



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2021 – 12:05 PM EDT

PDB ID : 6WHN  
Title : Histone deacetylases complex with peptide macrocycles  
Authors : Bera, A.K.; Hosseinzadeh, P.; Watson, P.; Baker, D.  
Deposited on : 2020-04-08  
Resolution : 1.54 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

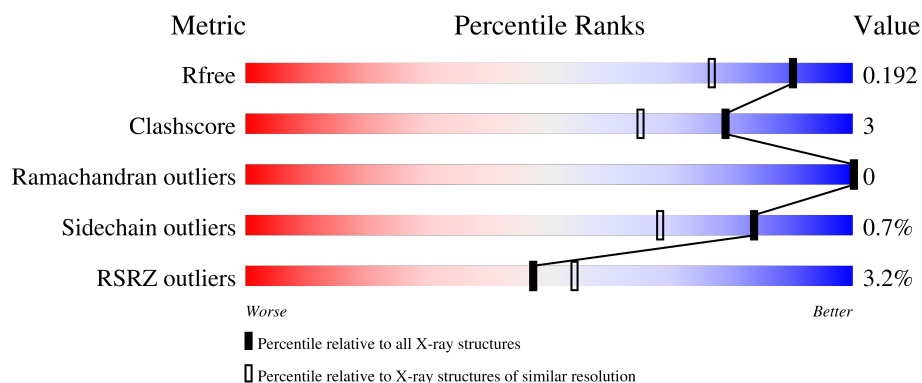
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.54 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))
$R_{free}$	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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  $\geq 3$ , 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	385	<div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	B	385	<div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	C	385	<div> <div>5%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	F	8	<div> <div>25%</div> <div>88%</div> <div>12%</div> </div>
2	G	8	<div> <div>38%</div> <div>62%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	8	<div><div></div><div></div><div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10346 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	9	0
			3048	1950	513	559	26			
1	B	367	Total	C	N	O	S	0	9	0
			2998	1919	501	551	27			
1	C	367	Total	C	N	O	S	0	5	0
			2973	1901	500	546	26			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP Q92769
B	5	ALA	-	expression tag	UNP Q92769
C	5	ALA	-	expression tag	UNP Q92769

- Molecule 2 is a protein called U2M-ASN-PRO-LYS-GLN-DLY-TRP-GLY peptide macro-cycle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	8	Total	C	N	O	S	0	0	0
			70	46	13	10	1			
2	G	8	Total	C	N	O	S	0	0	0
			70	46	13	10	1			
2	H	8	Total	C	N	O	S	0	0	0
			62	40	11	10	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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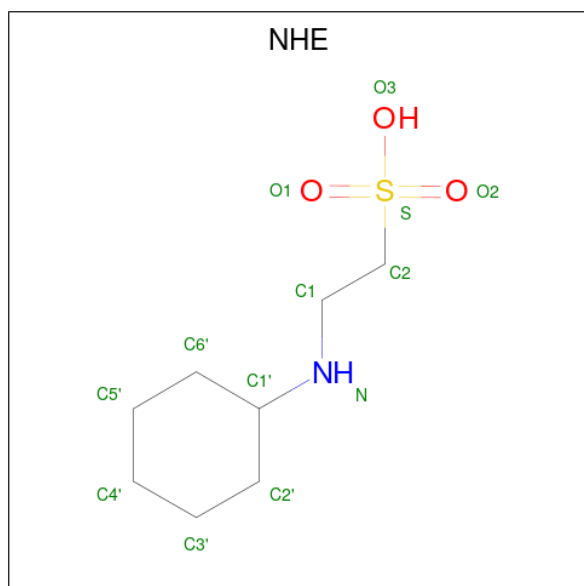
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		
4	C	2	Total	Na	0	0
			2	2		

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



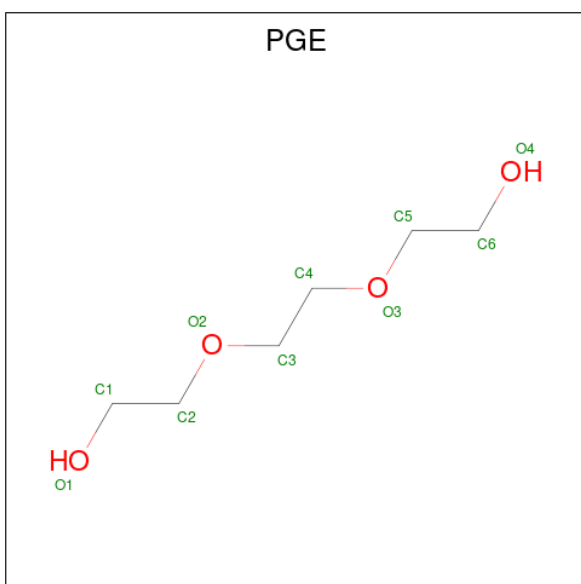
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



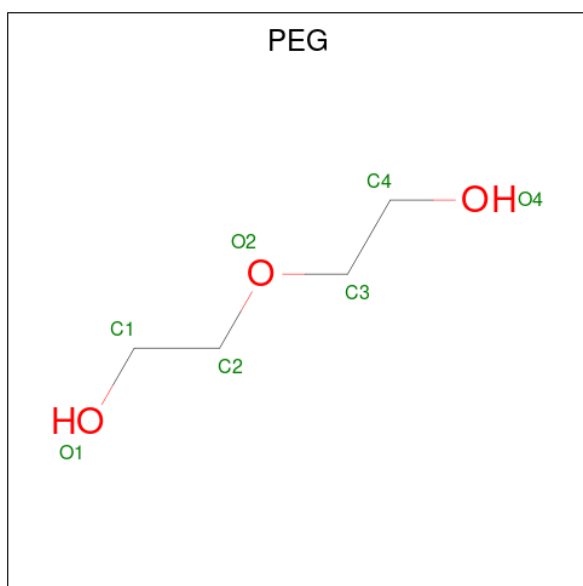
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	326	Total	O	0	0
			326	326		
9	B	377	Total	O	0	0
			377	377		
9	C	250	Total	O	0	0
			250	250		
9	F	6	Total	O	0	0
			6	6		

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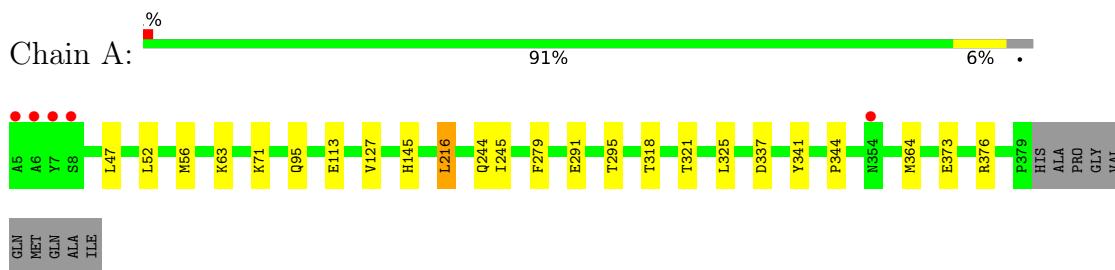
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	6	Total	O	0	0
			6	6		
9	H	3	Total	O	0	0
			3	3		



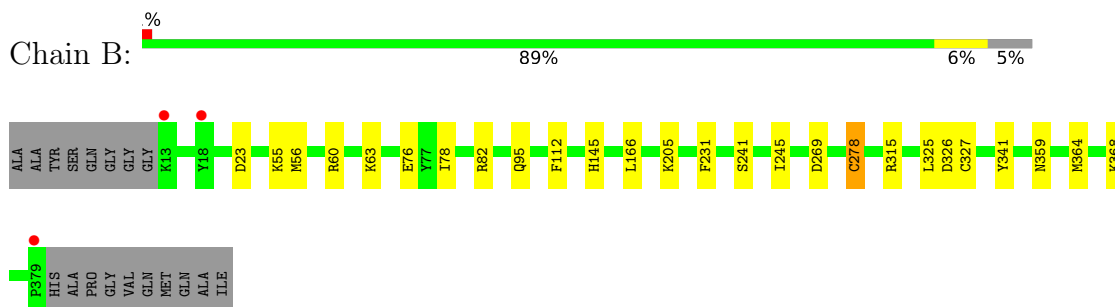
### 3 Residue-property plots [i](#)

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.

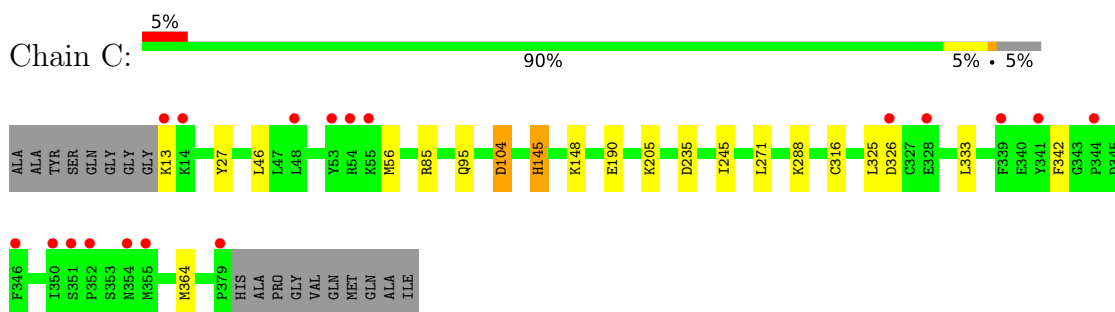
- Molecule 1: Histone deacetylase 2



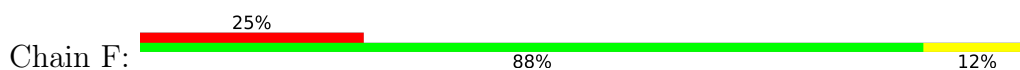
- Molecule 1: Histone deacetylase 2

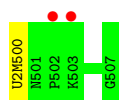


- Molecule 1: Histone deacetylase 2

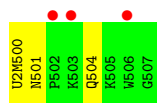


- Molecule 2: U2M-ASN-PRO-LYS-GLN-DLY-TRP-GLY peptide macrocycle

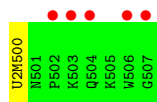
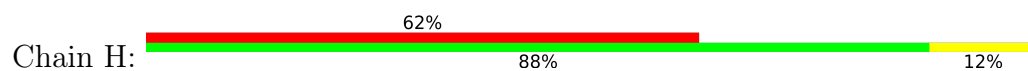




- Molecule 2: U2M-ASN-PRO-LYS-GLN-DLY-TRP-GLY peptide macrocycle



- Molecule 2: U2M-ASN-PRO-LYS-GLN-DLY-TRP-GLY peptide macrocycle



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.35Å 97.67Å 138.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.82 – 1.54 43.82 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.82-1.54) 99.3 (43.82-1.54)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 1.54Å)	Xtriage
Refinement program	PHENIX 1.17rc1_3605	Depositor
R, $R_{free}$	0.163 , 0.192 0.163 , 0.192	Depositor DCC
$R_{free}$ test set	9349 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10346	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: PGE, U2M, NHE, ZN, DLY, PG4, NA, PEG

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	0.64	0/3159	0.76	2/4264 (0.0%)
1	B	0.68	3/3108 (0.1%)	0.78	2/4195 (0.0%)
1	C	0.52	0/3065	0.67	0/4137
2	F	0.45	0/52	0.51	0/68
2	G	0.47	0/52	0.44	0/68
2	H	0.34	0/48	0.43	0/64
All	All	0.62	3/9484 (0.0%)	0.73	4/12796 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278[A]	CYS	CB-SG	-5.45	1.73	1.81
1	B	278[B]	CYS	CB-SG	-5.45	1.73	1.81
1	B	327	CYS	CB-SG	-5.30	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	216	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	B	269	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	279	PHE	CB-CG-CD1	-5.13	117.21	120.80

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	3048	0	2966	17	0
1	B	2998	0	2908	17	0
1	C	2973	0	2880	14	0
2	F	70	0	58	0	0
2	G	70	0	58	1	0
2	H	62	0	37	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	13	0	17	0	0
5	B	13	0	17	5	0
6	A	39	0	54	3	0
6	B	13	0	18	0	0
6	C	13	0	18	0	0
7	A	10	0	14	0	0
7	B	20	0	28	2	0
7	C	20	0	28	1	0
8	A	7	0	10	0	0
9	A	326	0	0	4	0
9	B	377	0	0	4	0
9	C	250	0	0	3	0
9	F	6	0	0	0	0
9	G	6	0	0	0	0
9	H	3	0	0	0	0
All	All	10346	0	9111	51	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 3.

All (51) 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:205:LYS:HD2	1:B:278[A]:CYS:SG	2.27	0.73
1:C:104:ASP:HB2	9:C:694:HOH:O	1.88	0.73
1:A:291:GLU:O	1:A:295:THR:HG23	1.95	0.67
1:B:63:LYS:HE3	5:B:404:NHE:H5'2	1.78	0.65
1:B:241:SER:HB3	1:B:364[B]:MET:SD	2.44	0.58
1:A:71:LYS:NZ	9:A:503:HOH:O	2.36	0.57
1:B:78:ILE:O	1:B:82:ARG:HG3	2.05	0.56
1:B:82:ARG:HG2	1:B:112:PHE:CZ	2.41	0.54
1:A:63:LYS:NZ	1:A:113[B]:GLU:OE1	2.32	0.53
1:B:23:ASP:OD2	5:B:404:NHE:HC22	2.08	0.52
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.89	0.52
1:A:337:ASP:HA	9:A:649:HOH:O	2.11	0.51
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.93	0.50
1:C:46[B]:LEU:HD11	1:C:342:PHE:CZ	2.46	0.50
1:C:245:ILE:HG21	1:C:364[A]:MET:HE3	1.92	0.50
1:A:47[B]:LEU:CD2	1:A:52:LEU:HD12	2.41	0.49
1:C:95:GLN:NE2	9:C:501:HOH:O	2.29	0.49
1:C:13:LYS:HD3	1:C:326:ASP:HB2	1.94	0.49
2:G:501:ASN:ND2	2:G:504:GLN:OE1	2.41	0.48
1:B:76:GLU:HG2	9:B:511:HOH:O	2.13	0.48
1:A:47[B]:LEU:HD23	1:A:52:LEU:HD12	1.95	0.48
1:A:341:TYR:HA	6:A:406:PG4:H82	1.96	0.47
1:C:46[A]:LEU:HD11	1:C:333:LEU:HD22	1.97	0.47
1:A:47[B]:LEU:HD21	1:A:321:THR:HB	1.96	0.47
1:B:245:ILE:HG22	1:B:368:LYS:HE2	1.97	0.47
1:C:85:ARG:NH2	9:C:512:HOH:O	2.49	0.46
1:A:95:GLN:HG3	9:A:691:HOH:O	2.16	0.46
1:C:271:LEU:HD11	1:C:316:CYS:HB2	1.98	0.46
1:A:127:VAL:HG11	5:B:404:NHE:H3'2	1.99	0.45
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.98	0.45
1:C:205:LYS:HE2	1:C:235:ASP:OD1	2.17	0.45
1:C:46[B]:LEU:HD21	1:C:342:PHE:CE1	2.52	0.44
1:B:166:LEU:HD21	7:B:407:PGE:H6	2.00	0.44
1:C:27:TYR:CE2	7:C:406:PGE:H32	2.53	0.44
1:B:60:ARG:NH2	5:B:404:NHE:O1	2.52	0.43
1:A:244:GLN:NE2	9:A:515:HOH:O	2.51	0.43
6:A:405:PG4:O5	6:A:405:PG4:H62	2.16	0.42
1:A:344:PRO:HD3	6:A:406:PG4:H22	2.01	0.42
1:B:231:PHE:CE1	1:B:245:ILE:HD13	2.55	0.42
1:C:145:HIS:CD2	1:C:145:HIS:H	2.38	0.42
1:B:95:GLN:HG3	9:B:705:HOH:O	2.20	0.41
7:B:407:PGE:H5	9:B:788:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ILE:HG12	1:A:364:MET:CE	2.51	0.41
1:A:373:GLU:HG2	1:A:376[A]:ARG:NH2	2.36	0.41
1:B:55:LYS:NZ	9:B:519:HOH:O	2.54	0.41
1:A:216:LEU:N	1:A:216:LEU:HD23	2.35	0.41
1:A:47[B]:LEU:HD23	1:A:318:THR:HG23	2.02	0.41
1:B:245:ILE:HG12	1:B:364[A]:MET:CE	2.51	0.40
1:B:359:ASN:HB3	1:B:364[A]:MET:SD	2.62	0.40
1:C:148:LYS:HD2	1:C:190:GLU:OE1	2.20	0.40
1:B:63:LYS:NZ	5:B:404:NHE:H4'1	2.36	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	382/385 (99%)	376 (98%)	6 (2%)	0	100	100
1	B	374/385 (97%)	368 (98%)	6 (2%)	0	100	100
1	C	369/385 (96%)	364 (99%)	5 (1%)	0	100	100
2	F	5/8 (62%)	5 (100%)	0	0	100	100
2	G	5/8 (62%)	5 (100%)	0	0	100	100
2	H	5/8 (62%)	5 (100%)	0	0	100	100
All	All	1140/1179 (97%)	1123 (98%)	17 (2%)	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	329/327 (101%)	328 (100%)	1 (0%)	92	84
1	B	326/327 (100%)	323 (99%)	3 (1%)	78	60
1	C	321/327 (98%)	318 (99%)	3 (1%)	78	60
2	F	5/5 (100%)	5 (100%)	0	100	100
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	4/5 (80%)	4 (100%)	0	100	100
All	All	990/996 (99%)	983 (99%)	7 (1%)	84	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	B	145	HIS
1	B	326	ASP
1	B	341	TYR
1	C	104	ASP
1	C	145	HIS
1	C	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	U2M	F	500	2,3	8,9,10	2.74	3 (37%)	4,9,11	1.20	1 (25%)
2	U2M	H	500	2,3	8,9,10	2.96	2 (25%)	4,9,11	1.95	1 (25%)
2	U2M	G	500	2,3	8,9,10	2.60	3 (37%)	4,9,11	1.38	1 (25%)

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	U2M	F	500	2,3	-	1/7/8/10	-
2	U2M	H	500	2,3	-	2/7/8/10	-
2	U2M	G	500	2,3	-	1/7/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	U2M	CA-N	-6.52	1.28	1.48
2	F	500	U2M	CA-N	-6.07	1.29	1.48
2	G	500	U2M	CA-N	-5.90	1.30	1.48
2	H	500	U2M	CZ-SH	-4.89	1.63	1.80
2	G	500	U2M	CZ-SH	-3.55	1.68	1.80
2	F	500	U2M	CZ-SH	-3.33	1.69	1.80
2	F	500	U2M	CB-CA	3.07	1.57	1.53
2	G	500	U2M	CB-CA	2.04	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	U2M	CE-CZ-SH	3.78	125.11	112.96
2	F	500	U2M	CE-CZ-SH	2.39	120.64	112.96
2	G	500	U2M	CE-CZ-SH	2.38	120.60	112.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	500	U2M	O-C-CA-CB
2	H	500	U2M	CG-CD-CE-CZ
2	F	500	U2M	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	G	500	U2M	CG-CD-CE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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
7	PGE	C	404	-	9,9,9	0.48	0	8,8,8	0.39	0
8	PEG	A	409	-	6,6,6	0.51	0	5,5,5	0.32	0
7	PGE	B	407	-	9,9,9	0.47	0	8,8,8	0.39	0
6	PG4	B	406	-	12,12,12	0.54	0	11,11,11	0.32	0
7	PGE	C	406	-	9,9,9	0.53	0	8,8,8	0.32	0
7	PGE	A	408	-	9,9,9	0.49	0	8,8,8	0.50	0
6	PG4	A	407	-	12,12,12	0.53	0	11,11,11	0.40	0
5	NHE	B	404	-	13,13,13	1.29	2 (15%)	16,17,17	2.34	7 (43%)
7	PGE	B	405	-	9,9,9	0.47	0	8,8,8	0.36	0
6	PG4	C	405	-	12,12,12	0.52	0	11,11,11	0.26	0
5	NHE	A	404	-	13,13,13	1.49	2 (15%)	16,17,17	2.21	4 (25%)
6	PG4	A	405	-	12,12,12	0.52	0	11,11,11	0.33	0
6	PG4	A	406	-	12,12,12	0.48	0	11,11,11	0.27	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
7	PGE	C	404	-	-	2/7/7/7	-
8	PEG	A	409	-	-	1/4/4/4	-
7	PGE	B	407	-	-	5/7/7/7	-
6	PG4	B	406	-	-	1/10/10/10	-
7	PGE	C	406	-	-	2/7/7/7	-
7	PGE	A	408	-	-	4/7/7/7	-
6	PG4	A	407	-	-	4/10/10/10	-
5	NHE	B	404	-	-	3/7/15/15	0/1/1/1
7	PGE	B	405	-	-	3/7/7/7	-
6	PG4	C	405	-	-	1/10/10/10	-
5	NHE	A	404	-	-	2/7/15/15	0/1/1/1
6	PG4	A	405	-	-	9/10/10/10	-
6	PG4	A	406	-	-	7/10/10/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	NHE	C2-S	4.11	1.83	1.77
5	B	404	NHE	C2-S	2.76	1.81	1.77
5	A	404	NHE	O2-S	2.75	1.53	1.45
5	B	404	NHE	O2-S	2.50	1.52	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	NHE	O3-S-O1	-5.92	96.82	111.27
5	B	404	NHE	O3-S-C2	4.83	113.59	105.77
5	A	404	NHE	O3-S-C2	3.68	111.72	105.77
5	B	404	NHE	O2-S-O1	-3.59	101.51	113.95
5	B	404	NHE	C2-C1-N	-3.46	101.43	111.25
5	A	404	NHE	O2-S-C2	3.29	110.88	106.92
5	B	404	NHE	C4'-C3'-C2'	2.99	117.52	111.42
5	B	404	NHE	O2-S-C2	2.86	110.36	106.92
5	B	404	NHE	C1-N-C1'	2.75	119.55	114.14
5	B	404	NHE	C5'-C6'-C1'	-2.29	106.79	111.11
5	A	404	NHE	C6'-C1'-C2'	-2.02	107.32	110.82

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	NHE	C2'-C1'-N-C1
5	B	404	NHE	C2'-C1'-N-C1
6	A	405	PG4	C8-C7-O4-C6
6	A	405	PG4	O2-C3-C4-O3
7	A	408	PGE	O2-C3-C4-O3
6	A	405	PG4	O3-C5-C6-O4
7	A	408	PGE	C6-C5-O3-C4
6	A	407	PG4	O3-C5-C6-O4
7	B	407	PGE	O2-C3-C4-O3
7	B	407	PGE	C6-C5-O3-C4
7	B	407	PGE	C4-C3-O2-C2
6	A	406	PG4	O1-C1-C2-O2
7	C	406	PGE	O1-C1-C2-O2
8	A	409	PEG	O2-C3-C4-O4
7	B	405	PGE	O1-C1-C2-O2
6	A	406	PG4	O2-C3-C4-O3
7	C	404	PGE	O3-C5-C6-O4
6	A	405	PG4	C1-C2-O2-C3
6	A	405	PG4	O1-C1-C2-O2
7	B	407	PGE	O1-C1-C2-O2
7	B	407	PGE	O3-C5-C6-O4
5	A	404	NHE	C6'-C1'-N-C1
6	A	405	PG4	C6-C5-O3-C4
5	B	404	NHE	C2-C1-N-C1'
7	A	408	PGE	C4-C3-O2-C2
6	A	405	PG4	O4-C7-C8-O5
6	A	407	PG4	O4-C7-C8-O5
7	C	404	PGE	O1-C1-C2-O2
6	A	405	PG4	C3-C4-O3-C5
6	A	406	PG4	C3-C4-O3-C5
6	A	405	PG4	C5-C6-O4-C7
6	A	407	PG4	C1-C2-O2-C3
6	C	405	PG4	O1-C1-C2-O2
6	B	406	PG4	C1-C2-O2-C3
6	A	406	PG4	C1-C2-O2-C3
6	A	407	PG4	C6-C5-O3-C4
7	B	405	PGE	C3-C4-O3-C5
6	A	406	PG4	C4-C3-O2-C2
5	B	404	NHE	C6'-C1'-N-C1
7	B	405	PGE	C6-C5-O3-C4
6	A	406	PG4	C6-C5-O3-C4
7	A	408	PGE	O1-C1-C2-O2
7	C	406	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
6	A	406	PG4	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	407	PGE	2	0
7	C	406	PGE	1	0
5	B	404	NHE	5	0
6	A	405	PG4	1	0
6	A	406	PG4	2	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 ⓘ

### 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, 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(Å²)	Q<0.9	
1	A	375/385 (97%)	-0.27	5 (1%)	77	81	11, 18, 38, 60	1 (0%)
1	B	367/385 (95%)	-0.11	3 (0%)	86	88	9, 16, 35, 59	1 (0%)
1	C	367/385 (95%)	0.08	18 (4%)	29	33	14, 25, 45, 71	1 (0%)
2	F	6/8 (75%)	1.49	2 (33%)	0	0	27, 29, 50, 55	0
2	G	6/8 (75%)	2.28	3 (50%)	0	0	25, 37, 41, 48	0
2	H	6/8 (75%)	4.13	5 (83%)	0	0	51, 69, 77, 78	1 (16%)
All	All	1127/1179 (95%)	-0.06	36 (3%)	47	54	9, 20, 42, 78	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	506	TRP	9.4
1	A	5	ALA	8.9
1	C	379	PRO	5.8
2	G	506	TRP	5.6
2	H	503	LYS	5.1
1	C	354	ASN	4.8
1	A	7	TYR	4.8
1	A	6	ALA	4.7
1	C	341	TYR	4.4
1	C	13	LYS	4.2
2	H	502	PRO	3.8
2	F	503	LYS	3.4
2	F	502	PRO	3.2
1	C	339	PHE	3.1
1	B	379	PRO	3.0
1	C	54	ARG	2.9
1	C	344	PRO	2.8
1	C	53	TYR	2.8
1	B	13	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	503	LYS	2.7
1	C	352	PRO	2.6
1	A	354	ASN	2.6
2	G	502	PRO	2.6
1	C	350	ILE	2.6
2	H	504	GLN	2.5
2	H	507	GLY	2.5
1	C	14	LYS	2.5
1	A	8	SER	2.5
1	C	346	PHE	2.4
1	C	55	LYS	2.4
1	B	18	TYR	2.1
1	C	326	ASP	2.1
1	C	351	SER	2.1
1	C	48	LEU	2.1
1	C	328	GLU	2.0
1	C	355	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	DLY	H	505	5/10	0.66	0.31	76,78,82,85	1
2	DLY	G	505	9/10	0.87	0.24	37,42,67,71	0
2	DLY	F	505	9/10	0.93	0.13	29,34,48,49	0
2	U2M	H	500	10/11	0.96	0.10	16,21,41,41	0
2	U2M	F	500	10/11	0.97	0.09	13,19,28,30	0
2	U2M	G	500	10/11	0.97	0.09	12,17,25,25	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
7	PGE	B	407	10/10	0.81	0.12	41,45,52,54	0
6	PG4	A	407	13/13	0.82	0.19	37,40,57,59	0
5	NHE	B	404	13/13	0.84	0.20	24,31,35,49	13
6	PG4	C	405	13/13	0.85	0.16	36,44,53,58	0
6	PG4	A	406	13/13	0.85	0.17	35,46,56,57	0
8	PEG	A	409	7/7	0.85	0.11	36,40,52,55	0
6	PG4	A	405	13/13	0.86	0.29	45,51,63,65	0
7	PGE	A	408	10/10	0.87	0.13	31,41,48,49	0
6	PG4	B	406	13/13	0.88	0.11	26,38,45,52	0
7	PGE	B	405	10/10	0.88	0.15	32,43,48,50	0
7	PGE	C	406	10/10	0.89	0.16	37,46,56,59	0
5	NHE	A	404	13/13	0.91	0.17	31,40,47,49	7
7	PGE	C	404	10/10	0.93	0.09	28,33,49,55	0
4	NA	B	403	1/1	0.98	0.08	17,17,17,17	0
4	NA	A	403	1/1	0.98	0.05	19,19,19,19	0
4	NA	C	402	1/1	0.99	0.12	14,14,14,14	0
4	NA	C	403	1/1	0.99	0.06	18,18,18,18	0
3	ZN	C	401	1/1	0.99	0.06	15,15,15,15	1
4	NA	B	402	1/1	0.99	0.13	7,7,7,7	0
4	NA	A	402	1/1	0.99	0.14	10,10,10,10	0
3	ZN	A	401	1/1	1.00	0.07	13,13,13,13	0
3	ZN	B	401	1/1	1.00	0.07	10,10,10,10	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.