28/62/62	0/5/5/5
5	GOL	A	1992	-	-	2/4/4/4	-
5	GOL	A	1989	-	-	2/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	CNA	C2N-N1N	15.20	1.51	1.35
4	A	1001	CNA	O7N-C7N	10.02	1.42	1.24
4	A	1001	CNA	PA-O3	-9.92	1.48	1.59
4	A	1001	CNA	PN-O3	-9.64	1.49	1.59
4	A	1001	CNA	C4A-N3A	8.84	1.50	1.34
4	A	1001	CNA	C6N-N1N	8.30	1.54	1.35
5	A	1992	GOL	C3-C2	-7.85	1.21	1.51
5	A	1989	GOL	C3-C2	-7.76	1.22	1.51
5	A	1990	GOL	C3-C2	-7.76	1.22	1.51
5	A	1991	GOL	C3-C2	-7.58	1.22	1.51
4	A	1001	CNA	C4N-C3N	7.08	1.50	1.39
4	A	1001	CNA	C2A-N1A	7.06	1.46	1.33
4	A	1001	CNA	C4D-C3D	-6.37	1.36	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	CNA	C5N-C4N	5.30	1.48	1.38
4	A	1001	CNA	C7N-N7N	5.23	1.42	1.33
4	A	1001	CNA	C6A-N1A	4.56	1.48	1.35
4	A	1001	CNA	C4'-C4D	-4.45	1.42	1.53
4	A	1001	CNA	C4'-C1D	-4.43	1.38	1.53
4	A	1001	CNA	C2A-N3A	4.28	1.41	1.33
4	A	1001	CNA	O2D-C2D	-4.05	1.32	1.43
4	A	1001	CNA	C6N-C5N	3.93	1.46	1.38
4	A	1001	CNA	C2N-C3N	3.77	1.45	1.39
4	A	1001	CNA	C8A-N7A	3.71	1.38	1.31
4	A	1001	CNA	C5A-C4A	3.56	1.45	1.39
5	A	1992	GOL	C1-C2	-3.26	1.39	1.51
4	A	1001	CNA	C5A-C6A	3.24	1.50	1.41
5	A	1991	GOL	C1-C2	-3.10	1.40	1.51
5	A	1990	GOL	C1-C2	-3.06	1.40	1.51
4	A	1001	CNA	PN-O2N	-3.01	1.41	1.55
5	A	1989	GOL	C1-C2	-2.97	1.40	1.51
5	A	1989	GOL	O2-C2	-2.93	1.34	1.43
5	A	1990	GOL	O2-C2	-2.91	1.34	1.43
5	A	1992	GOL	O2-C2	-2.90	1.34	1.43
5	A	1991	GOL	O2-C2	-2.89	1.35	1.43
4	A	1001	CNA	C8A-N9A	2.73	1.42	1.37
4	A	1001	CNA	O3D-C3D	2.61	1.49	1.43
4	A	1001	CNA	C2B-C1B	-2.51	1.45	1.53
4	A	1001	CNA	C3B-C4B	-2.27	1.47	1.53
4	A	1001	CNA	PN-O5D	-2.17	1.50	1.59
4	A	1001	CNA	PA-O5B	-2.04	1.51	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1991	GOL	O2-C2-C3	9.88	150.09	109.18
5	A	1990	GOL	O2-C2-C3	9.87	150.05	109.18
5	A	1992	GOL	O2-C2-C3	9.86	150.02	109.18
5	A	1989	GOL	O2-C2-C3	9.81	149.79	109.18
4	A	1001	CNA	C4'-C1D-N1N	-7.59	103.97	113.50
4	A	1001	CNA	O3D-C3D-C4D	6.68	130.00	112.56
5	A	1991	GOL	O3-C3-C2	6.66	140.35	110.38
5	A	1990	GOL	O3-C3-C2	6.61	140.12	110.38
5	A	1992	GOL	O3-C3-C2	6.59	140.06	110.38
5	A	1989	GOL	O3-C3-C2	6.51	139.71	110.38
4	A	1001	CNA	O2N-PN-O5D	6.38	136.48	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	CNA	O5D-PN-O1N	-5.39	87.59	108.94
4	A	1001	CNA	C5N-C6N-N1N	-5.00	113.56	120.38
4	A	1001	CNA	O2N-PN-O3	4.90	120.50	107.27
4	A	1001	CNA	N3A-C2A-N1A	-4.70	121.47	128.58
4	A	1001	CNA	O7N-C7N-C3N	-4.41	114.21	119.60
4	A	1001	CNA	C4A-N9A-C1B	-4.40	116.33	126.63
4	A	1001	CNA	C1B-N9A-C8A	4.10	136.19	127.09
4	A	1001	CNA	C4'-C4D-C5D	4.03	120.75	112.78
4	A	1001	CNA	O2D-C2D-C1D	3.91	121.86	111.71
4	A	1001	CNA	O3B-C3B-C4B	-3.80	100.17	111.08
4	A	1001	CNA	C4'-C4D-C3D	3.77	112.46	102.89
4	A	1001	CNA	C3N-C7N-N7N	3.77	122.38	117.74
4	A	1001	CNA	C2B-C3B-C4B	3.76	109.88	102.61
5	A	1992	GOL	C3-C2-C1	-3.66	98.37	111.80
5	A	1990	GOL	C3-C2-C1	-3.49	99.00	111.80
5	A	1989	GOL	C3-C2-C1	-3.47	99.07	111.80
5	A	1991	GOL	C3-C2-C1	-3.46	99.11	111.80
4	A	1001	CNA	C6A-C5A-C4A	-3.11	112.94	117.18
4	A	1001	CNA	C6N-N1N-C2N	3.10	124.52	121.88
4	A	1001	CNA	PN-O5D-C5D	-3.08	103.70	121.35
4	A	1001	CNA	O2N-PN-O1N	-2.85	99.21	112.44
4	A	1001	CNA	C2B-C1B-N9A	2.77	120.20	113.30
4	A	1001	CNA	C6N-C5N-C4N	2.66	123.28	119.45
4	A	1001	CNA	C6A-C5A-N7A	2.44	136.79	132.09
5	A	1990	GOL	O1-C1-C2	2.34	120.92	110.38
5	A	1992	GOL	O1-C1-C2	2.26	120.54	110.38
5	A	1989	GOL	O1-C1-C2	2.16	120.10	110.38
4	A	1001	CNA	O2B-C2B-C3B	2.12	118.60	111.82
5	A	1991	GOL	O1-C1-C2	2.12	119.90	110.38
4	A	1001	CNA	C4D-C4'-C1D	2.03	109.04	102.60
4	A	1001	CNA	C3B-C2B-C1B	2.01	105.26	101.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	CNA	C4D

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	CNA	C5D-O5D-PN-O3
4	A	1001	CNA	C5D-O5D-PN-O1N

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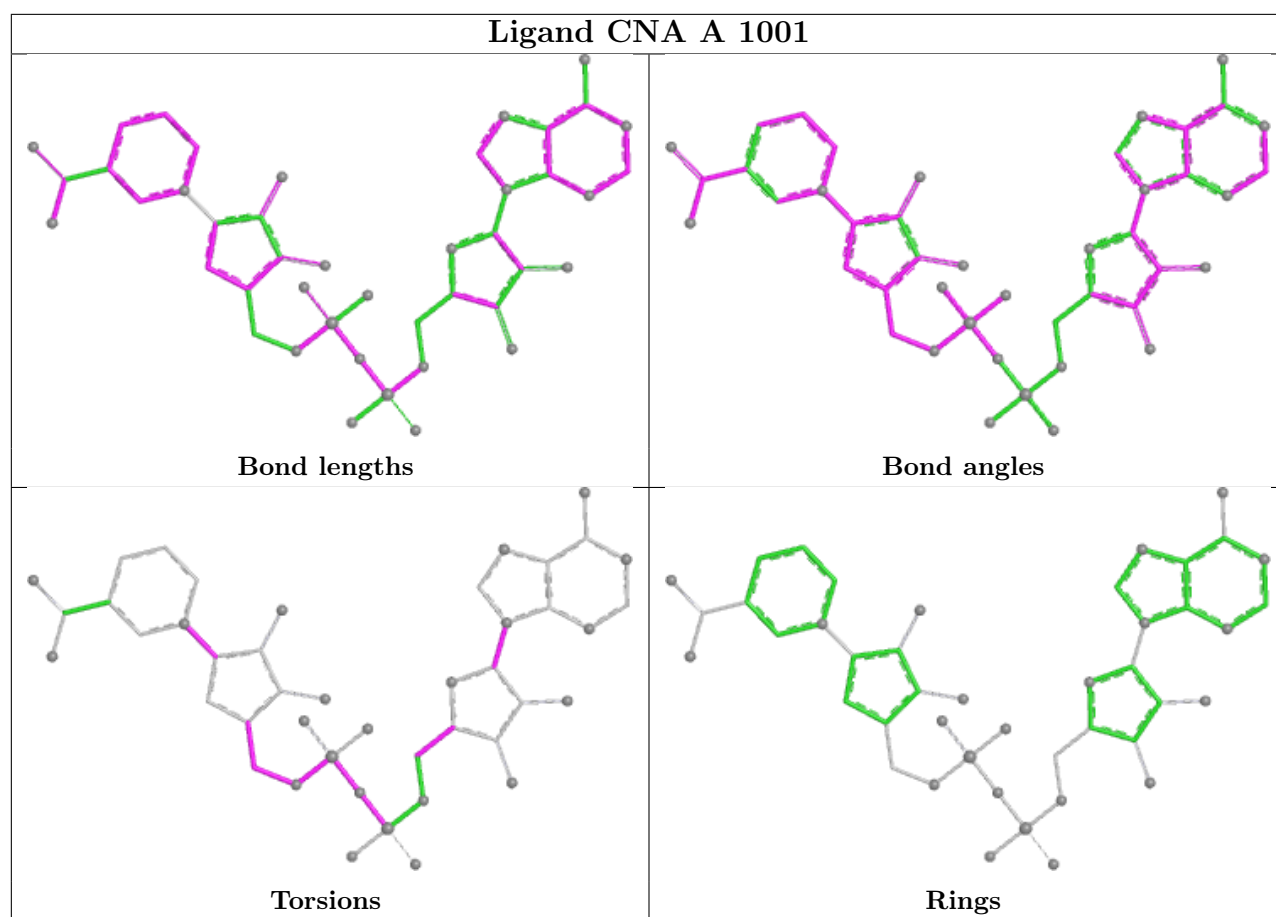
Mol	Chain	Res	Type	Atoms
4	A	1001	CNA	C3D-C4D-C5D-O5D
4	A	1001	CNA	C2D-C1D-N1N-C2N
4	A	1001	CNA	C2D-C1D-N1N-C6N
5	A	1989	GOL	O1-C1-C2-C3
5	A	1989	GOL	O2-C2-C3-O3
5	A	1990	GOL	O1-C1-C2-C3
5	A	1990	GOL	O2-C2-C3-O3
5	A	1991	GOL	O2-C2-C3-O3
5	A	1992	GOL	O2-C2-C3-O3
5	A	1991	GOL	O1-C1-C2-C3
5	A	1992	GOL	O1-C1-C2-O2
4	A	1001	CNA	PN-O3-PA-O5B
4	A	1001	CNA	PA-O3-PN-O1N
4	A	1001	CNA	C4D-C5D-O5D-PN
4	A	1001	CNA	O4B-C4B-C5B-O5B
4	A	1001	CNA	C2B-C1B-N9A-C8A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1990	GOL	1	0
5	A	1992	GOL	1	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	291/308 (94%)	0.78	41 (14%) 6 5	22, 36, 74, 122	0
2	B	6/14 (42%)	2.88	3 (50%) 0 1	37, 49, 68, 77	0
All	All	297/322 (92%)	0.83	44 (14%) 5 5	22, 36, 74, 122	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	ALA	9.5
1	A	292	THR	7.3
1	A	209	THR	5.3
1	A	23	PRO	5.2
2	B	18	HIS	5.0
1	A	166	ASP	4.9
2	B	12	LYS	4.8
1	A	10	MET	4.6
1	A	208	THR	4.4
1	A	265	ILE	4.0
1	A	24	ASN	3.8
1	A	204	ARG	3.7
1	A	22	ASN	3.5
1	A	163	PRO	3.5
1	A	215	GLN	3.2
1	A	117	PHE	3.1
1	A	162	HIS	3.1
1	A	207	ILE	3.1
1	A	13	ARG	3.0
1	A	257	ALA	2.9
1	A	205	GLU	2.9
1	A	280	GLU	2.9
1	A	259	LYS	2.8
1	A	107	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	254	ASP	2.5
1	A	144	ILE	2.5
1	A	16	ALA	2.5
1	A	11	SER	2.4
1	A	240	ARG	2.4
1	A	12	VAL	2.4
1	A	256	LYS	2.3
1	A	165	LYS	2.2
1	A	220	ILE	2.2
1	A	14	LYS	2.2
1	A	6	ALA	2.1
1	A	17	ALA	2.1
1	A	15	ILE	2.1
2	B	14	GLY	2.1
1	A	21	SER	2.1
1	A	198	ASN	2.0
1	A	127	LYS	2.0
1	A	291	LEU	2.0
1	A	286	ASP	2.0
1	A	57	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	ALY	B	16	12/13	0.94	0.10	28,31,41,43	0

6.3 Carbohydrates [i](#)

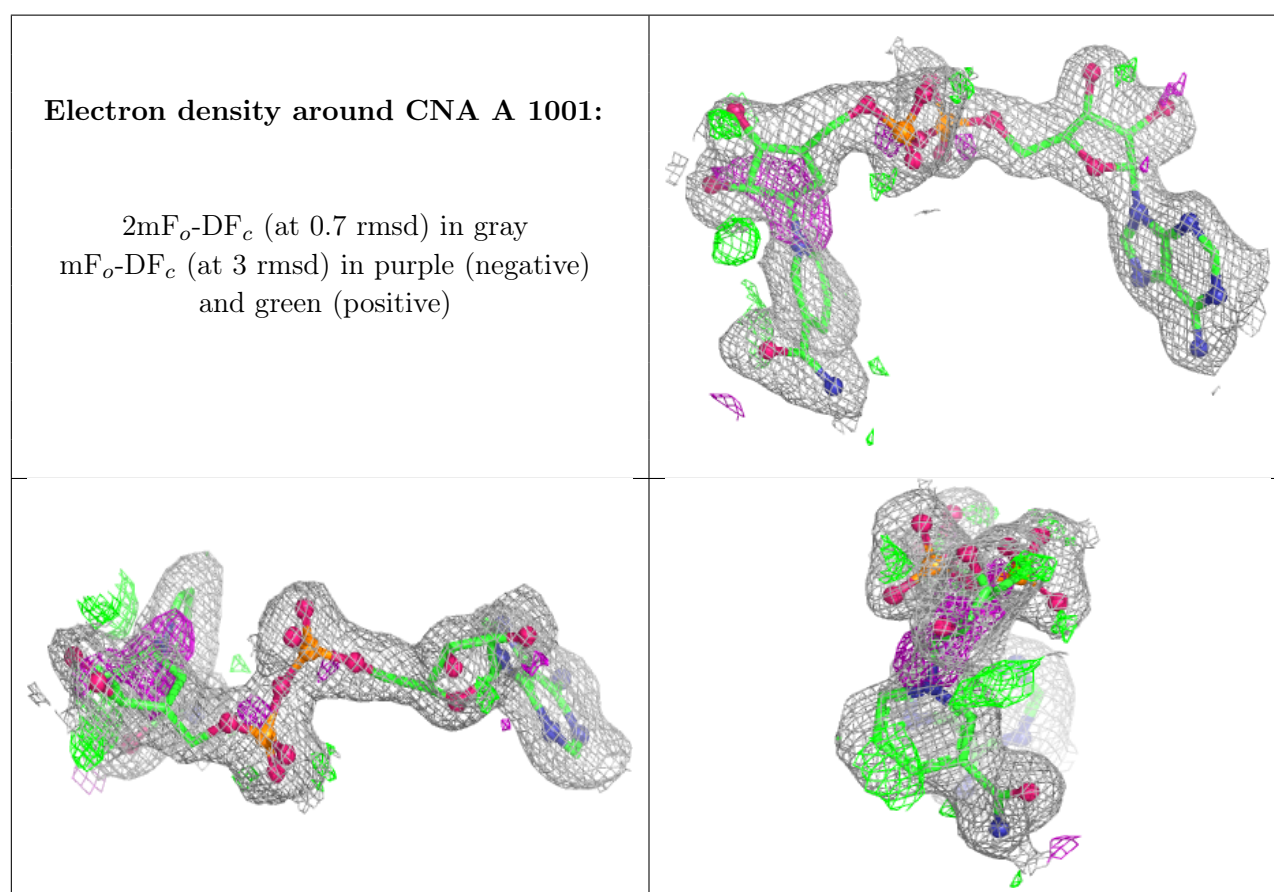
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	1992	6/6	0.68	0.19	36,40,44,51	0
5	GOL	A	1991	6/6	0.78	0.16	35,48,52,55	0
3	ZN	A	701	1/1	0.79	0.16	31,31,31,31	0
5	GOL	A	1990	6/6	0.80	0.14	40,50,55,56	0
5	GOL	A	1989	6/6	0.83	0.14	42,42,48,51	0
4	CNA	A	1001	44/44	0.90	0.13	31,42,53,61	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.