



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2025 – 10:24 AM JST

PDB ID : 9JV3 / pdb_00009jv3
Title : Structure of Human HDAC2
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Deposited on : 2024-10-08
Resolution : 2.57 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

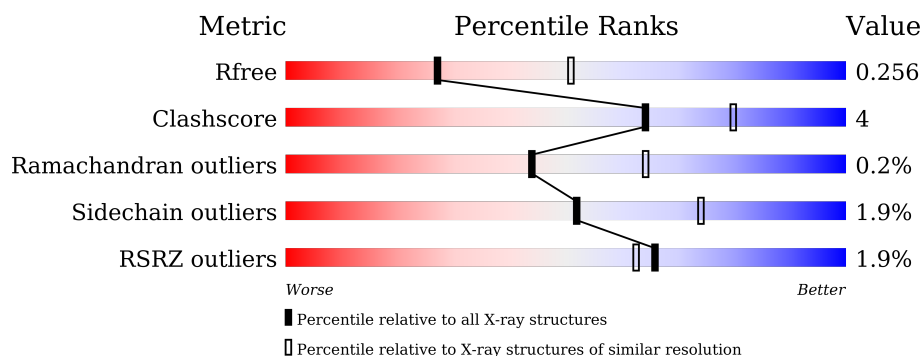
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 1%, yellow 8%, green 82%, grey 9%);"></div> </div> <div> 3% 82% 8% 9% </div> </div>
1	B	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 79%, grey 9%);"></div> </div> <div> 79% 11% 9% </div> </div>
1	C	404	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 3%, orange 1%, yellow 13%, green 76%, grey 9%);"></div> </div> <div> 76% 13% 9% </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9316 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	369	Total	C	N	O	S	27	1	0
			2966	1894	503	544	25			
1	B	366	Total	C	N	O	S	22	1	0
			2959	1890	501	544	24			
1	C	367	Total	C	N	O	S	75	0	0
			2944	1882	499	539	24			

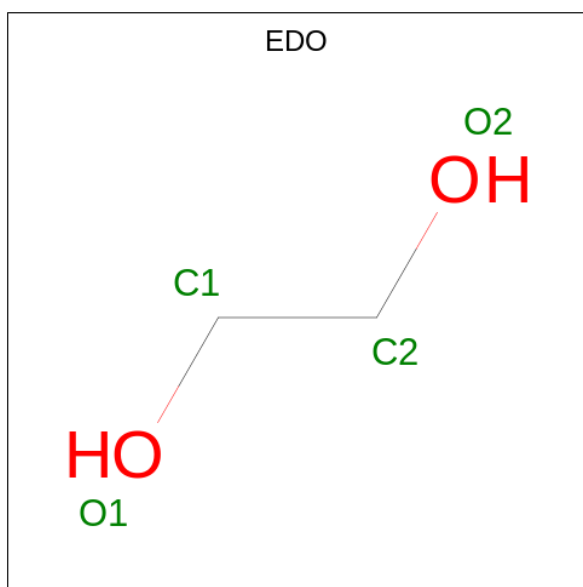
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

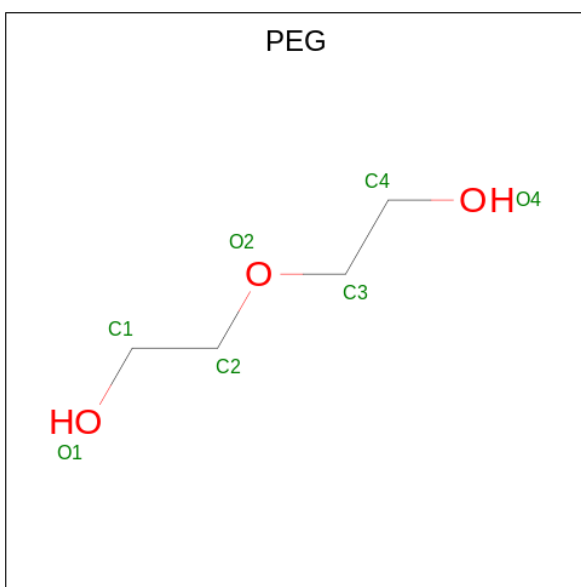
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



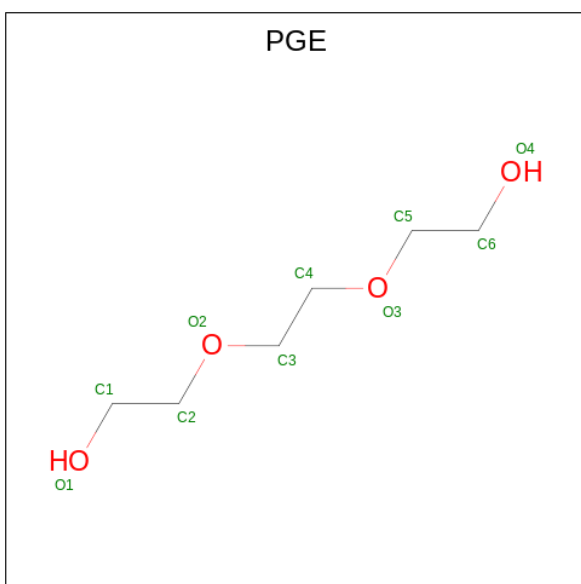
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



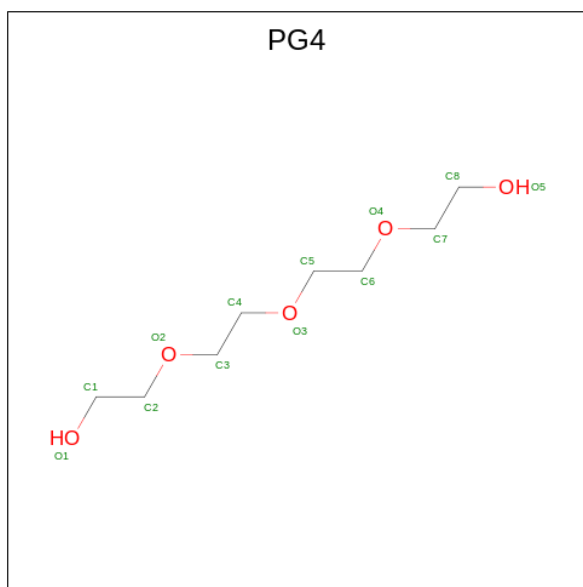
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



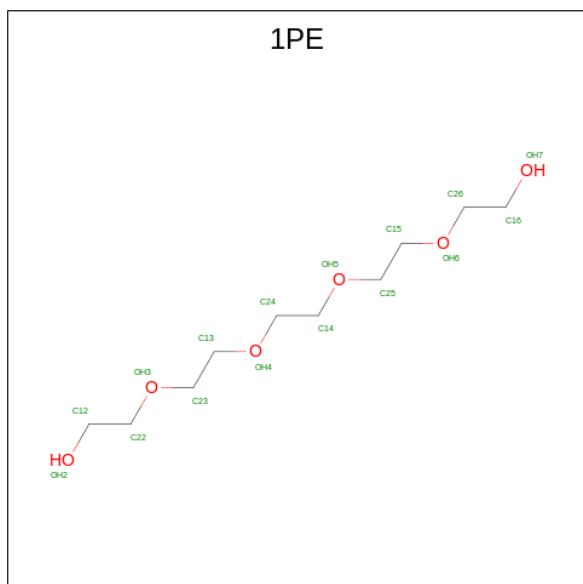
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			16	10	6		

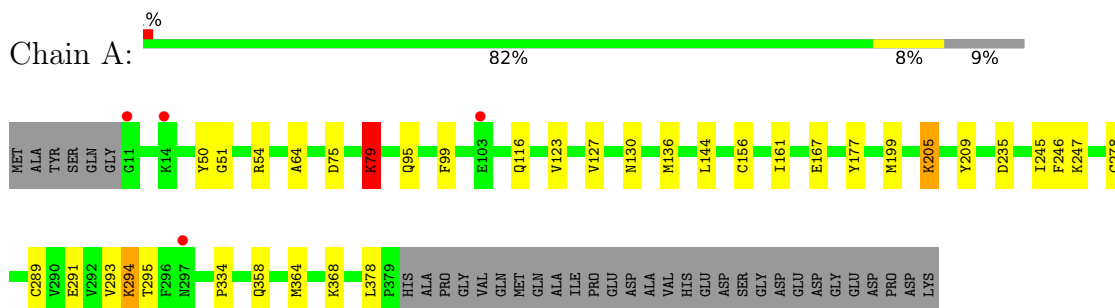
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	122	Total	O	0	0
			122	122		
9	B	117	Total	O	0	1
			118	118		
9	C	62	Total	O	0	0
			62	62		

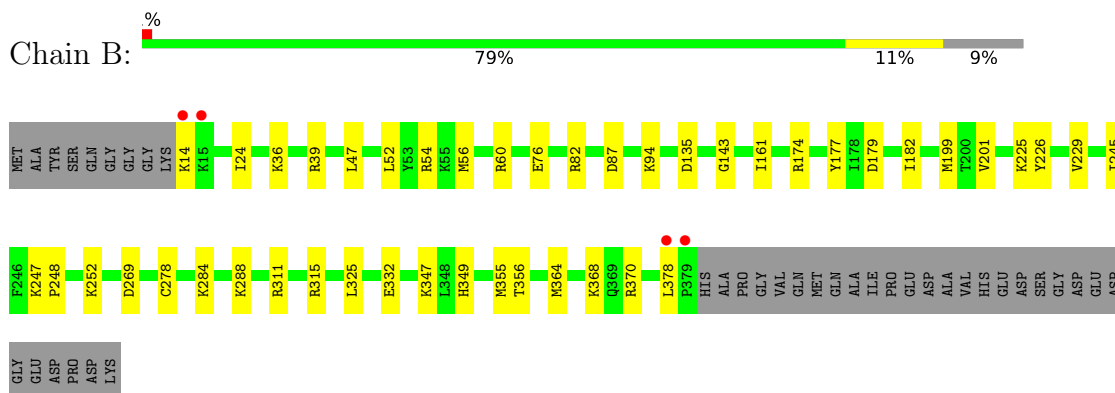
3 Residue-property plots [i](#)

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.

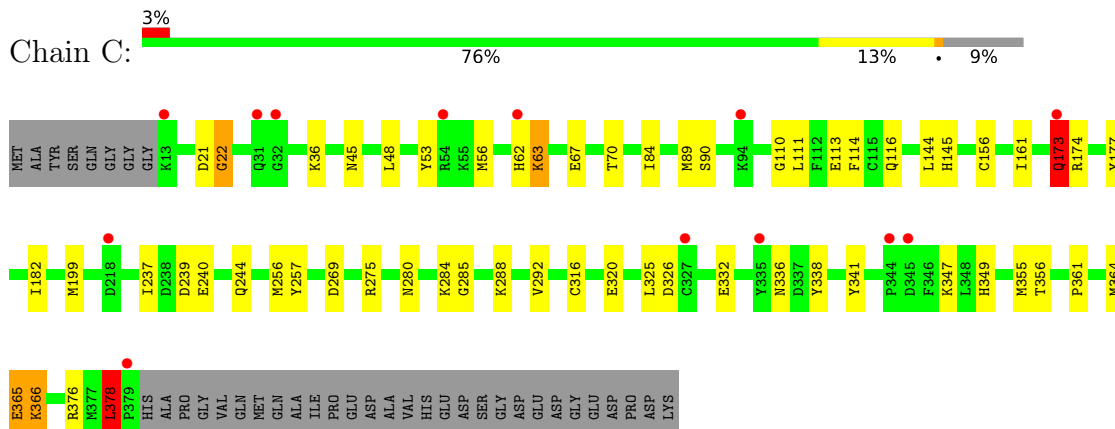
• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 97.58Å 138.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 50.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.57) 97.4 (50.00-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.181 , 0.256 0.189 , 0.256	Depositor DCC
R_{free} test set	953 reflections (2.35%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9316	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: CA, 1PE, ZN, PGE, EDO, PG4, 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	0.62	2/3043 (0.1%)	0.89	2/4108 (0.0%)
1	B	0.63	1/3039 (0.0%)	1.22	11/4104 (0.3%)
1	C	0.75	7/3020 (0.2%)	0.95	12/4078 (0.3%)
All	All	0.67	10/9102 (0.1%)	1.03	25/12290 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	366	LYS	CG-CD	14.59	1.96	1.52
1	C	62	HIS	CB-CG	-13.65	1.31	1.50
1	C	173	GLN	CG-CD	11.44	1.80	1.52
1	B	368	LYS	CD-CE	-10.55	1.20	1.52
1	A	368	LYS	CD-CE	10.11	1.82	1.52
1	C	275	ARG	CG-CD	-9.59	1.23	1.52
1	C	376	ARG	CB-CG	-8.37	1.27	1.52
1	C	63	LYS	CD-CE	7.88	1.76	1.52
1	C	365	GLU	CG-CD	7.00	1.69	1.52
1	A	247	LYS	CE-NZ	5.78	1.66	1.49

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	NE-CZ-NH2	31.62	147.66	119.20
1	B	54	ARG	CD-NE-CZ	27.62	163.07	124.40
1	B	54	ARG	NE-CZ-NH1	-27.37	94.13	121.50
1	B	368	LYS	CG-CD-CE	15.08	145.98	111.30
1	A	79	LYS	CG-CD-CE	11.54	137.84	111.30
1	C	366	LYS	CB-CG-CD	-10.84	86.36	111.30
1	C	365	GLU	CB-CG-CD	9.29	128.39	112.60
1	B	288	LYS	CG-CD-CE	8.03	129.77	111.30
1	C	62	HIS	CA-CB-CG	7.44	121.24	113.80
1	C	347	LYS	CG-CD-CE	7.15	127.75	111.30
1	C	36	LYS	CD-CE-NZ	-7.11	89.15	111.90
1	C	376	ARG	CA-CB-CG	6.51	127.11	114.10
1	C	145	HIS	N-CA-C	6.35	120.49	112.87
1	B	60[A]	ARG	CA-C-N	-6.19	114.25	120.31
1	B	60[A]	ARG	C-N-CA	-6.19	114.25	120.31
1	B	60[B]	ARG	CA-C-N	-6.19	114.25	120.31
1	B	60[B]	ARG	C-N-CA	-6.19	114.25	120.31
1	C	63	LYS	CG-CD-CE	-6.01	97.48	111.30
1	B	76	GLU	CA-CB-CG	5.78	125.66	114.10
1	C	275	ARG	CB-CG-CD	5.63	124.26	111.30
1	C	244	GLN	CA-CB-CG	5.58	125.26	114.10
1	C	173	GLN	CG-CD-NE2	-5.32	108.43	116.40
1	C	366	LYS	CG-CD-CE	5.27	123.43	111.30
1	A	79	LYS	CB-CG-CD	5.17	123.19	111.30
1	B	76	GLU	CB-CG-CD	5.15	121.35	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	173	GLN	Sidechain
1	C	378	LEU	Peptide

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	2966	0	2870	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2959	0	2868	23	0
1	C	2944	0	2843	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	16	0	24	0	0
4	B	20	0	30	3	0
4	C	16	0	24	1	0
5	A	14	0	20	0	0
5	B	7	0	10	0	0
5	C	14	0	20	0	0
6	A	10	0	14	0	0
6	B	10	0	14	0	0
7	B	13	0	18	5	0
8	B	16	0	22	0	0
9	A	122	0	0	0	0
9	B	118	0	0	2	0
9	C	62	0	0	0	0
All	All	9316	0	8777	67	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 4.

All (67) 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:284:LYS:HZ2	7:B:506:PG4:H41	1.00	1.06
1:B:284:LYS:NZ	7:B:506:PG4:H41	1.82	0.94
1:B:245:ILE:HG21	1:B:364:MET:HE3	1.62	0.79
1:C:199:MET:HE1	1:C:378:LEU:HD11	1.78	0.66
1:B:199:MET:HE1	1:B:378:LEU:HD11	1.79	0.65
1:B:349:HIS:CD2	7:B:506:PG4:H42	2.33	0.64
1:A:205:LYS:HG3	1:A:278[A]:CYS:SG	2.41	0.61
7:B:506:PG4:H31	9:B:629:HOH:O	2.01	0.60
1:A:75:ASP:O	1:A:79:LYS:HB2	2.02	0.59
1:A:144:LEU:HB3	1:A:156:CYS:HB3	1.86	0.57
1:A:199:MET:HE1	1:A:378:LEU:HD11	1.87	0.57
1:C:316:CYS:O	1:C:320:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.86	0.56
1:B:247:LYS:HB3	1:B:248:PRO:HD3	1.88	0.55
1:C:45:ASN:OD1	1:C:336:ASN:HB2	2.06	0.55
1:B:174:ARG:HD3	4:B:508:EDO:H21	1.90	0.54
1:C:338:TYR:O	1:C:341:TYR:HB2	2.07	0.54
1:A:95:GLN:HG2	1:A:99:PHE:HE2	1.74	0.52
1:C:182:ILE:HG22	1:C:269:ASP:CG	2.34	0.52
1:A:95:GLN:HG2	1:A:99:PHE:CE2	2.45	0.52
1:A:245:ILE:HG12	1:A:364:MET:HE3	1.90	0.52
1:C:239:ASP:OD1	1:C:285:GLY:HA3	2.10	0.52
1:B:47:LEU:HB2	1:B:52:LEU:HD12	1.90	0.52
1:B:14:LYS:HD3	4:B:507:EDO:H11	1.92	0.51
1:A:64:ALA:O	1:A:116:GLN:HG2	2.10	0.51
1:C:361:PRO:HA	1:C:364:MET:HE2	1.93	0.50
1:C:288:LYS:O	1:C:292:VAL:HG23	2.12	0.50
1:B:143:GLY:HA2	1:B:161:ILE:HD11	1.94	0.50
1:B:225:LYS:O	1:B:226:TYR:HB2	2.13	0.48
1:B:311:ARG:O	1:B:315:ARG:HG3	2.13	0.48
1:C:84:ILE:HD11	1:C:89:MET:HA	1.94	0.48
1:C:284:LYS:HG3	1:C:349:HIS:CD2	2.48	0.48
1:B:370:ARG:HB3	9:B:661:HOH:O	2.14	0.48
1:B:182:ILE:HG22	1:B:269:ASP:CG	2.39	0.47
1:C:111:LEU:O	1:C:114:PHE:HB3	2.14	0.47
1:A:136:MET:HE1	1:A:294:LYS:HE3	1.96	0.47
1:B:177:TYR:CE2	1:B:179:ASP:HB2	2.50	0.47
1:A:50:TYR:CZ	1:A:334:PRO:HD3	2.50	0.47
1:B:332:GLU:OE1	1:B:347:LYS:NZ	2.48	0.46
1:A:51:GLY:HA3	1:A:54:ARG:HH21	1.81	0.46
1:C:161:ILE:HG21	1:C:177:TYR:CE1	2.51	0.46
1:B:135:ASP:HB3	4:B:507:EDO:H22	1.97	0.46
1:C:67:GLU:O	1:C:70:THR:OG1	2.27	0.46
1:C:256:MET:HB3	1:C:378:LEU:HD12	1.97	0.46
1:A:291:GLU:O	1:A:295:THR:HG23	2.17	0.45
1:A:245:ILE:C	1:A:245:ILE:HD12	2.43	0.44
1:A:161:ILE:HG21	1:A:177:TYR:CE1	2.51	0.44
1:A:123:VAL:O	1:A:127:VAL:HG23	2.18	0.44
1:B:36:LYS:O	1:B:39:ARG:HD3	2.18	0.44
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.98	0.44
1:A:245:ILE:HD12	1:A:246:PHE:N	2.32	0.43
1:C:63:LYS:HB3	1:C:116:GLN:HB3	2.01	0.43
1:A:289:CYS:O	1:A:293:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HD2	1:B:252:LYS:HA	1.77	0.43
1:C:144:LEU:HB3	1:C:156:CYS:HB3	2.00	0.42
1:B:245:ILE:HG12	1:B:364:MET:CE	2.49	0.42
1:B:284:LYS:HZ2	7:B:506:PG4:H21	1.83	0.42
1:C:174:ARG:HB3	1:C:257:TYR:CE2	2.54	0.42
1:C:280:ASN:ND2	1:C:355:MET:HG2	2.35	0.42
1:A:235:ASP:HB2	1:A:358:GLN:HG3	2.00	0.42
1:A:205:LYS:HD2	1:A:209:TYR:CG	2.54	0.42
1:B:201:VAL:HG22	1:B:229:VAL:HB	2.02	0.42
1:C:173:GLN:HG3	4:C:505:EDO:H21	2.02	0.41
1:C:110:GLY:HA2	1:C:113:GLU:OE1	2.20	0.41
1:C:21:ASP:O	1:C:22:GLY:C	2.63	0.41
1:C:48:LEU:HD23	1:C:53:TYR:HB3	2.03	0.41
1:A:130:ASN:ND2	1:A:167:GLU:HG3	2.37	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	368/404 (91%)	354 (96%)	14 (4%)	0	100	100
1	B	365/404 (90%)	357 (98%)	8 (2%)	0	100	100
1	C	365/404 (90%)	345 (94%)	18 (5%)	2 (0%)	25	45
All	All	1098/1212 (91%)	1056 (96%)	40 (4%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	22	GLY
1	C	378	LEU

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	316/344 (92%)	313 (99%)	3 (1%)	75	89
1	B	317/344 (92%)	310 (98%)	7 (2%)	47	70
1	C	312/344 (91%)	304 (97%)	8 (3%)	41	65
All	All	945/1032 (92%)	927 (98%)	18 (2%)	52	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	205	LYS
1	A	294	LYS
1	B	24	ILE
1	B	82	ARG
1	B	87	ASP
1	B	94	LYS
1	B	278	CYS
1	B	355	MET
1	B	356	THR
1	C	90	SER
1	C	237	ILE
1	C	240	GLU
1	C	326	ASP
1	C	332	GLU
1	C	356	THR
1	C	365	GLU
1	C	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	358	GLN
1	B	133	GLN

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Mol	Chain	Res	Type
1	B	173	GLN
1	B	349	HIS
1	C	38	HIS
1	C	116	GLN
1	C	133	GLN
1	C	172	HIS
1	C	280	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 9 are monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	504	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	C	507	-	3,3,3	0.49	0	2,2,2	0.36	0
8	1PE	B	511	-	15,15,15	0.49	0	14,14,14	0.23	0
6	PGE	A	506	-	9,9,9	0.56	0	8,8,8	0.34	0
4	EDO	B	512	-	3,3,3	0.63	0	2,2,2	0.07	0
4	EDO	B	510	-	3,3,3	0.61	0	2,2,2	0.20	0
5	PEG	C	504	-	6,6,6	0.47	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	B	505	-	6,6,6	0.47	0	5,5,5	0.24	0
4	EDO	B	508	-	3,3,3	0.49	0	2,2,2	0.22	0
4	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	508	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	B	509	-	3,3,3	0.54	0	2,2,2	0.12	0
6	PGE	B	504	-	9,9,9	0.58	0	8,8,8	0.31	0
4	EDO	A	509	-	3,3,3	0.46	0	2,2,2	0.33	0
4	EDO	C	505	-	3,3,3	0.60	0	2,2,2	0.09	0
5	PEG	A	507	-	6,6,6	0.53	0	5,5,5	0.28	0
4	EDO	C	508	-	3,3,3	0.53	0	2,2,2	0.08	0
4	EDO	A	510	-	3,3,3	0.60	0	2,2,2	0.14	0
5	PEG	A	505	-	6,6,6	0.53	0	5,5,5	0.48	0
5	PEG	C	509	-	6,6,6	0.48	0	5,5,5	0.31	0
4	EDO	B	507	-	3,3,3	0.55	0	2,2,2	0.18	0
7	PG4	B	506	-	12,12,12	0.51	0	11,11,11	0.37	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
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
8	1PE	B	511	-	-	4/13/13/13	-
6	PGE	A	506	-	-	2/7/7/7	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
5	PEG	C	504	-	-	2/4/4/4	-
5	PEG	B	505	-	-	1/4/4/4	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
6	PGE	B	504	-	-	2/7/7/7	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
5	PEG	A	507	-	-	2/4/4/4	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
5	PEG	A	505	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	509	-	-	4/4/4/4	-
4	EDO	B	507	-	-	1/1/1/1	-
7	PG4	B	506	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	507	PEG	O1-C1-C2-O2
7	B	506	PG4	O4-C7-C8-O5
5	A	505	PEG	C1-C2-O2-C3
5	A	507	PEG	O2-C3-C4-O4
5	B	505	PEG	O2-C3-C4-O4
5	C	504	PEG	O2-C3-C4-O4
5	C	509	PEG	O1-C1-C2-O2
7	B	506	PG4	O1-C1-C2-O2
6	B	504	PGE	O2-C3-C4-O3
4	A	504	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
4	B	507	EDO	O1-C1-C2-O2
4	B	509	EDO	O1-C1-C2-O2
4	B	510	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
7	B	506	PG4	O2-C3-C4-O3
4	C	505	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
5	A	505	PEG	C4-C3-O2-C2
8	B	511	1PE	C16-C26-OH6-C15
6	A	506	PGE	C3-C4-O3-C5
7	B	506	PG4	C5-C6-O4-C7
6	A	506	PGE	C1-C2-O2-C3
7	B	506	PG4	C6-C5-O3-C4
8	B	511	1PE	OH2-C12-C22-OH3
5	C	504	PEG	C4-C3-O2-C2
6	B	504	PGE	C4-C3-O2-C2
8	B	511	1PE	C25-C15-OH6-C26
8	B	511	1PE	OH5-C14-C24-OH4
7	B	506	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	B	512	EDO	O1-C1-C2-O2
5	C	509	PEG	C4-C3-O2-C2
5	C	509	PEG	C1-C2-O2-C3
5	C	509	PEG	O2-C3-C4-O4
4	A	508	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	508	EDO	1	0
4	C	505	EDO	1	0
4	B	507	EDO	2	0
7	B	506	PG4	5	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, 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	369/404 (91%)	0.06	4 (1%) 77 75	29, 56, 76, 96	12 (3%)
1	B	366/404 (90%)	-0.09	4 (1%) 77 75	30, 54, 74, 102	8 (2%)
1	C	367/404 (90%)	0.43	13 (3%) 47 43	28, 66, 89, 119	21 (5%)
All	All	1102/1212 (90%)	0.13	21 (1%) 66 62	28, 57, 82, 119	41 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	379	PRO	4.5
1	A	11	GLY	3.6
1	C	31	GLN	3.2
1	C	344	PRO	3.2
1	B	379	PRO	3.0
1	C	54	ARG	2.9
1	C	218	ASP	2.9
1	A	103	GLU	2.7
1	C	62	HIS	2.6
1	C	345	ASP	2.4
1	C	13	LYS	2.3
1	B	378	LEU	2.2
1	C	32	GLY	2.2
1	C	327	CYS	2.2
1	C	335	TYR	2.1
1	C	94	LYS	2.1
1	A	14	LYS	2.1
1	A	297	ASN	2.1
1	B	14	LYS	2.0
1	C	173	GLN	2.0
1	B	15	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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, 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
4	EDO	B	507	4/4	0.76	0.24	86,88,88,92	0
4	EDO	A	508	4/4	0.79	0.25	98,103,104,105	0
4	EDO	B	510	4/4	0.80	0.17	73,75,80,81	0
4	EDO	B	508	4/4	0.81	0.25	93,94,99,99	0
4	EDO	C	507	4/4	0.81	0.23	81,84,88,88	0
4	EDO	C	508	4/4	0.82	0.21	83,83,84,87	0
4	EDO	A	504	4/4	0.87	0.15	60,63,68,71	0
5	PEG	A	505	7/7	0.87	0.18	79,86,90,94	0
5	PEG	B	505	7/7	0.87	0.16	79,83,86,87	0
6	PGE	A	506	10/10	0.87	0.17	67,81,88,90	0
4	EDO	C	506	4/4	0.88	0.18	81,84,88,89	0
5	PEG	C	509	7/7	0.89	0.17	82,83,93,97	0
5	PEG	A	507	7/7	0.89	0.17	70,75,93,97	0
4	EDO	A	510	4/4	0.90	0.17	60,71,73,73	0
6	PGE	B	504	10/10	0.90	0.15	68,75,78,87	0
4	EDO	B	509	4/4	0.91	0.17	73,74,76,80	0
4	EDO	B	512	4/4	0.91	0.14	76,81,81,86	0
5	PEG	C	504	7/7	0.91	0.18	65,67,79,80	0
4	EDO	C	505	4/4	0.92	0.15	62,63,63,64	0
8	1PE	B	511	16/16	0.93	0.14	67,78,90,94	0
7	PG4	B	506	13/13	0.94	0.13	69,75,83,83	0
2	ZN	C	501	1/1	0.95	0.10	63,63,63,63	0
4	EDO	A	509	4/4	0.95	0.09	73,80,86,93	0
2	ZN	A	501	1/1	0.95	0.07	55,55,55,55	0
2	ZN	B	501	1/1	0.97	0.09	54,54,54,54	0
3	CA	C	502	1/1	0.97	0.15	65,65,65,65	0
3	CA	B	503	1/1	0.98	0.05	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	503	1/1	0.98	0.09	56,56,56,56	0
3	CA	B	502	1/1	0.98	0.10	55,55,55,55	0
3	CA	A	502	1/1	0.99	0.13	54,54,54,54	0
3	CA	C	503	1/1	0.99	0.15	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.