



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:39 AM UTC

PDB ID : 6WHZ / pdb_00006whz
Title : Histone deacetylases complex with peptide macrocycles
Authors : Bera, A.K.; Hosseinzadeh, P.; Watson, P.; Baker, D.
Deposited on : 2020-04-08
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

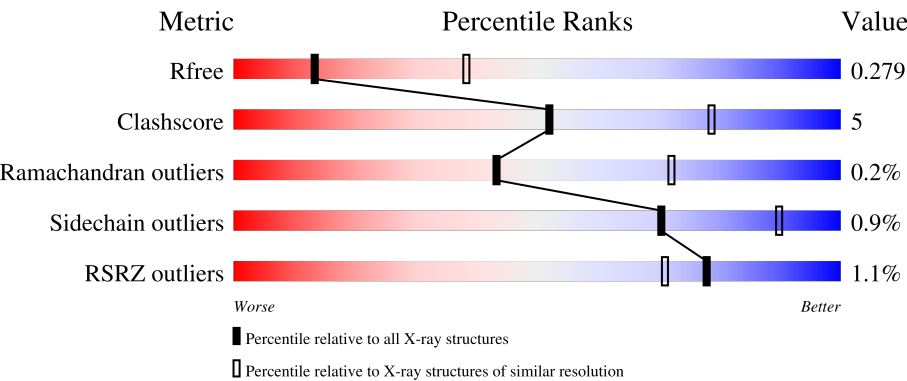
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	84%12%.
1	B	385	82%12%5%
1	C	385	2% 80%14%.5%
2	D	8	38%38%25%
2	F	8	12% 62%38%

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Mol	Chain	Length	Quality of chain
2	G	8	25% 75% 12% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9197 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	372	Total	C	N	O	S	0	0	0
			2980	1901	505	550	24			
1	B	364	Total	C	N	O	S	0	0	0
			2935	1874	495	542	24			
1	C	365	Total	C	N	O	S	0	0	0
			2936	1874	495	543	24			

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-HYP-LYS-GLN-DLY-TRP-GLY peptide macrocycle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	S	0	0	0
			71	46	13	11	1			
2	F	8	Total	C	N	O	S	0	0	0
			54	32	10	11	1			
2	G	8	Total	C	N	O	S	0	0	0
			54	32	10	11	1			

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

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

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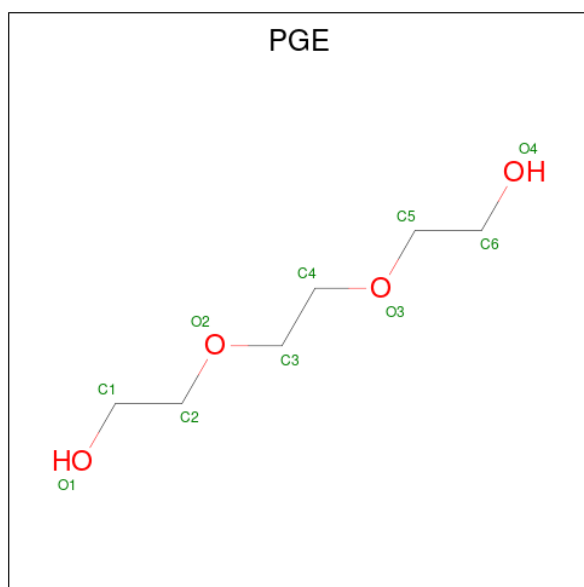
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

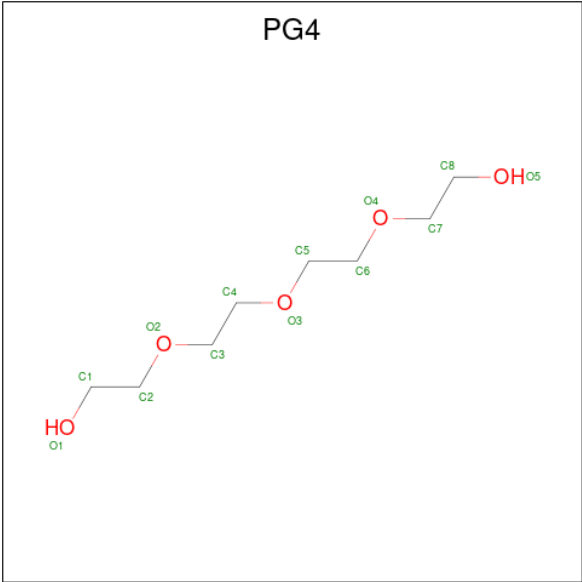
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

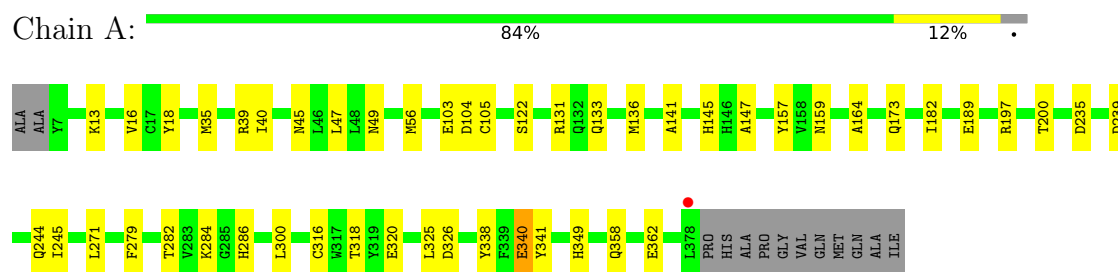
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	46	Total	O	0	0
			46	46		
7	B	32	Total	O	0	0
			32	32		
7	C	22	Total	O	0	0
			22	22		
7	D	5	Total	O	0	0
			5	5		
7	G	1	Total	O	0	0
			1	1		

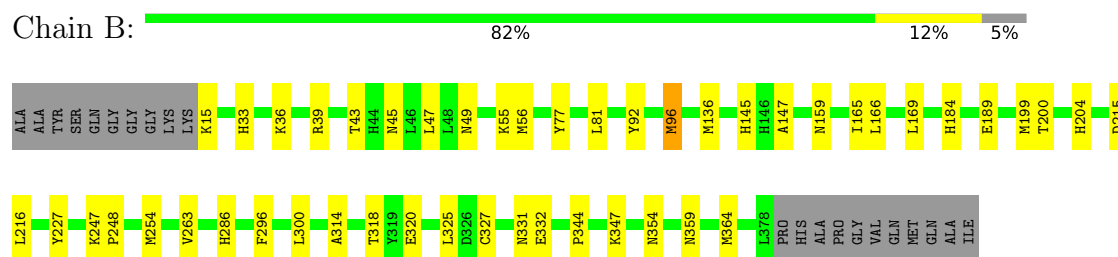
3 Residue-property plots [i](#)

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.

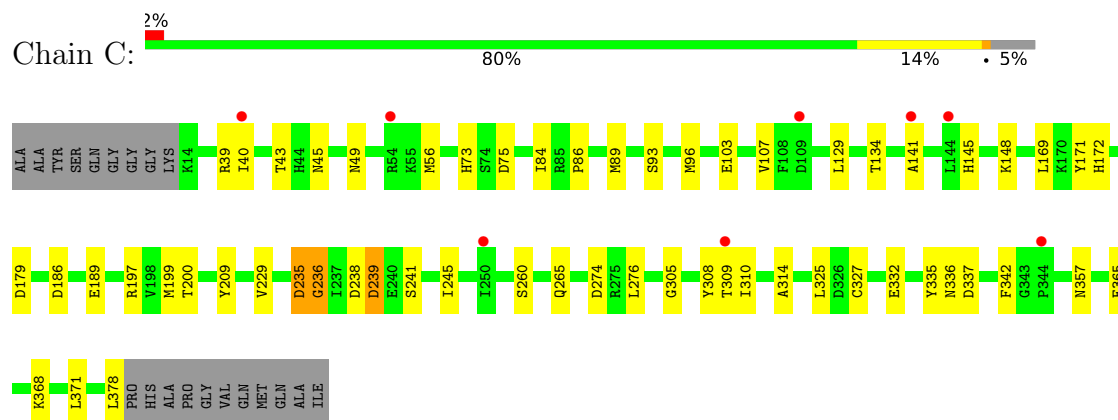
• Molecule 1: Histone deacetylase 2



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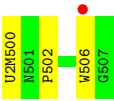


• Molecule 2: U2M-ASN-HYP-LYS-GLN-DLY-TRP-GLY peptide macrocycle

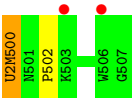
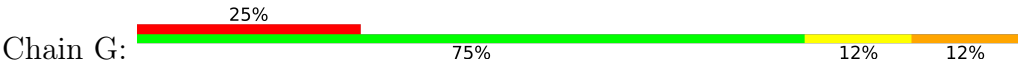




• Molecule 2: U2M-ASN-HYP-LYS-GLN-DLY-TRP-GLY peptide macrocycle



• Molecule 2: U2M-ASN-HYP-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, α , β , γ	92.48Å 94.80Å 138.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.90 47.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.90-2.90) 99.9 (47.90-2.90)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17rc1 _3605	Depositor
R, R_{free}	0.227 , 0.281 0.227 , 0.279	Depositor DCC
R_{free} test set	1312 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9197	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, DLY, ZN, HYP, PGE, U2M, 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	0.09	0/3056	0.26	0/4124
1	B	0.09	0/3011	0.26	0/4066
1	C	0.09	0/3012	0.26	0/4069
2	D	0.08	0/43	0.17	0/53
2	F	0.11	0/28	0.55	0/33
2	G	0.10	0/28	0.25	0/33
All	All	0.09	0/9178	0.26	0/12378

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	2980	0	2876	28	0
1	B	2935	0	2835	29	0
1	C	2936	0	2826	33	0
2	D	71	0	58	4	0
2	F	54	0	29	0	0
2	G	54	0	29	1	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	1	0	0	0	0
5	A	20	0	28	0	0
5	B	10	0	14	0	0
5	C	10	0	14	0	0
6	B	13	0	18	1	0
7	A	46	0	0	0	0
7	B	32	0	0	1	0
7	C	22	0	0	0	0
7	D	5	0	0	0	0
7	G	1	0	0	0	0
All	All	9197	0	8727	90	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 5.

All (90) 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:43:THR:HG22	1:B:314:ALA:HA	1.63	0.79
1:B:55:LYS:NZ	1:B:327:CYS:SG	2.64	0.70
1:A:136:MET:HG2	1:A:300:LEU:HB3	1.73	0.69
1:C:235:ASP:OD1	1:C:235:ASP:N	2.25	0.67
1:C:239:ASP:N	1:C:239:ASP:OD1	2.27	0.67
1:A:18:TYR:HB2	1:A:56:MET:HE2	1.79	0.65
1:A:35:MET:HE1	1:A:39:ARG:HH21	1.63	0.63
1:C:49:ASN:ND2	1:C:335:TYR:O	2.25	0.63
1:C:43:THR:HG22	1:C:314:ALA:HA	1.81	0.61
1:B:33:HIS:O	1:B:36:LYS:NZ	2.32	0.61
1:B:332:GLU:OE1	1:B:347:LYS:NZ	2.35	0.60
1:B:136:MET:HG2	1:B:300:LEU:HB3	1.83	0.59
1:B:199:MET:HE2	1:B:227:TYR:HA	1.85	0.59
1:B:354:ASN:HD22	1:C:171:TYR:HA	1.69	0.58
1:C:189:GLU:HA	1:C:200:THR:HG21	1.85	0.58
1:C:39:ARG:NH1	1:C:305:GLY:O	2.32	0.57
1:A:244:GLN:HG3	1:A:245:ILE:HG23	1.88	0.56
1:C:40:ILE:HD13	1:C:141:ALA:HA	1.88	0.55
1:C:308:TYR:OH	2:G:500:U2M:SH	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:HIS:ND1	1:B:320:GLU:OE2	2.40	0.55
1:C:39:ARG:HB3	1:C:310:ILE:HG22	1.88	0.54
1:A:103:GLU:OE2	2:D:504:GLN:NE2	2.39	0.54
1:C:274:ASP:OD1	1:C:309:THR:OG1	2.24	0.54
1:B:15:LYS:N	7:B:501:HOH:O	2.40	0.53
1:A:16:VAL:HG22	1:A:136:MET:HE3	1.91	0.53
1:C:45:ASN:ND2	1:C:337:ASP:OD1	2.43	0.52
1:A:235:ASP:HB2	1:A:358:GLN:HG3	1.92	0.51
1:C:229:VAL:HG13	1:C:371:LEU:HD22	1.92	0.50
1:C:336:ASN:HD21	1:C:342:PHE:HE2	1.60	0.50
1:A:271:LEU:HD11	1:A:316:CYS:HB2	1.94	0.50
1:A:47:LEU:HD23	1:A:318:THR:HG23	1.94	0.50
1:C:365:GLU:HA	1:C:368:LYS:HE2	1.94	0.50
1:C:209:TYR:OH	1:C:276:LEU:O	2.28	0.49
1:A:284:LYS:HG3	1:A:349:HIS:CD2	2.48	0.49
1:A:145:HIS:H	1:A:145:HIS:CD2	2.31	0.49
1:A:286:HIS:ND1	1:A:320:GLU:OE2	2.44	0.49
2:D:505:DLY:HB3	2:D:506:TRP:CD2	2.47	0.48
1:C:93:SER:HA	1:C:96:MET:HE2	1.94	0.48
1:C:145:HIS:ND1	1:C:179:ASP:OD2	2.40	0.48
1:B:215:ASP:OD1	1:B:216:LEU:N	2.47	0.48
1:C:236:GLY:O	1:C:357:ASN:HA	2.13	0.48
1:C:238:ASP:OD1	1:C:241:SER:N	2.36	0.48
1:C:39:ARG:HG3	1:C:40:ILE:HG13	1.95	0.48
1:B:184:HIS:HB2	1:B:204:HIS:CD2	2.49	0.47
1:A:45:ASN:O	1:A:49:ASN:ND2	2.44	0.47
1:B:147:ALA:HB3	1:B:159:ASN:HB2	1.97	0.47
1:A:362:GLU:HG2	1:B:344:PRO:HB3	1.95	0.47
1:B:166:LEU:HD23	1:B:169:LEU:HD12	1.95	0.47
1:B:189:GLU:HA	1:B:200:THR:HG21	1.96	0.47
1:A:340:GLU:H	1:A:340:GLU:HG3	1.45	0.46
1:B:331:ASN:N	1:C:75:ASP:OD2	2.48	0.46
1:A:131:ARG:HH11	1:A:133:GLN:HE22	1.64	0.46
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.97	0.46
1:A:239:ASP:OD2	1:A:282:THR:OG1	2.32	0.46
1:B:47:LEU:HD23	1:B:318:THR:HG23	1.96	0.46
1:C:169:LEU:O	1:C:197:ARG:NH1	2.49	0.46
2:D:504:GLN:HG2	2:D:505:DLY:HG3	1.98	0.46
1:B:45:ASN:O	1:B:49:ASN:ND2	2.38	0.46
1:A:173:GLN:HA	1:A:197:ARG:HH11	1.81	0.45
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.99	0.45
1:B:36:LYS:O	1:B:39:ARG:HG2	2.16	0.45
1:B:359:ASN:HB3	1:B:364:MET:SD	2.57	0.45
1:C:245:ILE:HG13	1:C:368:LYS:HD3	1.98	0.44
1:C:84:ILE:HG13	1:C:107:VAL:HG11	2.00	0.44
1:A:13:LYS:HE2	1:A:326:ASP:HB2	2.00	0.43
1:A:105:CYS:HB3	1:A:157:TYR:CE2	2.52	0.43
1:B:92:TYR:O	1:B:96:MET:HB2	2.19	0.43
1:B:77:TYR:CZ	1:B:81:LEU:HD11	2.53	0.43
1:A:122:SER:HB3	1:A:164:ALA:HB2	2.00	0.43
1:A:147:ALA:HB3	1:A:159:ASN:HB2	2.00	0.42
1:B:39:ARG:O	1:B:43:THR:HG23	2.18	0.42
1:A:189:GLU:HA	1:A:200:THR:HG21	2.00	0.42
1:B:347:LYS:NZ	1:C:73:HIS:O	2.44	0.42
2:D:505:DLY:HB3	2:D:506:TRP:CE3	2.54	0.42
1:C:172:HIS:HB3	1:C:260:SER:HB2	2.01	0.42
1:B:145:HIS:CD2	1:B:145:HIS:H	2.36	0.42
6:B:404:PG4:H51	6:B:404:PG4:H72	1.81	0.42
1:C:129:LEU:HD23	1:C:134:THR:HG23	2.02	0.41
1:C:199:MET:HE1	1:C:378:LEU:HD11	2.01	0.41
1:C:265:GLN:NE2	1:C:305:GLY:HA3	2.35	0.41
1:B:247:LYS:HB3	1:B:248:PRO:HD3	2.02	0.41
1:A:182:ILE:HG13	1:A:279:PHE:CE1	2.56	0.41
1:C:148:LYS:NZ	1:C:186:ASP:OD1	2.48	0.41
1:A:40:ILE:HD13	1:A:141:ALA:HA	2.02	0.41
1:A:338:TYR:HB3	1:A:341:TYR:CD1	2.56	0.41
1:A:103:GLU:HB3	1:A:104:ASP:H	1.74	0.40
1:B:165:ILE:HG12	1:B:263:VAL:HG21	2.03	0.40
1:B:254:MET:HG3	1:B:296:PHE:CZ	2.56	0.40
1:C:86:PRO:HA	1:C:89:MET:HG3	2.02	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	370/385 (96%)	355 (96%)	15 (4%)	0	100	100
1	B	362/385 (94%)	345 (95%)	17 (5%)	0	100	100
1	C	363/385 (94%)	340 (94%)	22 (6%)	1 (0%)	36	65
2	D	4/8 (50%)	4 (100%)	0	0	100	100
2	F	4/8 (50%)	2 (50%)	1 (25%)	1 (25%)	0	0
2	G	4/8 (50%)	2 (50%)	2 (50%)	0	100	100
All	All	1107/1179 (94%)	1048 (95%)	57 (5%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	506	TRP
1	C	236	GLY

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	316/327 (97%)	315 (100%)	1 (0%)	86	96
1	B	314/327 (96%)	313 (100%)	1 (0%)	86	96
1	C	313/327 (96%)	308 (98%)	5 (2%)	55	83
2	D	4/4 (100%)	2 (50%)	2 (50%)	0	0
2	F	2/4 (50%)	2 (100%)	0	100	100
2	G	2/4 (50%)	2 (100%)	0	100	100
All	All	951/993 (96%)	942 (99%)	9 (1%)	70	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	GLU
1	B	96	MET
1	C	103	GLU
1	C	235	ASP
1	C	239	ASP
1	C	327	CYS
1	C	332	GLU
2	D	504	GLN
2	D	506	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	374	ASN
1	B	116	GLN
1	B	354	ASN
1	C	33	HIS
1	C	95	GLN
1	C	139	ASN
1	C	230	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 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	3,2	8,9,10	3.29	2 (25%)	4,9,11	1.47	1 (25%)
2	HYP	D	502	2	7,8,9	5.61	5 (71%)	5,10,12	1.87	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	U2M	D	500	3,2	8,9,10	3.32	2 (25%)	4,9,11	1.30	0
2	U2M	F	500	3,2	8,9,10	3.22	2 (25%)	4,9,11	1.15	0
2	HYP	F	502	2	7,8,9	5.59	5 (71%)	5,10,12	1.12	0
2	HYP	G	502	2	7,8,9	5.52	5 (71%)	5,10,12	2.32	2 (40%)

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	3,2	-	3/7/8/10	-
2	HYP	D	502	2	-	0/0/11/13	0/1/1/1
2	U2M	D	500	3,2	-	4/7/8/10	-
2	U2M	F	500	3,2	-	1/7/8/10	-
2	HYP	F	502	2	-	0/0/11/13	0/1/1/1
2	HYP	G	502	2	-	0/0/11/13	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	502	HYP	CB-CG	-10.75	1.33	1.52
2	D	502	HYP	CB-CG	-10.66	1.33	1.52
2	G	502	HYP	CB-CG	-10.53	1.33	1.52
2	D	502	HYP	CA-N	-7.89	1.34	1.48
2	D	500	U2M	CA-N	-7.88	1.26	1.48
2	G	500	U2M	CA-N	-7.82	1.26	1.48
2	F	502	HYP	CA-N	-7.77	1.35	1.48
2	F	500	U2M	CA-N	-7.62	1.26	1.48
2	G	502	HYP	CA-N	-7.61	1.35	1.48
2	G	502	HYP	CB-CA	5.17	1.65	1.54
2	D	500	U2M	CZ-SH	-5.05	1.60	1.80
2	D	502	HYP	CB-CA	5.05	1.65	1.54
2	G	500	U2M	CZ-SH	-5.00	1.60	1.80
2	F	500	U2M	CZ-SH	-4.94	1.60	1.80
2	F	502	HYP	CB-CA	4.93	1.65	1.54
2	F	502	HYP	CD-N	2.97	1.57	1.47
2	D	502	HYP	CD-N	2.91	1.57	1.47
2	G	502	HYP	CD-N	2.85	1.57	1.47
2	F	502	HYP	CD-CG	2.47	1.58	1.53
2	D	502	HYP	CD-CG	2.43	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	502	HYP	CD-CG	2.35	1.58	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	502	HYP	CG-CB-CA	3.89	108.25	103.75
2	G	502	HYP	CB-CG-CD	2.96	106.46	103.16
2	D	502	HYP	CG-CB-CA	2.71	106.88	103.75
2	D	502	HYP	CB-CG-CD	2.57	106.02	103.16
2	G	500	U2M	CD-CE-CZ	-2.44	108.74	113.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	500	U2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are 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
6	PG4	B	404	-	12,12,12	0.54	0	11,11,11	0.25	0
5	PGE	A	405	-	9,9,9	0.53	0	8,8,8	0.24	0
5	PGE	C	403	-	9,9,9	0.53	0	8,8,8	0.26	0
5	PGE	B	405	-	9,9,9	0.53	0	8,8,8	0.24	0
5	PGE	A	404	-	9,9,9	0.53	0	8,8,8	0.24	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	404	-	-	8/10/10/10	-
5	PGE	A	405	-	-	4/7/7/7	-
5	PGE	C	403	-	-	1/7/7/7	-
5	PGE	B	405	-	-	4/7/7/7	-
5	PGE	A	404	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	404	PG4	C3-C4-O3-C5
5	A	404	PGE	O3-C5-C6-O4
6	B	404	PG4	O2-C3-C4-O3
5	A	405	PGE	O2-C3-C4-O3
6	B	404	PG4	C4-C3-O2-C2
5	A	405	PGE	C6-C5-O3-C4
5	B	405	PGE	O3-C5-C6-O4
5	C	403	PGE	C3-C4-O3-C5
5	B	405	PGE	C1-C2-O2-C3
6	B	404	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
6	B	404	PG4	O4-C7-C8-O5
5	B	405	PGE	C3-C4-O3-C5
5	A	405	PGE	C3-C4-O3-C5
6	B	404	PG4	C5-C6-O4-C7
5	A	404	PGE	O2-C3-C4-O3
5	A	405	PGE	O1-C1-C2-O2
6	B	404	PG4	O1-C1-C2-O2
6	B	404	PG4	O3-C5-C6-O4
5	B	405	PGE	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	404	PG4	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, 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	372/385 (96%)	-0.07	1 (0%) 90 87	34, 48, 68, 82	0
1	B	364/385 (94%)	-0.05	0 100 100	32, 51, 74, 85	2 (0%)
1	C	365/385 (94%)	0.47	8 (2%) 62 53	55, 86, 96, 108	64 (17%)
2	D	5/8 (62%)	0.06	0 100 100	59, 62, 72, 73	0
2	F	5/8 (62%)	0.97	1 (20%) 3 2	78, 92, 105, 113	2 (40%)
2	G	5/8 (62%)	1.68	2 (40%) 1 0	57, 77, 96, 107	4 (80%)
All	All	1116/1179 (94%)	0.13	12 (1%) 78 71	32, 57, 93, 113	72 (6%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	503	LYS	2.5
2	F	506	TRP	2.4
2	G	506	TRP	2.4
1	C	141	ALA	2.3
1	C	309	THR	2.3
1	A	378	LEU	2.2
1	C	109	ASP	2.2
1	C	250	ILE	2.2
1	C	344	PRO	2.1
1	C	144	LEU	2.1
1	C	54	ARG	2.0
1	C	40	ILE	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($\text{\AA}^2$)	Q<0.9
2	DLY	F	505	5/10	-0.04	0.24	109,110,111,111	0
2	DLY	G	505	5/10	0.44	0.34	113,114,122,123	5
2	HYP	F	502	8/9	0.61	0.15	105,108,111,120	0
2	HYP	G	502	8/9	0.67	0.17	98,112,116,119	8
2	DLY	D	505	9/10	0.83	0.12	63,67,79,79	0
2	U2M	G	500	10/11	0.85	0.13	79,85,101,105	2
2	HYP	D	502	8/9	0.86	0.08	47,62,69,76	0
2	U2M	F	500	10/11	0.94	0.11	37,63,83,84	0
2	U2M	D	500	10/11	0.96	0.10	42,47,58,60	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PG4	B	404	13/13	0.70	0.13	64,69,80,81	0
5	PGE	A	405	10/10	0.76	0.11	61,71,75,76	0
5	PGE	A	404	10/10	0.76	0.14	58,68,69,70	0
5	PGE	B	405	10/10	0.77	0.14	61,73,79,83	0
5	PGE	C	403	10/10	0.79	0.15	59,68,75,76	0
4	NA	B	403	1/1	0.82	0.20	59,59,59,59	0
4	NA	A	403	1/1	0.86	0.15	45,45,45,45	0
4	NA	C	402	1/1	0.96	0.05	73,73,73,73	0
4	NA	A	402	1/1	0.98	0.06	25,25,25,25	0
4	NA	B	402	1/1	0.99	0.05	30,30,30,30	0
3	ZN	C	401	1/1	0.99	0.03	73,73,73,73	0
3	ZN	A	401	1/1	0.99	0.04	44,44,44,44	0
3	ZN	B	401	1/1	0.99	0.03	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.