



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 11:33 AM EDT

PDB ID : 2OD2  
Title : Crystal Structure of yHst2 I117F mutant bound to carba-NAD<sup>+</sup> and an acetylated H4 peptide  
Authors : Sanders, B.D.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

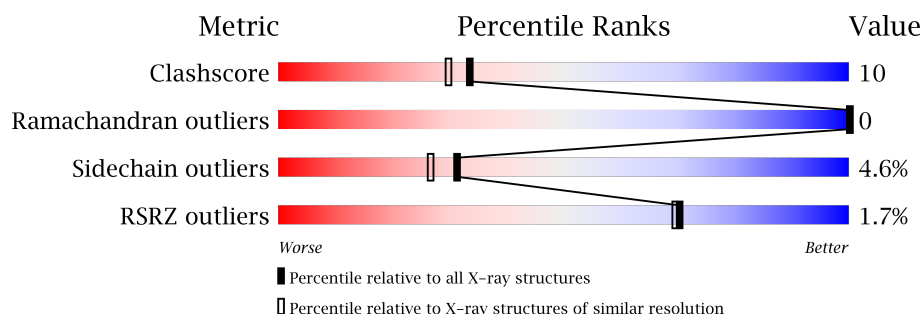
# 1 Overall quality at a glance

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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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
3	ZN	A	701	-	-	-	X
4	CNA	A	1001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1989	-	X	-	-
5	GOL	A	1990	-	X	-	X
5	GOL	A	1991	-	X	-	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	UNP P53686

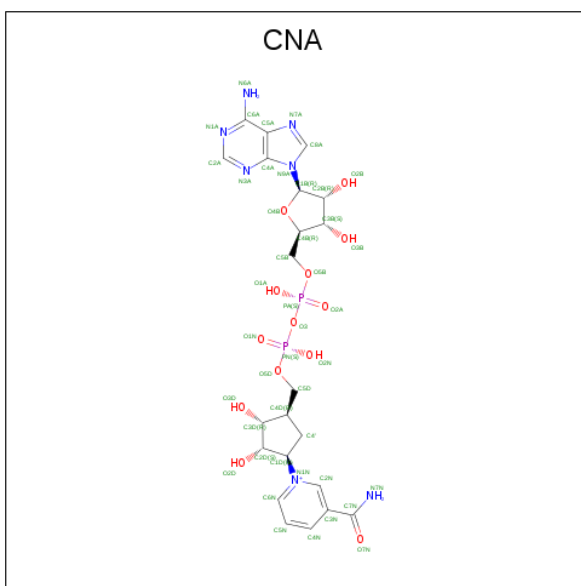
- Molecule 2 is a protein called Acetylated H4 peptide.

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 (three-letter code: ZN) (formula: Zn).

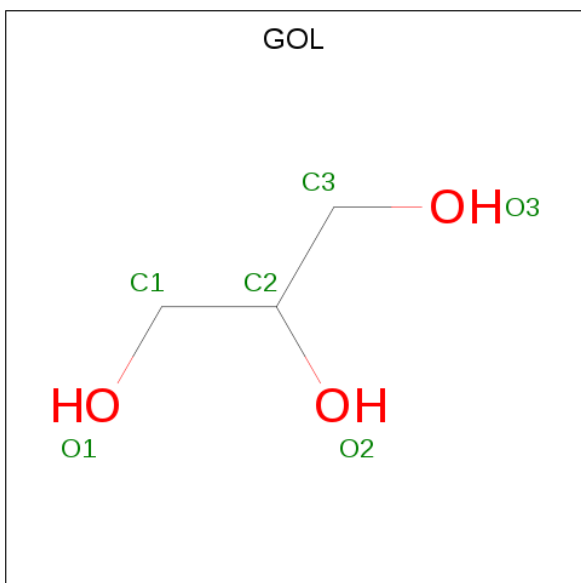
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is CARBA-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: CNA) (formula:  $C_{22}H_{30}N_7O_{13}P_2$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



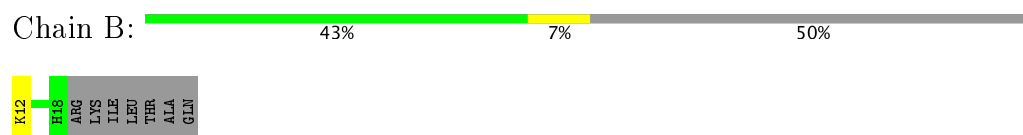
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

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



- Molecule 1: NAD-dependent deacetylase HST2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.64 Å   106.64 Å   67.72 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	41.89 – 2.00 41.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.0 (41.89-2.00) 84.3 (41.89-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 1.89 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 ,   0.233 0.240 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2602	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, CNA, ALY

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	2.01	48/2372 (2.0%)	1.62	45/3215 (1.4%)
2	B	0.37	0/42	0.54	0/51
All	All	1.99	48/2414 (2.0%)	1.61	45/3266 (1.4%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	ASP	N-CA	9.80	1.66	1.46
1	A	173	CYS	CB-SG	-9.47	1.66	1.82
1	A	156	LYS	CD-CE	9.14	1.74	1.51
1	A	79	PHE	CB-CG	7.67	1.64	1.51
1	A	166	ASP	CB-CG	7.31	1.67	1.51
1	A	183	PHE	CD1-CE1	-7.26	1.24	1.39
1	A	79	PHE	C-O	7.14	1.36	1.23
1	A	122	ARG	CG-CD	6.86	1.69	1.51
1	A	198	ASN	CB-CG	6.84	1.66	1.51
1	A	273	PHE	CE2-CZ	6.66	1.50	1.37
1	A	269	TYR	C-O	6.58	1.35	1.23
1	A	193	SER	C-O	6.56	1.35	1.23
1	A	272	GLU	CD-OE1	-6.44	1.18	1.25
1	A	143	CYS	C-O	6.42	1.35	1.23
1	A	122	ARG	C-O	6.34	1.35	1.23
1	A	205	GLU	CG-CD	6.32	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	SER	CA-CB	6.26	1.62	1.52
1	A	95	LYS	CD-CE	6.25	1.66	1.51
1	A	137	SER	CA-CB	6.23	1.62	1.52
1	A	98	TYR	CE1-CZ	-6.22	1.30	1.38
1	A	126	VAL	CB-CG1	6.20	1.65	1.52
1	A	52	TYR	CD2-CE2	6.12	1.48	1.39
1	A	169	LYS	CD-CE	6.04	1.66	1.51
1	A	48	GLY	N-CA	6.04	1.55	1.46
1	A	86	LEU	CG-CD2	5.99	1.74	1.51
1	A	116	ASN	CG-OD1	5.99	1.37	1.24
1	A	156	LYS	C-O	5.91	1.34	1.23
1	A	263	ASP	CB-CG	-5.88	1.39	1.51
1	A	243	LYS	CD-CE	5.72	1.65	1.51
1	A	127	LYS	CD-CE	5.71	1.65	1.51
1	A	175	GLU	CG-CD	5.70	1.60	1.51
1	A	32	GLY	N-CA	5.69	1.54	1.46
1	A	95	LYS	CG-CD	5.62	1.71	1.52
1	A	3	VAL	CB-CG2	5.58	1.64	1.52
1	A	236	GLU	CG-CD	5.55	1.60	1.51
1	A	28	ILE	CA-CB	-5.50	1.42	1.54
1	A	88	PRO	CA-C	-5.41	1.42	1.52
1	A	64	GLU	CD-OE1	5.36	1.31	1.25
1	A	148	LYS	CD-CE	5.35	1.64	1.51
1	A	191	SER	C-O	5.35	1.33	1.23
1	A	243	LYS	CB-CG	5.32	1.67	1.52
1	A	149	VAL	CB-CG2	5.24	1.63	1.52
1	A	120	LEU	C-O	5.23	1.33	1.23
1	A	229	TYR	CD1-CE1	5.17	1.47	1.39
1	A	47	PRO	C-N	-5.11	1.23	1.33
1	A	269	TYR	CB-CG	5.04	1.59	1.51
1	A	52	TYR	CD1-CE1	5.02	1.46	1.39
1	A	174	GLY	N-CA	5.01	1.53	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASP	CB-CG-OD2	13.82	130.74	118.30
1	A	166	ASP	CB-CG-OD2	11.16	128.34	118.30
1	A	47	PRO	C-N-CA	-10.46	100.33	122.30
1	A	92	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	68	ASP	CB-CG-OD1	-9.75	109.52	118.30
1	A	92	ARG	NE-CZ-NH2	-9.47	115.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASP	N-CA-C	8.93	135.10	111.00
1	A	129	ASP	CB-CG-OD1	8.87	126.28	118.30
1	A	107	ASP	CB-CG-OD2	8.68	126.11	118.30
1	A	68	ASP	CB-CG-OD2	8.14	125.62	118.30
1	A	128	ASP	CB-CG-OD2	7.97	125.48	118.30
1	A	171	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	143	CYS	CA-CB-SG	-7.51	100.48	114.00
1	A	57	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	190	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	118	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	272	GLU	OE1-CD-OE2	-6.84	115.09	123.30
1	A	187	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	43	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	49	THR	N-CA-CB	-6.35	98.24	110.30
1	A	183	PHE	CB-CG-CD1	6.23	125.16	120.80
1	A	286	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	57	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	244	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	204	ARG	CG-CD-NE	-5.83	99.55	111.80
1	A	130	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	87	TYR	CB-CG-CD2	5.76	124.46	121.00
1	A	118	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	177	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	A	205	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	27	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	A	166	ASP	OD1-CG-OD2	-5.49	112.86	123.30
1	A	199	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	251	THR	OG1-CB-CG2	-5.40	97.59	110.00
1	A	95	LYS	CD-CE-NZ	5.36	124.03	111.70
1	A	47	PRO	O-C-N	-5.36	114.09	123.20
1	A	122	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	70	ASP	OD1-CG-OD2	-5.32	113.19	123.30
1	A	52	TYR	CG-CD2-CE2	-5.30	117.06	121.30
1	A	169	LYS	CD-CE-NZ	5.18	123.62	111.70
1	A	52	TYR	CD1-CE1-CZ	-5.14	115.18	119.80
1	A	221	VAL	CA-CB-CG1	5.13	118.59	110.90
1	A	165	LYS	CD-CE-NZ	5.10	123.43	111.70
1	A	-2	MET	N-CA-C	5.05	124.62	111.00
1	A	183	PHE	CB-CG-CD2	-5.01	117.29	120.80

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	6	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:144:ILE:HD12	1.76	0.49
1:A:207:ILE:CG2	1:A:207:ILE:O	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
2:B:12:LYS:HG3	6:B:49:HOH:O	2.17	0.45
1:A:204:ARG:NH1	1:A:204:ARG:HG2	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
1:A:58:LEU:O	1:A:59:LYS:CB	2.68	0.41
1:A:218:LEU:HA	1:A:218:LEU:HD12	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
1:A:193:SER:CB	2:B:12:LYS:HZ3	2.34	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 ⓘ

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%)	30	26
2	B	3/9 (33%)	3 (100%)	0	100	100
All	All	259/280 (92%)	247 (95%)	12 (5%)	31	27

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	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	259	LYS
1	A	275	GLU
1	A	286	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	HIS
1	A	104	GLN
1	A	153	GLN
1	A	215	GLN

### 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	11,11,12	1.59	3 (27%)	9,12,14	1.83	1 (11%)

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	-	0/8/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	16	ALY	CA-C	2.18	1.53	1.50
2	B	16	ALY	OH-CH	2.98	1.30	1.23
2	B	16	ALY	CH-NZ	3.22	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	-4.88	114.63	122.49

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 carbohydrates 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
4	CNA	A	1001	-	42,48,48	3.83	21 (50%)	45,73,73	3.30	20 (44%)
5	GOL	A	1989	-	5,5,5	4.16	3 (60%)	5,5,5	4.98	3 (60%)
5	GOL	A	1990	-	5,5,5	4.17	3 (60%)	5,5,5	5.03	4 (80%)
5	GOL	A	1991	-	5,5,5	4.10	3 (60%)	5,5,5	5.02	3 (60%)
5	GOL	A	1992	-	5,5,5	4.23	3 (60%)	5,5,5	5.04	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
4	CNA	A	1001	-	1/1/11/11	0/22/62/62	0/5/5/5
5	GOL	A	1989	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1990	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1991	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1992	-	-	0/4/4/4	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1992	GOL	C3-C2	-8.20	1.21	1.52
5	A	1989	GOL	C3-C2	-8.12	1.22	1.52
5	A	1990	GOL	C3-C2	-8.12	1.22	1.52
5	A	1991	GOL	C3-C2	-7.93	1.22	1.52
4	A	1001	CNA	C4D-C3D	-5.94	1.36	1.54
4	A	1001	CNA	C2B-C1B	-5.06	1.45	1.53
4	A	1001	CNA	C4'-C1D	-4.38	1.38	1.53
4	A	1001	CNA	O2D-C2D	-4.36	1.32	1.43
4	A	1001	CNA	C4'-C4D	-4.26	1.42	1.53
5	A	1992	GOL	C1-C2	-3.49	1.39	1.52
5	A	1991	GOL	C1-C2	-3.32	1.40	1.52
5	A	1990	GOL	C1-C2	-3.28	1.40	1.52
5	A	1989	GOL	C1-C2	-3.18	1.40	1.52
5	A	1989	GOL	O2-C2	-2.91	1.34	1.43
5	A	1990	GOL	O2-C2	-2.89	1.34	1.43
5	A	1992	GOL	O2-C2	-2.88	1.34	1.43
5	A	1991	GOL	O2-C2	-2.87	1.35	1.43
4	A	1001	CNA	PN-O2N	-2.73	1.41	1.55
4	A	1001	CNA	C3B-C4B	-2.21	1.47	1.53
4	A	1001	CNA	C5A-C4A	2.19	1.45	1.40
4	A	1001	CNA	C8A-N7A	2.21	1.38	1.34
4	A	1001	CNA	C6A-N1A	2.50	1.48	1.37
4	A	1001	CNA	O3D-C3D	2.81	1.49	1.43
4	A	1001	CNA	C6N-C5N	3.71	1.46	1.38
4	A	1001	CNA	C2N-C3N	3.94	1.45	1.39
4	A	1001	CNA	C5N-C4N	4.75	1.48	1.38
4	A	1001	CNA	C7N-N7N	4.92	1.42	1.33
4	A	1001	CNA	C2A-N3A	5.63	1.41	1.32
4	A	1001	CNA	C4N-C3N	6.56	1.50	1.39
4	A	1001	CNA	C2A-N1A	6.68	1.46	1.33
4	A	1001	CNA	C6N-N1N	7.29	1.54	1.35
4	A	1001	CNA	O7N-C7N	9.03	1.42	1.24
4	A	1001	CNA	C4A-N3A	10.44	1.50	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	CNA	N3A-C2A-N1A	-8.48	121.47	128.86
4	A	1001	CNA	C6N-N1N-C1D	-7.15	108.46	119.74
4	A	1001	CNA	C1B-N9A-C4A	-5.96	116.33	126.64
4	A	1001	CNA	O5D-PN-O1N	-5.37	87.59	109.25
4	A	1001	CNA	O7N-C7N-C3N	-4.63	114.21	119.62
4	A	1001	CNA	C5N-C6N-N1N	-4.45	113.56	120.40
4	A	1001	CNA	O3B-C3B-C4B	-3.74	100.17	111.09
5	A	1992	GOL	C3-C2-C1	-3.31	98.37	111.52
5	A	1990	GOL	C3-C2-C1	-3.15	99.00	111.52
5	A	1989	GOL	C3-C2-C1	-3.13	99.07	111.52
5	A	1991	GOL	C3-C2-C1	-3.12	99.11	111.52
4	A	1001	CNA	C3N-C2N-N1N	-2.88	117.53	120.43
4	A	1001	CNA	O2N-PN-O1N	-2.53	99.21	112.28
5	A	1992	GOL	O1-C1-C2	2.08	120.54	110.07
4	A	1001	CNA	O2B-C2B-C3B	2.12	118.60	111.83
5	A	1990	GOL	O1-C1-C2	2.15	120.92	110.07
4	A	1001	CNA	C4B-O4B-C1B	2.51	112.44	109.77
4	A	1001	CNA	C6N-C5N-C4N	2.55	123.28	119.44
4	A	1001	CNA	C2B-C3B-C4B	3.73	109.88	102.62
4	A	1001	CNA	C3N-C7N-N7N	4.03	122.38	117.77
4	A	1001	CNA	O2D-C2D-C1D	4.28	121.86	111.47
4	A	1001	CNA	C4'-C4D-C3D	4.38	112.46	102.31
4	A	1001	CNA	C2N-N1N-C1D	4.62	127.03	119.74
4	A	1001	CNA	C4'-C4D-C5D	4.64	120.75	112.40
5	A	1989	GOL	O3-C3-C2	5.88	139.71	110.07
5	A	1992	GOL	O3-C3-C2	5.95	140.06	110.07
5	A	1990	GOL	O3-C3-C2	5.97	140.12	110.07
4	A	1001	CNA	O2N-PN-O5D	6.00	136.48	108.14
5	A	1991	GOL	O3-C3-C2	6.01	140.35	110.07
4	A	1001	CNA	O3D-C3D-C4D	6.66	130.00	112.97
5	A	1989	GOL	O2-C2-C3	8.67	149.79	108.84
5	A	1992	GOL	O2-C2-C3	8.72	150.02	108.84
5	A	1990	GOL	O2-C2-C3	8.73	150.05	108.84
5	A	1991	GOL	O2-C2-C3	8.73	150.09	108.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	CNA	C4D

There are no torsion outliers.

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	291/308 (94%)	-0.26	5 (1%) 70 69	22, 36, 74, 122	0
2	B	6/14 (42%)	0.71	0 100 100	37, 49, 68, 77	0
All	All	297/322 (92%)	-0.24	5 (1%) 70 69	22, 36, 74, 122	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	THR	5.9
1	A	24	ASN	3.4
1	A	162	HIS	2.5
1	A	166	ASP	2.3
1	A	293	ALA	2.2

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	B	16	12/13	0.93	0.11	-	28,31,41,43	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	1991	6/6	0.79	0.39	15.18	35,48,52,55	0
5	GOL	A	1990	6/6	0.82	0.22	12.35	40,50,55,56	0
3	ZN	A	701	1/1	0.82	0.11	2.72	31,31,31,31	0
5	GOL	A	1989	6/6	0.82	0.23	1.59	42,42,48,51	0
4	CNA	A	1001	44/44	0.92	0.14	0.59	31,42,53,61	0
5	GOL	A	1992	6/6	0.84	0.21	-	36,40,44,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.