



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2021 – 08:03 AM EDT

PDB ID : 6WHO  
Title : Histone deacetylases complex with peptide macrocycles  
Authors : Bera, A.K.; Hosseinzadeh, P.; Watson, P.; Baker, D.  
Deposited on : 2020-04-08  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

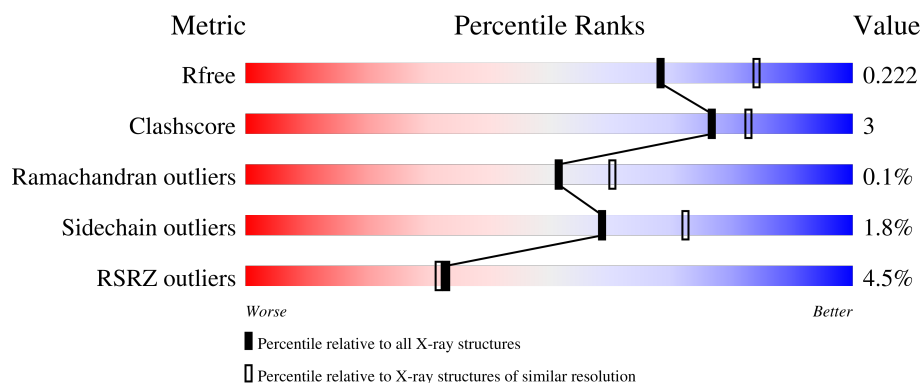
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 3%;"></div> </div> 90% 7% •
1	B	385	<div> <div style="width: 89%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> </div> 89% 5% • 5%
1	C	385	<div> <div style="width: 12%;"></div> <div style="width: 85%;"></div> <div style="width: 9%;"></div> <div style="width: 5%;"></div> </div> 12% 85% 9% • 5%
2	F	8	<div> <div style="width: 88%;"></div> <div style="width: 12%;"></div> </div> 88% 12%
2	G	8	<div> <div style="width: 25%;"></div> <div style="width: 50%;"></div> <div style="width: 38%;"></div> <div style="width: 12%;"></div> </div> 25% 50% 38% 12%

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Mol	Chain	Length	Quality of chain
2	H	8	<div><div></div><div>25%</div><div></div><div>75%</div><div></div><div>12%</div><div></div><div>12%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9863 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	374	Total	C	N	O	S	0	6	0
			3027	1933	512	556	26			
1	B	366	Total	C	N	O	S	0	3	0
			2957	1888	498	544	27			
1	C	365	Total	C	N	O	S	0	5	0
			2963	1894	500	544	25			

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-GLU-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	45	12	12	1			
2	G	8	Total	C	N	O	S	0	0	0
			70	45	12	12	1			
2	H	7	Total	C	N	O	S	0	0	0
			61	39	10	11	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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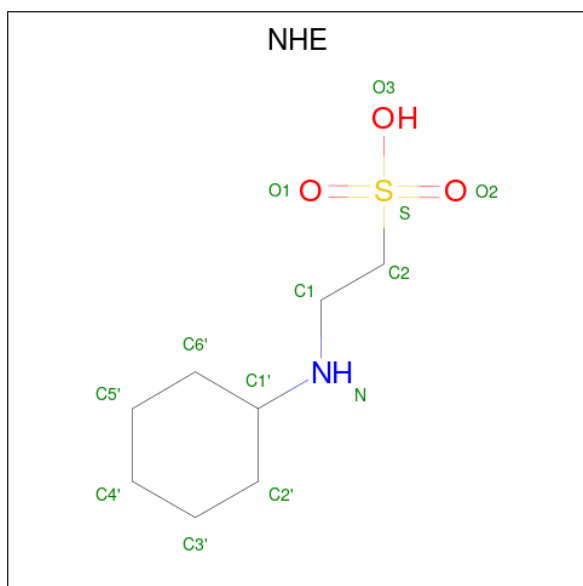
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

- 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	A	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	B	1	Total	C	O	0	0
			13	8	5		
6	B	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<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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	C	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		

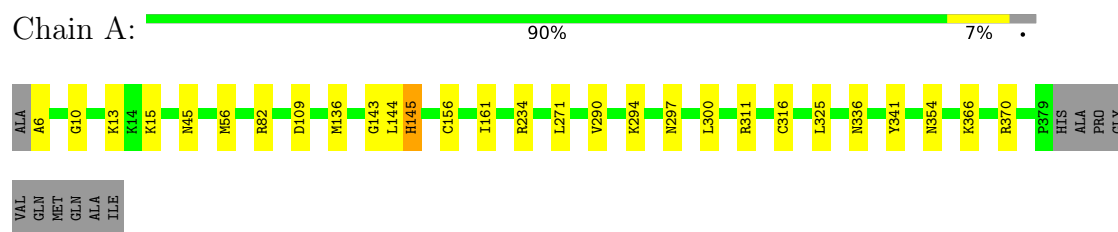
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	233	Total	O	0	0
			233	233		
8	B	213	Total	O	0	0
			213	213		
8	C	106	Total	O	0	0
			106	106		
8	F	4	Total	O	0	0
			4	4		
8	G	4	Total	O	0	0
			4	4		
8	H	2	Total	O	0	0
			2	2		

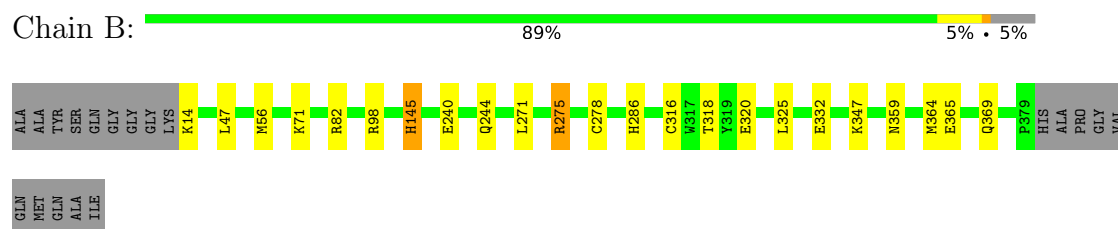
### 3 Residue-property plots

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.

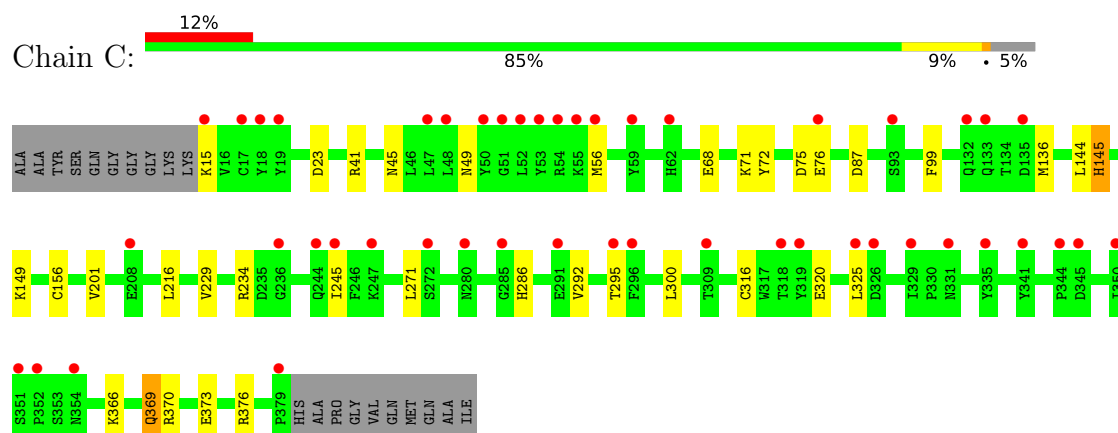
#### • Molecule 1: Histone deacetylase 2



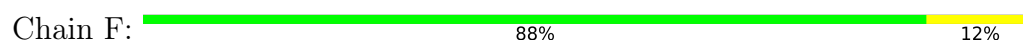
#### • Molecule 1: Histone deacetylase 2



#### • Molecule 1: Histone deacetylase 2



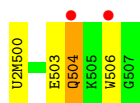
#### • Molecule 2: U2M-ASN-PRO-GLU-GLN-DLY-TRP-GLY peptide macrocycle



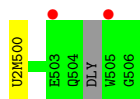
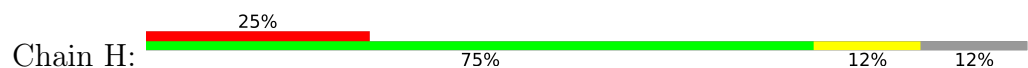




- Molecule 2: U2M-ASN-PRO-GLU-GLN-DLY-TRP-GLY peptide macrocycle



- Molecule 2: U2M-ASN-PRO-GLU-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, $\alpha$ , $\beta$ , $\gamma$	92.54Å 97.48Å 138.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.20 48.74 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.20) 100.0 (48.74-2.20)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.17rc1_3605	Depositor
R, $R_{free}$	0.184 , 0.221 0.186 , 0.222	Depositor DCC
$R_{free}$ test set	3279 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9863	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 2.98% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, NA, ZN, U2M, DLY, NHE, PG4

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	0.25	0/3128	0.41	0/4222
1	B	0.25	0/3046	0.41	0/4113
1	C	0.25	0/3059	0.40	0/4132
2	F	0.22	0/52	0.32	0/69
2	G	0.38	0/52	0.41	0/69
2	H	0.20	0/52	0.29	0/69
All	All	0.25	0/9389	0.40	0/12674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3027	0	2936	19	0
1	B	2957	0	2856	14	0
1	C	2963	0	2873	21	0
2	F	70	0	51	0	0
2	G	70	0	51	1	0
2	H	61	0	39	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	26	0	34	2	0
6	A	26	0	36	1	0
6	B	39	0	52	1	0
6	C	13	0	18	0	0
7	A	10	0	14	2	0
7	B	10	0	14	0	0
7	C	20	0	28	2	0
8	A	233	0	0	2	0
8	B	213	0	0	2	0
8	C	106	0	0	3	0
8	F	4	0	0	0	0
8	G	4	0	0	0	0
8	H	2	0	0	0	0
All	All	9863	0	9002	55	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.

The worst 5 of 55 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:109:ASP:HB3	6:A:408:PG4:H72	1.73	0.69
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.76	0.66
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.80	0.64
1:C:15:LYS:N	8:C:502:HOH:O	2.32	0.63
1:B:14:LYS:N	8:B:501:HOH:O	2.32	0.62

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	378/385 (98%)	374 (99%)	4 (1%)	0	100	100
1	B	367/385 (95%)	361 (98%)	6 (2%)	0	100	100
1	C	368/385 (96%)	362 (98%)	6 (2%)	0	100	100
2	F	5/8 (62%)	5 (100%)	0	0	100	100
2	G	5/8 (62%)	3 (60%)	1 (20%)	1 (20%)	0	0
2	H	3/8 (38%)	3 (100%)	0	0	100	100
All	All	1126/1179 (96%)	1108 (98%)	17 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	504	GLN

### 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	326/327 (100%)	323 (99%)	3 (1%)	78	88
1	B	319/327 (98%)	313 (98%)	6 (2%)	57	71
1	C	320/327 (98%)	313 (98%)	7 (2%)	52	65
2	F	5/5 (100%)	5 (100%)	0	100	100
2	G	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	H	5/5 (100%)	5 (100%)	0	100	100
All	All	980/996 (98%)	962 (98%)	18 (2%)	59	72

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	366	LYS
2	G	506	TRP

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Mol	Chain	Res	Type
2	G	504	GLN
1	B	278[C]	CYS
1	C	245	ILE

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 ⓘ

5 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	G	500	2,3	8,9,10	3.35	2 (25%)	4,9,11	1.32	1 (25%)
2	U2M	F	500	2,3	8,9,10	3.28	2 (25%)	4,9,11	1.07	0
2	U2M	H	500	2,3	8,9,10	3.29	2 (25%)	4,9,11	1.35	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	G	500	2,3	-	2/7/8/10	-
2	U2M	F	500	2,3	-	1/7/8/10	-
2	U2M	H	500	2,3	-	3/7/8/10	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	U2M	CA-N	-7.41	1.25	1.48
2	F	500	U2M	CA-N	-7.21	1.26	1.48
2	H	500	U2M	CA-N	-7.19	1.26	1.48
2	H	500	U2M	CZ-SH	-5.89	1.60	1.80
2	G	500	U2M	CZ-SH	-5.86	1.60	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	U2M	CD-CE-CZ	-2.22	109.14	113.09
2	G	500	U2M	CD-CE-CZ	-2.14	109.27	113.09

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

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

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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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
6	PG4	B	407	-	12,12,12	0.52	0	11,11,11	0.22	0
7	PGE	C	404	-	9,9,9	0.52	0	8,8,8	0.24	0
7	PGE	C	406	-	9,9,9	0.52	0	8,8,8	0.24	0
5	NHE	A	405	-	13,13,13	1.32	3 (23%)	16,17,17	1.87	5 (31%)
6	PG4	A	406	-	12,12,12	0.52	0	11,11,11	0.22	0
6	PG4	C	405	-	12,12,12	0.53	0	11,11,11	0.23	0
5	NHE	A	404	-	13,13,13	1.32	3 (23%)	16,17,17	1.83	5 (31%)
6	PG4	B	404	-	12,12,12	0.52	0	11,11,11	0.22	0
6	PG4	B	406	-	12,12,12	0.53	0	11,11,11	0.30	0
7	PGE	B	405	-	9,9,9	0.52	0	8,8,8	0.25	0
6	PG4	A	408	-	12,12,12	0.53	0	11,11,11	0.27	0
7	PGE	A	407	-	9,9,9	0.51	0	8,8,8	0.25	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
6	PG4	B	407	-	-	3/10/10/10	-
7	PGE	C	404	-	-	1/7/7/7	-
7	PGE	C	406	-	-	4/7/7/7	-
5	NHE	A	405	-	-	4/7/15/15	0/1/1/1
6	PG4	A	406	-	-	5/10/10/10	-
6	PG4	C	405	-	-	2/10/10/10	-
5	NHE	A	404	-	-	2/7/15/15	0/1/1/1
6	PG4	B	404	-	-	5/10/10/10	-
6	PG4	B	406	-	-	7/10/10/10	-
7	PGE	B	405	-	-	3/7/7/7	-
6	PG4	A	408	-	-	2/10/10/10	-
7	PGE	A	407	-	-	4/7/7/7	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	NHE	C2-S	3.15	1.82	1.77
5	A	404	NHE	C2-S	3.08	1.81	1.77
5	A	404	NHE	O2-S	2.19	1.51	1.45
5	A	404	NHE	O1-S	2.19	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	NHE	O2-S	2.18	1.51	1.45

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	404	NHE	O3-S-O1	-4.07	101.33	111.27
5	A	405	NHE	O2-S-O1	-3.83	100.70	113.95
5	A	405	NHE	O1-S-C2	3.67	111.33	106.92
5	A	405	NHE	O2-S-C2	3.56	111.20	106.92
5	A	404	NHE	O3-S-C2	3.30	111.10	105.77

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	405	NHE	C1-C2-S-O2
5	A	405	NHE	C1-C2-S-O3
6	B	404	PG4	O2-C3-C4-O3
6	A	406	PG4	O2-C3-C4-O3
7	A	407	PGE	O3-C5-C6-O4

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	406	PGE	2	0
5	A	405	NHE	2	0
6	B	404	PG4	1	0
6	A	408	PG4	1	0
7	A	407	PGE	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 [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	374/385 (97%)	-0.41	0	100 100	21, 30, 49, 64	1 (0%)
1	B	366/385 (95%)	-0.36	0	100 100	19, 30, 50, 71	2 (0%)
1	C	365/385 (94%)	0.75	47 (12%)	3 3	36, 57, 80, 93	6 (1%)
2	F	6/8 (75%)	0.10	0	100 100	37, 46, 58, 60	0
2	G	6/8 (75%)	1.31	2 (33%)	0 0	53, 62, 74, 84	2 (33%)
2	H	6/8 (75%)	2.30	2 (33%)	0 0	67, 86, 89, 93	3 (50%)
All	All	1123/1179 (95%)	0.01	51 (4%)	33 32	19, 35, 72, 93	14 (1%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	505	TRP	7.3
1	C	52	LEU	4.8
2	G	506	TRP	4.7
1	C	379	PRO	4.6
1	C	51	GLY	4.4

### 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, 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	G	505	9/10	0.76	0.28	66,75,88,92	0
2	DLY	F	505	9/10	0.92	0.19	44,54,60,68	0
2	U2M	H	500	10/11	0.93	0.11	43,51,66,67	0
2	U2M	F	500	10/11	0.94	0.14	25,33,38,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	U2M	G	500	10/11	0.97	0.10	19,33,44,46	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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( $\text{\AA}^2$ )	Q<0.9
6	PG4	B	406	13/13	0.79	0.17	49,64,68,72	0
6	PG4	C	405	13/13	0.82	0.18	54,64,71,74	0
6	PG4	B	407	13/13	0.83	0.18	45,58,73,76	0
6	PG4	A	408	13/13	0.86	0.21	47,54,62,67	0
6	PG4	A	406	13/13	0.86	0.19	45,61,72,72	0
5	NHE	A	404	13/13	0.88	0.17	36,39,54,64	13
6	PG4	B	404	13/13	0.89	0.15	45,54,64,68	0
7	PGE	C	406	10/10	0.89	0.13	61,71,81,83	0
7	PGE	C	404	10/10	0.90	0.12	46,54,58,61	0
5	NHE	A	405	13/13	0.91	0.21	32,42,46,47	13
7	PGE	A	407	10/10	0.93	0.14	39,48,54,58	0
7	PGE	B	405	10/10	0.93	0.13	41,44,56,66	0
4	NA	C	403	1/1	0.95	0.08	45,45,45,45	0
4	NA	C	402	1/1	0.96	0.13	40,40,40,40	0
4	NA	A	403	1/1	0.97	0.09	31,31,31,31	0
4	NA	A	402	1/1	0.98	0.21	13,13,13,13	0
4	NA	B	402	1/1	0.99	0.16	14,14,14,14	0
4	NA	B	403	1/1	0.99	0.07	34,34,34,34	0
3	ZN	B	401	1/1	0.99	0.13	22,22,22,22	0
3	ZN	C	401	1/1	0.99	0.04	41,41,41,41	0
3	ZN	A	401	1/1	1.00	0.12	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.