Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 01:48 PM EST

PDB ID	:	6WHQ
Title	:	Histone deacetylases complex with peptide macrocycles
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Deposited on	:	2020-04-08
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

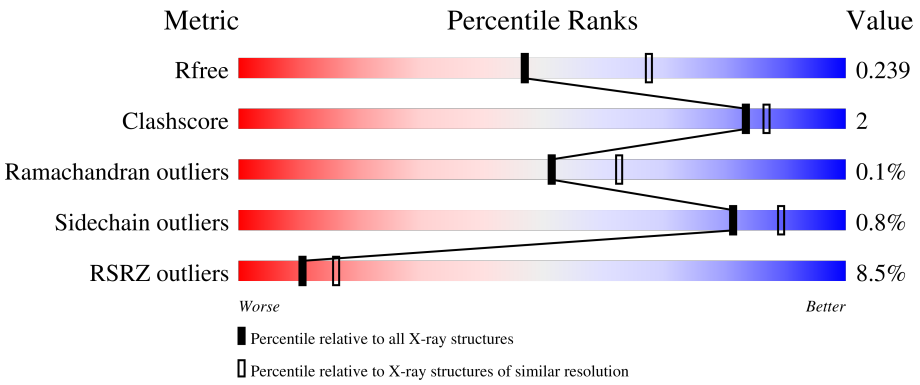
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	90% 7% •
1	B	385	% 90% 5% 5%
1	C	385	22% 86% 8% 5%
2	F	8	12% 88% 12%
2	G	8	50% 75% 25%

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Mol	Chain	Length	Quality of chain
2	H	8	38% 50% 12% 38%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9729 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
			Total	C	N	O	S			
1	A	374	3027	1933	512	556	26	0	6	0
1	B	366	2960	1891	498	544	27	0	3	0
1	C	365	2960	1892	500	543	25	0	4	0

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 macrocycle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	F	8	70	45	12	12	1	0	0	0
2	G	8	70	45	12	12	1	0	0	0
2	H	5	43	29	7	6	1	0	0	0

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

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

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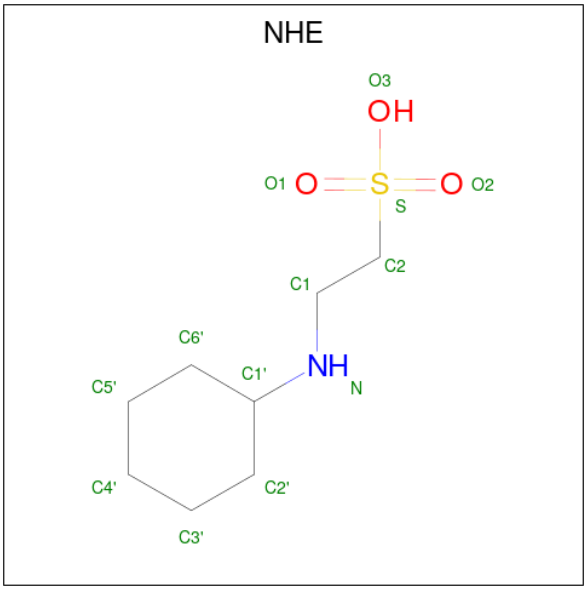
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	C	1	1	1	0	0

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

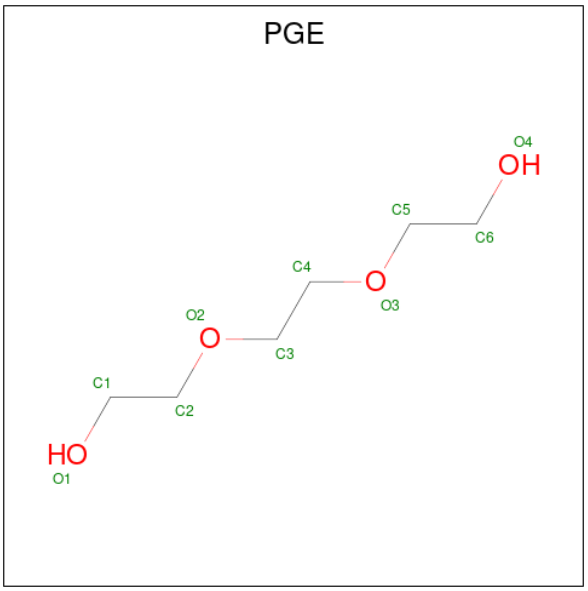
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
			Total	Na		
4	B	2	2	2	0	0
			Total	Na		
4	C	2	2	2	0	0

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



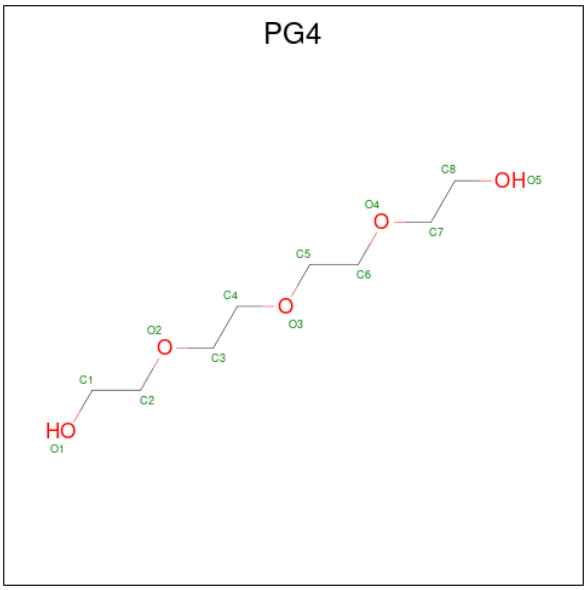
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	13	8	1	3	1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 8 is water.

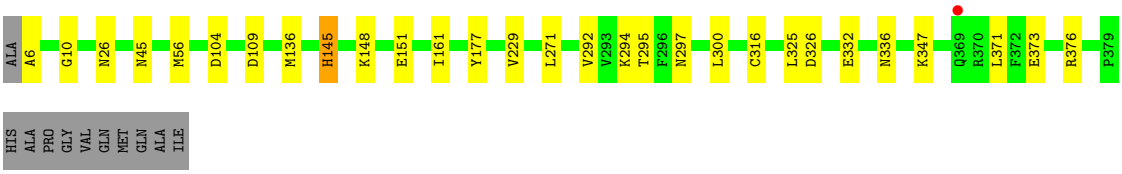
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	209	209	209	0	0
			Total	O		
8	B	194	194	194	0	0
			Total	O		
8	C	77	77	77	0	0
			Total	O		
8	F	4	4	4	0	0
			Total	O		
8	G	3	3	3	0	0
			Total	O		
8	H	1	1	1	0	0

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.

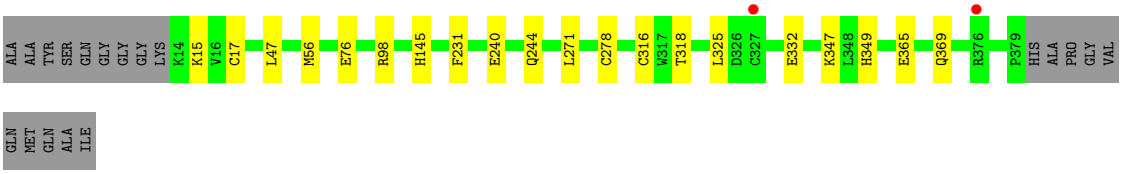
• Molecule 1: Histone deacetylase 2

Chain A:



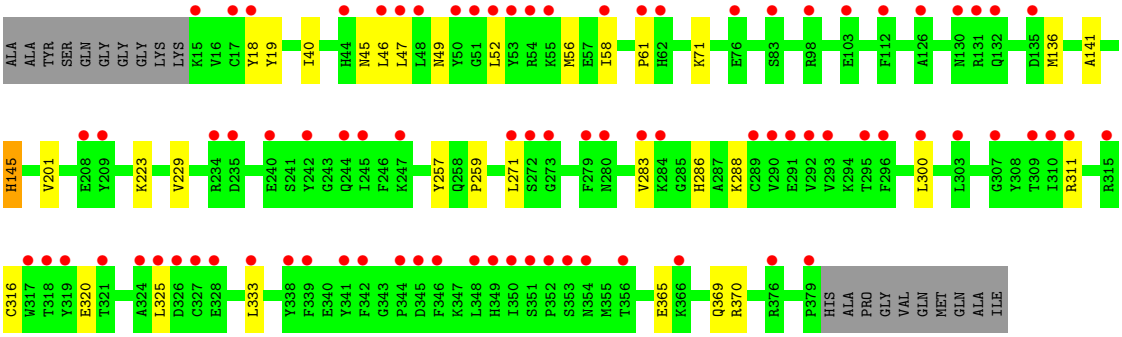
• Molecule 1: Histone deacetylase 2

Chain B:



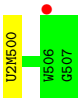
• Molecule 1: Histone deacetylase 2

Chain C:



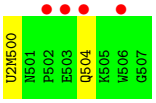
• Molecule 2: U2M-ASN-PRO-GLU-GLN-DLY-TRP-GLY peptide macrocycle

Chain F:



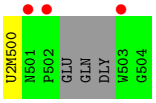
• Molecule 2: U2M-ASN-PRO-GLU-GLN-DLY-TRP-GLY peptide macrocycle

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.44Å 97.30Å 138.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.35 48.65 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.35) 100.0 (48.65-2.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.17rc1_3605	Depositor
R, R_{free}	0.196 , 0.241 0.196 , 0.239	Depositor DCC
R_{free} test set	2613 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9729	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: DLY, ZN, PGE, NHE, U2M, PG4, NA

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	0.24	0/3128	0.40	0/4222
1	B	0.25	0/3048	0.40	0/4115
1	C	0.24	0/3052	0.39	0/4122
2	F	0.20	0/52	0.34	0/69
2	G	0.23	0/52	0.40	0/69
2	H	0.15	0/34	0.32	0/45
All	All	0.24	0/9366	0.40	0/12642

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	16	0
1	B	2960	0	2866	9	0
1	C	2960	0	2870	18	0
2	F	70	0	51	0	0
2	G	70	0	51	0	0
2	H	43	0	25	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	13	0	17	0	0
6	A	20	0	28	0	0
6	B	10	0	14	0	0
6	C	20	0	28	0	0
7	A	13	0	18	2	0
7	B	26	0	36	2	0
8	A	209	0	0	1	0
8	B	194	0	0	0	0
8	C	77	0	0	1	0
8	F	4	0	0	0	0
8	G	3	0	0	0	0
8	H	1	0	0	0	0
All	All	9729	0	8940	43	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 2.

All (43) 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	7:A:407:PG4:H82	1.71	0.71
1:C:45:ASN:O	1:C:49:ASN:ND2	2.29	0.65
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.82	0.62
1:B:76:GLU:HG3	1:B:98:ARG:HH12	1.67	0.59
1:A:332:GLU:OE2	1:A:347:LYS:NZ	2.35	0.59
1:B:15:LYS:NZ	1:B:17[A]:CYS:SG	2.76	0.58
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.84	0.58
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.86	0.58
1:C:46:LEU:HD11	1:C:333:LEU:HD22	1.85	0.57
1:C:271:LEU:HD11	1:C:316:CYS:HB2	1.87	0.56
1:A:26:ASN:HB2	7:A:407:PG4:H41	1.88	0.55
1:C:19:TYR:HB3	1:C:61:PRO:HG3	1.90	0.53
1:C:136:MET:HG2	1:C:300:LEU:HB3	1.90	0.52
1:A:229:VAL:HG13	1:A:371:LEU:HD22	1.91	0.52
1:A:136:MET:HG2	1:A:300:LEU:HB3	1.91	0.52
1:C:283:VAL:HG13	1:C:316:CYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HZ3	1:A:326:ASP:CG	2.15	0.49
1:A:145:HIS:H	1:A:145:HIS:CD2	2.31	0.48
1:C:47:LEU:HB2	1:C:52:LEU:HD12	1.95	0.48
1:C:257:TYR:HD2	1:C:259:PRO:HG3	1.78	0.48
1:A:271:LEU:HD11	1:A:316:CYS:HB2	1.94	0.48
1:B:240:GLU:OE2	1:B:244:GLN:NE2	2.47	0.48
1:C:201:VAL:HG22	1:C:229:VAL:HB	1.96	0.47
1:B:271:LEU:HD11	1:B:316:CYS:HB2	1.96	0.46
7:B:406:PG4:H32	1:C:71:LYS:HE2	1.96	0.46
1:B:365:GLU:O	1:B:369:GLN:HG2	2.15	0.46
1:A:10:GLY:HA2	1:A:297:ASN:ND2	2.32	0.44
1:C:288:LYS:HE3	1:C:288:LYS:HB3	1.77	0.44
1:A:6:ALA:N	8:A:515:HOH:O	2.51	0.44
1:C:286:HIS:ND1	1:C:320:GLU:OE2	2.46	0.43
1:B:47:LEU:HD23	1:B:318:THR:HG23	2.01	0.43
1:A:45:ASN:OD1	1:A:336:ASN:HB2	2.19	0.43
1:C:40:ILE:HD13	1:C:141:ALA:HA	1.99	0.43
1:B:332:GLU:OE1	1:B:347:LYS:NZ	2.43	0.42
1:C:18:TYR:HB3	1:C:58:ILE:HG12	2.01	0.42
1:C:145:HIS:H	1:C:145:HIS:CD2	2.37	0.42
1:C:365:GLU:O	1:C:369:GLN:HG2	2.19	0.42
1:A:161:ILE:HG21	1:A:177:TYR:CE1	2.54	0.42
1:B:349:HIS:CD2	7:B:406:PG4:H52	2.55	0.42
1:A:148:LYS:HB2	1:A:151:GLU:HG2	2.01	0.41
1:A:373:GLU:HG2	1:A:376[A]:ARG:HH22	1.86	0.40
1:C:223:LYS:HG2	8:C:514:HOH:O	2.22	0.40
1:A:292:VAL:O	1:A:295[A]:THR:OG1	2.39	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	378/385 (98%)	372 (98%)	6 (2%)	0	100	100
1	B	367/385 (95%)	358 (98%)	9 (2%)	0	100	100
1	C	367/385 (95%)	354 (96%)	13 (4%)	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	1/8 (12%)	1 (100%)	0	0	100	100
All	All	1123/1179 (95%)	1093 (97%)	29 (3%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	504	GLN

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	326/327 (100%)	324 (99%)	2 (1%)	86	93
1	B	319/327 (98%)	316 (99%)	3 (1%)	78	87
1	C	319/327 (98%)	316 (99%)	3 (1%)	78	87
2	F	5/5 (100%)	5 (100%)	0	100	100
2	G	5/5 (100%)	5 (100%)	0	100	100
2	H	3/5 (60%)	3 (100%)	0	100	100
All	All	977/996 (98%)	969 (99%)	8 (1%)	81	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
1	A	145	HIS
1	B	145	HIS
1	B	231	PHE

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Mol	Chain	Res	Type
1	B	278	CYS
1	C	145	HIS
1	C	311	ARG
1	C	370	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	F	500	3,2	8,9,10	3.32	2 (25%)	4,9,11	1.48	1 (25%)
2	U2M	H	500	3,2	8,9,10	3.30	2 (25%)	4,9,11	1.39	1 (25%)
2	U2M	G	500	3,2	8,9,10	3.37	2 (25%)	4,9,11	1.26	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
2	U2M	F	500	3,2	-	4/7/8/10	-
2	U2M	H	500	3,2	-	3/7/8/10	-
2	U2M	G	500	3,2	-	4/7/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	U2M	CA-N	-7.44	1.25	1.48
2	F	500	U2M	CA-N	-7.25	1.26	1.48
2	H	500	U2M	CA-N	-7.23	1.26	1.48
2	G	500	U2M	CZ-SH	-5.95	1.60	1.80
2	F	500	U2M	CZ-SH	-5.94	1.60	1.80
2	H	500	U2M	CZ-SH	-5.89	1.60	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	U2M	CD-CE-CZ	-2.31	108.98	113.09
2	F	500	U2M	CD-CE-CZ	-2.24	109.11	113.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	500	U2M	N-CA-CB-CG
2	F	500	U2M	C-CA-CB-CG
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	C-CA-CB-CG
2	F	500	U2M	CE-CD-CG-CB
2	G	500	U2M	CG-CD-CE-CZ
2	F	500	U2M	CG-CD-CE-CZ
2	H	500	U2M	CG-CD-CE-CZ
2	G	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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	PG4	B	404	-	12,12,12	0.54	0	11,11,11	0.22	0
6	PGE	C	405	-	9,9,9	0.52	0	8,8,8	0.30	0
6	PGE	C	404	-	9,9,9	0.52	0	8,8,8	0.32	0
6	PGE	A	406	-	9,9,9	0.52	0	8,8,8	0.27	0
7	PG4	A	407	-	12,12,12	0.53	0	11,11,11	0.27	0
7	PG4	B	406	-	12,12,12	0.53	0	11,11,11	0.22	0
6	PGE	B	405	-	9,9,9	0.53	0	8,8,8	0.31	0
5	NHE	A	404	-	13,13,13	1.39	3 (23%)	16,17,17	1.97	5 (31%)
6	PGE	A	405	-	9,9,9	0.52	0	8,8,8	0.28	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	PG4	B	404	-	-	5/10/10/10	-
6	PGE	C	405	-	-	5/7/7/7	-
6	PGE	C	404	-	-	3/7/7/7	-
6	PGE	A	406	-	-	3/7/7/7	-
7	PG4	A	407	-	-	5/10/10/10	-
7	PG4	B	406	-	-	2/10/10/10	-
6	PGE	B	405	-	-	3/7/7/7	-
5	NHE	A	404	-	-	1/7/15/15	0/1/1/1
6	PGE	A	405	-	-	2/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	NHE	C2-S	3.32	1.82	1.77
5	A	404	NHE	O1-S	2.26	1.51	1.45
5	A	404	NHE	O2-S	2.25	1.51	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	404	NHE	O3-S-O1	-4.17	101.09	111.27
5	A	404	NHE	O1-S-C2	3.67	111.33	106.92
5	A	404	NHE	O3-S-C2	3.26	111.04	105.77
5	A	404	NHE	O2-S-C2	2.95	110.47	106.92
5	A	404	NHE	C1-N-C1'	-2.19	109.85	114.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	407	PG4	2	0
7	B	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 (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, 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	374/385 (97%)	-0.02	1 (0%)	94	97	27, 38, 57, 75	2 (0%)
1	B	366/385 (95%)	0.03	2 (0%)	91	95	27, 38, 56, 71	2 (0%)
1	C	365/385 (94%)	1.19	84 (23%)	0	1	50, 69, 86, 107	9 (2%)
2	F	6/8 (75%)	0.85	1 (16%)	1	2	53, 59, 74, 80	0
2	G	6/8 (75%)	2.45	4 (66%)	0	0	75, 88, 94, 106	1 (16%)
2	H	4/8 (50%)	3.54	3 (75%)	0	0	80, 91, 100, 101	1 (25%)
All	All	1121/1179 (95%)	0.42	95 (8%)	10	16	27, 43, 81, 107	15 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	503	TRP	7.0
2	G	506	TRP	6.3
1	C	350	ILE	6.3
1	C	51	GLY	5.3
1	C	52	LEU	5.2
1	C	345	ASP	4.5
1	C	271	LEU	4.4
1	C	309	THR	4.2
1	C	280	ASN	4.2
1	C	351	SER	4.2
1	C	341	TYR	4.1
1	C	319	TYR	4.0
2	H	502	PRO	4.0
1	C	325	LEU	3.8
1	C	291	GLU	3.7
1	C	352	PRO	3.6
1	C	293	VAL	3.5
1	C	53	TYR	3.2
1	C	103	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	369	GLN	3.1
1	C	55	LYS	3.1
1	C	62	HIS	3.1
1	C	48	LEU	3.1
1	C	54	ARG	3.1
1	C	348	LEU	3.1
1	C	328	GLU	3.1
1	C	326	ASP	3.0
1	C	245	ILE	3.0
1	C	17	CYS	3.0
1	C	354	ASN	2.9
1	C	240	GLU	2.9
1	C	61	PRO	2.9
1	C	310	ILE	2.8
1	C	47	LEU	2.8
1	C	324	ALA	2.8
1	C	50	TYR	2.8
1	C	130	ASN	2.8
1	C	333	LEU	2.8
1	C	242	TYR	2.8
1	C	342	PHE	2.7
1	C	344	PRO	2.7
1	C	346	PHE	2.7
1	C	349	HIS	2.7
1	C	76	GLU	2.7
1	C	296	PHE	2.7
1	C	318	THR	2.7
2	G	503	GLU	2.6
1	C	317	TRP	2.6
1	C	339	PHE	2.6
1	C	131	ARG	2.6
1	C	356	THR	2.6
1	C	376[A]	ARG	2.6
1	C	244	GLN	2.5
1	C	112	PHE	2.5
1	C	290	VAL	2.5
1	C	18	TYR	2.5
1	C	209	TYR	2.5
1	C	46	LEU	2.4
1	C	234	ARG	2.4
1	C	273	GLY	2.4
1	C	295	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	235	ASP	2.4
1	C	327	CYS	2.4
1	C	303	LEU	2.4
1	C	353	SER	2.4
1	C	292	VAL	2.3
1	B	376	ARG	2.3
1	C	284	LYS	2.3
2	G	502	PRO	2.3
1	C	366	LYS	2.2
1	C	135	ASP	2.2
1	C	379	PRO	2.2
1	C	272	SER	2.2
1	B	327[A]	CYS	2.2
1	C	247	LYS	2.2
2	H	501	ASN	2.2
1	C	289	CYS	2.2
2	F	506	TRP	2.1
1	C	44	HIS	2.1
2	G	504	GLN	2.1
1	C	300	LEU	2.1
1	C	315	ARG	2.1
1	C	283	VAL	2.1
1	C	338	TYR	2.1
1	C	132	GLN	2.1
1	C	279	PHE	2.1
1	C	208	GLU	2.1
1	C	311	ARG	2.1
1	C	83	SER	2.1
1	C	15	LYS	2.1
1	C	126	ALA	2.1
1	C	307	GLY	2.1
1	C	58	ILE	2.0
1	C	98	ARG	2.0
1	C	321	THR	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	DLY	G	505	9/10	0.65	0.32	77,85,97,98	0
2	DLY	F	505	9/10	0.86	0.28	64,68,72,74	0
2	U2M	H	500	10/11	0.90	0.17	54,66,83,83	0
2	U2M	G	500	10/11	0.96	0.14	32,42,62,62	0
2	U2M	F	500	10/11	0.97	0.13	30,44,49,51	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, 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
7	PG4	A	407	13/13	0.78	0.23	46,58,63,67	0
7	PG4	B	406	13/13	0.82	0.17	52,59,64,67	0
6	PGE	C	404	10/10	0.83	0.17	54,58,65,69	0
4	NA	C	402	1/1	0.87	0.11	47,47,47,47	0
6	PGE	C	405	10/10	0.87	0.19	56,63,69,76	0
7	PG4	B	404	13/13	0.88	0.19	39,54,64,76	0
6	PGE	B	405	10/10	0.88	0.15	46,49,54,55	0
4	NA	A	403	1/1	0.92	0.11	40,40,40,40	0
5	NHE	A	404	13/13	0.93	0.17	44,47,56,62	13
6	PGE	A	405	10/10	0.94	0.15	51,60,65,71	0
6	PGE	A	406	10/10	0.94	0.12	44,47,52,60	0
4	NA	C	403	1/1	0.95	0.15	56,56,56,56	0
4	NA	B	403	1/1	0.96	0.08	43,43,43,43	0
3	ZN	C	401	1/1	0.98	0.04	50,50,50,50	0
3	ZN	A	401	1/1	0.99	0.15	31,31,31,31	0
4	NA	A	402	1/1	0.99	0.20	20,20,20,20	0
3	ZN	B	401	1/1	0.99	0.15	30,30,30,30	0
4	NA	B	402	1/1	0.99	0.17	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.