



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:24 PM UTC

PDB ID : 4E0T / pdb_00004e0t
Title : Crystal structure of CdpNPT in its unbound state
Authors : Schuller, J.M.; Zocher, G.; Stehle, T.
Deposited on : 2012-03-05
Resolution : 2.25 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

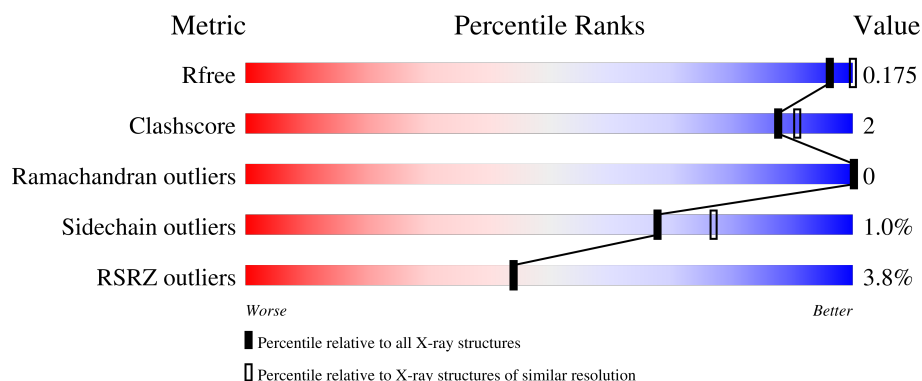
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	428	3% 89% 7% 5%
1	B	428	4% 86% 9% 5%
1	C	428	4% 88% 7% 5%
1	D	428	3% 89% 5% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13871 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 Cyclic dipeptide N-prenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	3	0
			3271	2106	550	595	20			
1	B	406	Total	C	N	O	S	0	3	0
			3241	2093	536	593	19			
1	C	406	Total	C	N	O	S	0	3	0
			3237	2086	537	595	19			
1	D	406	Total	C	N	O	S	0	3	0
			3249	2098	537	595	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	-	expression tag	UNP D1D8L6
A	14	HIS	-	expression tag	UNP D1D8L6
A	15	HIS	-	expression tag	UNP D1D8L6
A	16	HIS	-	expression tag	UNP D1D8L6
A	17	HIS	-	expression tag	UNP D1D8L6
A	18	HIS	-	expression tag	UNP D1D8L6
A	19	SER	-	expression tag	UNP D1D8L6
A	20	SER	-	expression tag	UNP D1D8L6
A	21	GLY	-	expression tag	UNP D1D8L6
A	22	LEU	-	expression tag	UNP D1D8L6
A	23	VAL	-	expression tag	UNP D1D8L6
A	24	PRO	-	expression tag	UNP D1D8L6
A	25	ARG	-	expression tag	UNP D1D8L6
A	26	GLY	-	expression tag	UNP D1D8L6
A	27	SER	-	expression tag	UNP D1D8L6
A	28	HIS	-	expression tag	UNP D1D8L6
B	13	HIS	-	expression tag	UNP D1D8L6
B	14	HIS	-	expression tag	UNP D1D8L6
B	15	HIS	-	expression tag	UNP D1D8L6
B	16	HIS	-	expression tag	UNP D1D8L6
B	17	HIS	-	expression tag	UNP D1D8L6

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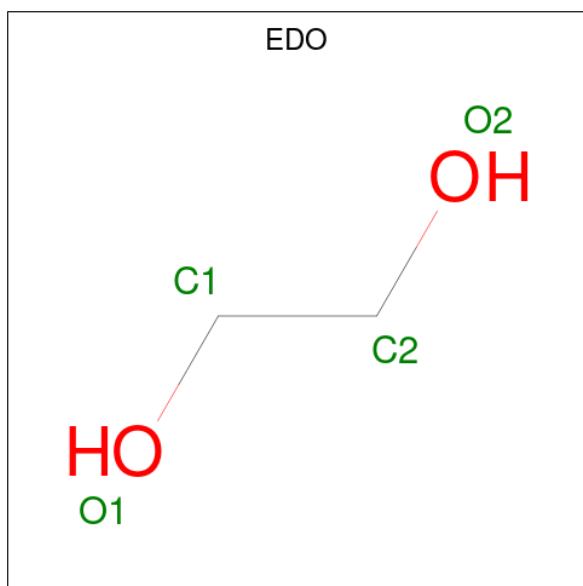
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	expression tag	UNP D1D8L6
B	19	SER	-	expression tag	UNP D1D8L6
B	20	SER	-	expression tag	UNP D1D8L6
B	21	GLY	-	expression tag	UNP D1D8L6
B	22	LEU	-	expression tag	UNP D1D8L6
B	23	VAL	-	expression tag	UNP D1D8L6
B	24	PRO	-	expression tag	UNP D1D8L6
B	25	ARG	-	expression tag	UNP D1D8L6
B	26	GLY	-	expression tag	UNP D1D8L6
B	27	SER	-	expression tag	UNP D1D8L6
B	28	HIS	-	expression tag	UNP D1D8L6
C	13	HIS	-	expression tag	UNP D1D8L6
C	14	HIS	-	expression tag	UNP D1D8L6
C	15	HIS	-	expression tag	UNP D1D8L6
C	16	HIS	-	expression tag	UNP D1D8L6
C	17	HIS	-	expression tag	UNP D1D8L6
C	18	HIS	-	expression tag	UNP D1D8L6
C	19	SER	-	expression tag	UNP D1D8L6
C	20	SER	-	expression tag	UNP D1D8L6
C	21	GLY	-	expression tag	UNP D1D8L6
C	22	LEU	-	expression tag	UNP D1D8L6
C	23	VAL	-	expression tag	UNP D1D8L6
C	24	PRO	-	expression tag	UNP D1D8L6
C	25	ARG	-	expression tag	UNP D1D8L6
C	26	GLY	-	expression tag	UNP D1D8L6
C	27	SER	-	expression tag	UNP D1D8L6
C	28	HIS	-	expression tag	UNP D1D8L6
D	13	HIS	-	expression tag	UNP D1D8L6
D	14	HIS	-	expression tag	UNP D1D8L6
D	15	HIS	-	expression tag	UNP D1D8L6
D	16	HIS	-	expression tag	UNP D1D8L6
D	17	HIS	-	expression tag	UNP D1D8L6
D	18	HIS	-	expression tag	UNP D1D8L6
D	19	SER	-	expression tag	UNP D1D8L6
D	20	SER	-	expression tag	UNP D1D8L6
D	21	GLY	-	expression tag	UNP D1D8L6
D	22	LEU	-	expression tag	UNP D1D8L6
D	23	VAL	-	expression tag	UNP D1D8L6
D	24	PRO	-	expression tag	UNP D1D8L6
D	25	ARG	-	expression tag	UNP D1D8L6
D	26	GLY	-	expression tag	UNP D1D8L6
D	27	SER	-	expression tag	UNP D1D8L6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	HIS	-	expression tag	UNP D1D8L6

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



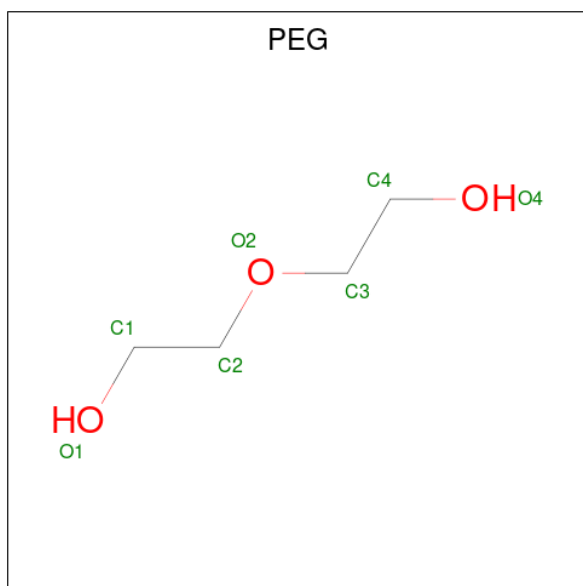
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Cl 3 3	0	0
4	B	3	Total Cl 3 3	0	0
4	C	3	Total Cl 3 3	0	0
4	D	3	Total Cl 3 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0

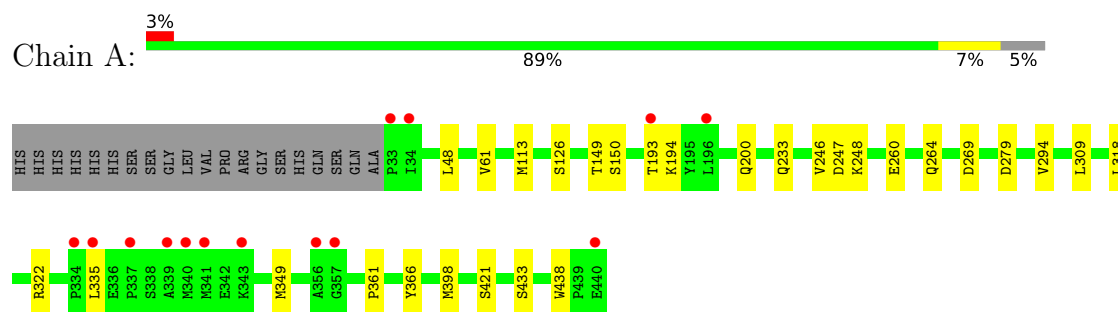
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	239	Total O 239 239	0	0
6	B	167	Total O 167 167	0	0
6	C	150	Total O 150 150	0	0
6	D	218	Total O 218 218	0	0

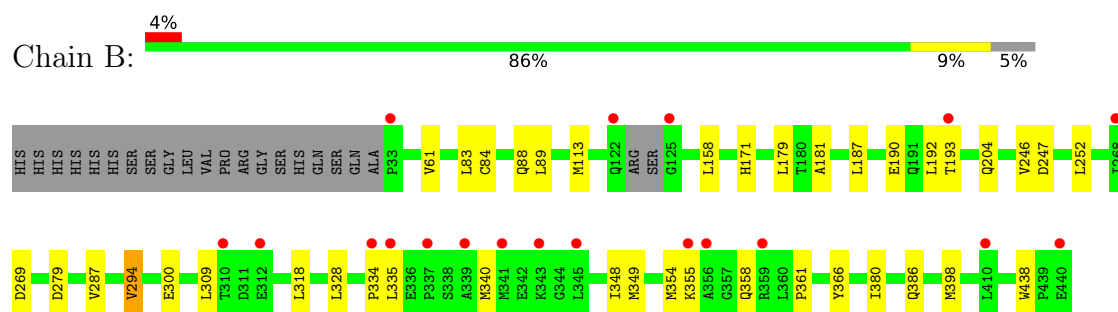
3 Residue-property plots [i](#)

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.

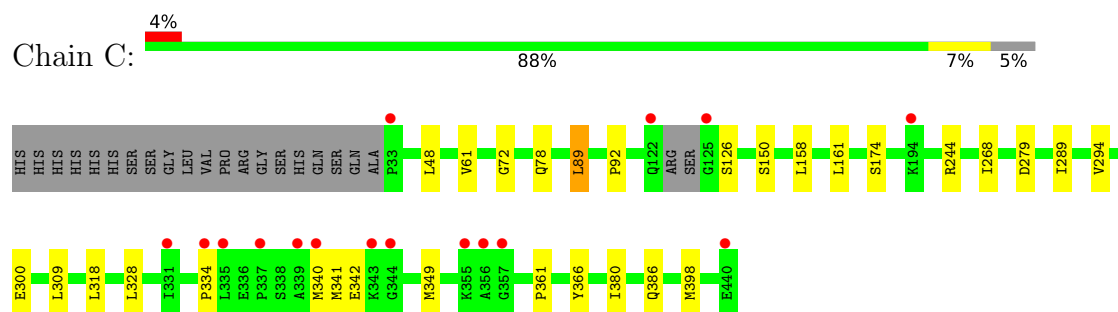
- Molecule 1: Cyclic dipeptide N-prenyltransferase



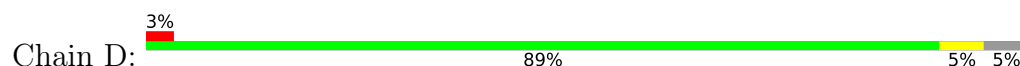
- Molecule 1: Cyclic dipeptide N-prenyltransferase

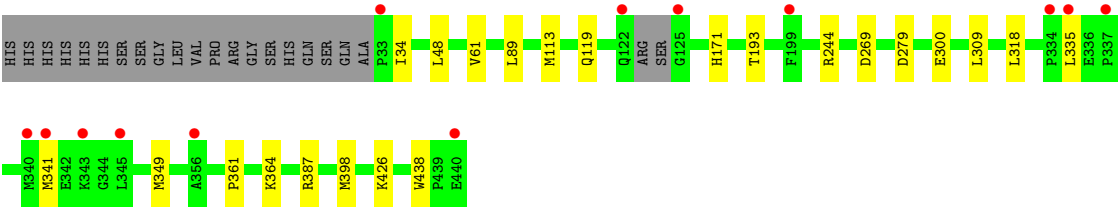


- Molecule 1: Cyclic dipeptide N-prenyltransferase



- Molecule 1: Cyclic dipeptide N-prenyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.51Å 137.02Å 172.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.25 29.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-2.25) 99.7 (29.83-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109, BUSTER 2.10.0	Depositor
R, R_{free}	0.166 , 0.193 0.172 , 0.175	Depositor DCC
R_{free} test set	5432 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13871	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, PEG, EDO

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	0.86	0/3364	1.26	12/4566 (0.3%)
1	B	0.84	2/3333 (0.1%)	1.25	15/4526 (0.3%)
1	C	0.82	0/3329	1.24	7/4522 (0.2%)
1	D	0.85	0/3342	1.24	9/4538 (0.2%)
All	All	0.84	2/13368 (0.0%)	1.25	43/18152 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84[A]	CYS	CA-C	-8.51	1.41	1.52
1	B	84[B]	CYS	CA-C	-8.51	1.41	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	MET	CA-C-N	6.52	129.35	120.54
1	A	398	MET	C-N-CA	6.52	129.35	120.54
1	C	61	VAL	N-CA-C	6.51	117.51	111.45
1	B	294	VAL	N-CA-C	6.49	113.15	106.21
1	D	398	MET	CA-C-N	6.35	129.11	120.54
1	D	398	MET	C-N-CA	6.35	129.11	120.54
1	B	398	MET	CA-C-N	6.24	128.96	120.54
1	B	398	MET	C-N-CA	6.24	128.96	120.54
1	C	398	MET	CA-C-N	6.15	128.84	120.54
1	C	398	MET	C-N-CA	6.15	128.84	120.54
1	A	61	VAL	N-CA-C	6.13	117.15	111.45
1	B	269	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	193	THR	CA-C-N	5.75	127.98	120.28
1	A	193	THR	C-N-CA	5.75	127.98	120.28
1	B	61	VAL	N-CA-C	5.72	117.10	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	THR	CA-C-N	5.66	128.14	120.38
1	D	193	THR	C-N-CA	5.66	128.14	120.38
1	B	193	THR	CA-C-N	5.52	127.68	120.28
1	B	193	THR	C-N-CA	5.52	127.68	120.28
1	B	386	GLN	CA-C-N	5.50	128.10	120.29
1	B	386	GLN	C-N-CA	5.50	128.10	120.29
1	D	61	VAL	N-CA-C	5.44	116.84	111.67
1	D	269	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	269	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	386	GLN	CA-C-N	5.39	127.94	120.29
1	C	386	GLN	C-N-CA	5.39	127.94	120.29
1	D	34	ILE	N-CA-CB	5.33	116.09	110.17
1	B	83	LEU	CA-C-N	5.30	127.82	120.29
1	B	83	LEU	C-N-CA	5.30	127.82	120.29
1	A	149	THR	N-CA-C	5.30	118.91	112.23
1	D	426	LYS	CA-C-N	5.28	128.13	120.79
1	D	426	LYS	C-N-CA	5.28	128.13	120.79
1	B	181	ALA	CA-C-N	5.25	127.31	120.28
1	B	181	ALA	C-N-CA	5.25	127.31	120.28
1	B	247	ASP	CA-C-N	5.23	127.55	120.38
1	B	247	ASP	C-N-CA	5.23	127.55	120.38
1	C	294	VAL	N-CA-C	5.22	111.80	106.21
1	A	150	SER	N-CA-C	5.20	116.94	111.28
1	C	150	SER	N-CA-C	5.09	116.83	111.28
1	A	247	ASP	CA-C-N	5.07	127.33	120.38
1	A	247	ASP	C-N-CA	5.07	127.33	120.38
1	A	294	VAL	N-CA-C	5.04	111.60	106.21
1	A	126	SER	N-CA-C	5.00	117.55	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3271	0	3231	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3241	0	3183	17	0
1	C	3237	0	3171	13	0
1	D	3249	0	3193	13	0
2	A	20	0	30	0	0
2	B	20	0	30	0	0
2	C	24	0	36	4	0
2	D	12	0	18	3	0
3	A	7	0	10	0	0
4	A	3	0	0	1	0
4	B	3	0	0	1	0
4	C	3	0	0	1	0
4	D	3	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	239	0	0	2	0
6	B	167	0	0	0	0
6	C	150	0	0	2	0
6	D	218	0	0	3	0
All	All	13871	0	12902	53	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 (53) 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:179:LEU:H	1:B:204:GLN:HE22	1.27	0.81
1:C:300:GLU:HG2	1:C:318:LEU:HD11	1.63	0.78
1:A:48:LEU:H	1:B:88:GLN:HE21	1.30	0.77
1:B:300:GLU:HG2	1:B:318:LEU:HD11	1.66	0.76
1:D:300:GLU:HG2	1:D:318:LEU:HD11	1.71	0.73
1:B:287:VAL:HG23	1:B:354:MET:HE1	1.73	0.69
1:C:244:ARG:HD2	6:C:911:HOH:O	2.00	0.61
1:D:349:MET:HE1	2:D:501:EDO:C2	2.30	0.61
1:C:92:PRO:HB2	2:C:702:EDO:H22	1.86	0.57
1:B:171:HIS:HD1	1:D:171:HIS:HD1	1.52	0.56
1:A:309:LEU:HD21	1:A:361:PRO:HD2	1.88	0.56
1:A:48:LEU:H	1:B:88:GLN:NE2	2.01	0.55
1:A:279:ASP:HB2	4:A:607:CL:CL	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:HG13	1:B:348:ILE:HG23	1.88	0.55
1:C:48:LEU:O	2:C:703:EDO:H12	2.09	0.52
1:C:89:LEU:HD21	1:C:158:LEU:HA	1.91	0.52
1:B:309:LEU:HD21	1:B:361:PRO:HD2	1.91	0.52
1:D:349:MET:HE1	2:D:501:EDO:H21	1.91	0.52
1:B:334:PRO:HD2	1:B:340:MET:HA	1.91	0.51
1:C:309:LEU:HD21	1:C:361:PRO:HD2	1.92	0.51
1:C:279:ASP:HB2	4:C:701:CL:CL	2.48	0.50
1:D:279:ASP:HB2	4:D:505:CL:CL	2.49	0.50
1:D:244:ARG:HD2	6:D:658:HOH:O	2.11	0.50
1:A:260:GLU:O	1:A:264:GLN:HG2	2.13	0.49
1:D:119:GLN:NE2	6:D:808:HOH:O	2.46	0.49
1:D:309:LEU:HD21	1:D:361:PRO:HD2	1.94	0.49
1:B:187:LEU:HB3	1:B:192:LEU:HD12	1.94	0.48
1:C:89:LEU:HD13	1:C:161:LEU:HD12	1.94	0.47
1:D:349:MET:HE1	2:D:501:EDO:H22	1.96	0.47
2:C:709:EDO:H21	1:D:48:LEU:O	2.15	0.46
1:A:421:SER:OG	1:A:433:SER:HB2	2.16	0.45
1:B:89:LEU:HD21	1:B:158:LEU:HA	1.99	0.45
2:C:702:EDO:H21	6:C:894:HOH:O	2.16	0.44
1:C:268:ILE:HG21	1:C:289:ILE:HG21	1.99	0.44
1:D:364:LYS:NZ	4:D:504:CL:CL	2.85	0.44
1:A:233:GLN:NE2	6:A:928:HOH:O	2.29	0.44
1:B:252:LEU:HD22	1:B:354:MET:HB3	2.00	0.44
1:B:349:MET:HB2	1:B:366:TYR:HB2	2.00	0.43
1:B:355:LYS:HD3	1:B:358:GLN:HG2	2.01	0.43
1:A:349:MET:HB2	1:A:366:TYR:HB2	1.99	0.43
1:D:113:MET:HG3	1:D:438:TRP:CD1	2.54	0.43
1:D:387:ARG:NH2	6:D:806:HOH:O	2.46	0.43
1:C:334:PRO:HD2	1:C:340:MET:HG3	2.01	0.42
1:A:194:LYS:HG2	1:A:200:GLN:HG3	2.00	0.42
1:A:248:LYS:HD2	6:A:931:HOH:O	2.18	0.42
1:A:113:MET:HG3	1:A:438:TRP:CD1	2.55	0.42
1:B:113:MET:HG3	1:B:438:TRP:CD1	2.55	0.42
1:B:279:ASP:HB2	4:B:506:CL:CL	2.57	0.41
1:C:72:GLY:HA2	1:C:126:SER:HB2	2.02	0.41
1:C:349:MET:HB2	1:C:366:TYR:HB2	2.02	0.41
1:A:318:LEU:O	1:A:322[A]:ARG:HG3	2.20	0.41
1:B:328:LEU:HA	1:B:380:ILE:HD13	2.03	0.41
1:C:328:LEU:HA	1:C:380:ILE:HD13	2.04	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	409/428 (96%)	399 (98%)	10 (2%)	0	100	100
1	B	405/428 (95%)	397 (98%)	8 (2%)	0	100	100
1	C	405/428 (95%)	396 (98%)	9 (2%)	0	100	100
1	D	405/428 (95%)	395 (98%)	10 (2%)	0	100	100
All	All	1624/1712 (95%)	1587 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	348/367 (95%)	346 (99%)	2 (1%)	78	84
1	B	342/367 (93%)	339 (99%)	3 (1%)	70	79
1	C	343/367 (94%)	338 (98%)	5 (2%)	57	68
1	D	345/367 (94%)	342 (99%)	3 (1%)	70	79
All	All	1378/1468 (94%)	1365 (99%)	13 (1%)	68	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	VAL
1	A	335	LEU

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Mol	Chain	Res	Type
1	B	190	GLU
1	B	246	VAL
1	B	335	LEU
1	C	78	GLN
1	C	89	LEU
1	C	174	SER
1	C	341	MET
1	C	342	GLU
1	D	89	LEU
1	D	335	LEU
1	D	341	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	332	GLN
1	A	417	GLN
1	B	57	HIS
1	B	78	GLN
1	B	88	GLN
1	B	122	GLN
1	B	204	GLN
1	B	417	GLN
1	C	57	HIS
1	C	78	GLN
1	C	79	GLN
1	C	122	GLN
1	C	417	GLN
1	D	57	HIS
1	D	251	HIS
1	D	332	GLN
1	D	417	GLN

5.3.3 RNA ⓘ

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 36 ligands modelled in this entry, 16 are monoatomic - leaving 20 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	$\# Z > 2$
2	EDO	B	501	-	3,3,3	0.61	0	2,2,2	0.20	0
2	EDO	C	710	-	3,3,3	0.72	0	2,2,2	0.20	0
2	EDO	B	502	-	3,3,3	0.62	0	2,2,2	0.31	0
3	PEG	A	605	-	6,6,6	0.28	0	5,5,5	0.14	0
2	EDO	B	504	-	3,3,3	0.58	0	2,2,2	0.33	0
2	EDO	C	702	-	3,3,3	0.60	0	2,2,2	0.69	0
2	EDO	A	604	-	3,3,3	0.55	0	2,2,2	0.40	0
2	EDO	C	705	-	3,3,3	0.47	0	2,2,2	0.38	0
2	EDO	C	703	-	3,3,3	0.36	0	2,2,2	0.59	0
2	EDO	A	602	-	3,3,3	0.55	0	2,2,2	0.36	0
2	EDO	A	601	-	3,3,3	0.59	0	2,2,2	0.32	0
2	EDO	B	503	-	3,3,3	0.57	0	2,2,2	0.36	0
2	EDO	C	704	-	3,3,3	0.45	0	2,2,2	0.62	0
2	EDO	A	603	-	3,3,3	0.58	0	2,2,2	0.07	0
2	EDO	B	509	-	3,3,3	0.75	0	2,2,2	0.06	0
2	EDO	C	709	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	610	-	3,3,3	0.51	0	2,2,2	0.40	0
2	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	D	507	-	3,3,3	0.63	0	2,2,2	0.24	0
2	EDO	D	502	-	3,3,3	0.56	0	2,2,2	0.43	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	EDO	B	501	-	-	1/1/1/1	-
2	EDO	C	710	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
3	PEG	A	605	-	-	2/4/4/4	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	C	702	-	-	1/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	C	705	-	-	1/1/1/1	-
2	EDO	C	703	-	-	0/1/1/1	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	C	704	-	-	0/1/1/1	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	509	-	-	1/1/1/1	-
2	EDO	C	709	-	-	0/1/1/1	-
2	EDO	A	610	-	-	1/1/1/1	-
2	EDO	D	501	-	-	0/1/1/1	-
2	EDO	D	507	-	-	0/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	705	EDO	O1-C1-C2-O2
2	B	504	EDO	O1-C1-C2-O2
2	A	604	EDO	O1-C1-C2-O2
2	A	610	EDO	O1-C1-C2-O2
2	B	509	EDO	O1-C1-C2-O2
3	A	605	PEG	C4-C3-O2-C2
2	B	501	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
2	C	702	EDO	O1-C1-C2-O2
3	A	605	PEG	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	702	EDO	2	0
2	C	703	EDO	1	0
2	C	709	EDO	1	0
2	D	501	EDO	3	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	408/428 (95%)	-0.24	14 (3%)	48 48	20, 42, 83, 114	3 (0%)
1	B	406/428 (94%)	0.09	19 (4%)	36 35	22, 56, 101, 143	3 (0%)
1	C	406/428 (94%)	-0.08	16 (3%)	43 43	20, 53, 94, 138	3 (0%)
1	D	406/428 (94%)	-0.28	13 (3%)	50 50	19, 42, 76, 125	3 (0%)
All	All	1626/1712 (94%)	-0.13	62 (3%)	44 44	19, 47, 92, 143	12 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	440	GLU	5.7
1	D	440	GLU	4.8
1	C	440	GLU	4.7
1	C	344	GLY	4.4
1	B	122	GLN	4.3
1	B	356	ALA	4.3
1	C	122	GLN	4.3
1	B	343	LYS	4.2
1	B	33	PRO	4.1
1	D	343	LYS	4.1
1	D	199	PHE	4.0
1	C	334	PRO	3.8
1	D	122	GLN	3.8
1	A	440	GLU	3.8
1	D	125	GLY	3.8
1	C	343	LYS	3.7
1	D	335	LEU	3.6
1	C	356	ALA	3.6
1	C	337	PRO	3.5
1	A	33	PRO	3.4
1	B	125	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	335	LEU	3.4
1	A	334	PRO	3.2
1	B	334	PRO	3.2
1	B	339	ALA	3.1
1	A	335	LEU	3.1
1	A	337	PRO	3.1
1	C	357	GLY	3.1
1	B	335	LEU	3.0
1	B	193	THR	2.9
1	D	337	PRO	2.7
1	B	355	LYS	2.7
1	C	125	GLY	2.6
1	D	33	PRO	2.6
1	D	340	MET	2.5
1	D	341	MET	2.5
1	B	359	ARG	2.5
1	C	355	LYS	2.4
1	A	196	LEU	2.4
1	B	345	LEU	2.4
1	D	345	LEU	2.4
1	B	312	GLU	2.4
1	B	310	THR	2.3
1	A	339	ALA	2.3
1	A	34	ILE	2.3
1	A	357	GLY	2.3
1	B	341	MET	2.2
1	A	356	ALA	2.2
1	B	268	ILE	2.2
1	C	339	ALA	2.2
1	D	356	ALA	2.2
1	C	33	PRO	2.2
1	D	334	PRO	2.2
1	C	340	MET	2.2
1	A	193	THR	2.2
1	A	340	MET	2.1
1	A	341	MET	2.1
1	C	194	LYS	2.1
1	C	331	ILE	2.1
1	A	343	LYS	2.0
1	B	410	LEU	2.0
1	B	337	PRO	2.0

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

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

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
2	EDO	D	502	4/4	0.82	0.15	58,62,66,70	0
3	PEG	A	605	7/7	0.82	0.16	77,78,79,79	0
2	EDO	B	509	4/4	0.85	0.18	72,74,76,77	0
2	EDO	A	604	4/4	0.88	0.17	54,56,61,66	0
2	EDO	B	504	4/4	0.89	0.20	63,63,67,71	0
2	EDO	C	705	4/4	0.90	0.14	61,61,62,64	0
2	EDO	D	501	4/4	0.92	0.14	54,54,56,56	0
2	EDO	A	610	4/4	0.92	0.10	54,58,61,64	0
2	EDO	C	710	4/4	0.92	0.12	57,58,59,60	0
4	CL	B	506	1/1	0.92	0.10	80,80,80,80	0
2	EDO	D	507	4/4	0.93	0.10	55,57,57,58	0
2	EDO	A	603	4/4	0.93	0.16	55,56,57,58	0
2	EDO	C	702	4/4	0.93	0.15	34,40,41,46	0
2	EDO	A	602	4/4	0.94	0.15	51,57,60,62	0
2	EDO	A	601	4/4	0.94	0.10	51,53,54,54	0
2	EDO	B	501	4/4	0.94	0.11	46,50,56,61	0
2	EDO	C	704	4/4	0.94	0.10	59,59,59,60	0
2	EDO	B	502	4/4	0.94	0.09	50,51,55,55	0
2	EDO	C	709	4/4	0.94	0.10	40,47,53,57	0
4	CL	D	505	1/1	0.94	0.09	70,70,70,70	0
4	CL	A	607	1/1	0.95	0.08	71,71,71,71	0
2	EDO	B	503	4/4	0.95	0.08	50,50,50,52	0
4	CL	C	701	1/1	0.95	0.11	64,64,64,64	0
2	EDO	C	703	4/4	0.95	0.15	38,43,50,56	0
4	CL	A	606	1/1	0.96	0.13	67,67,67,67	0
4	CL	C	706	1/1	0.97	0.17	72,72,72,72	0
4	CL	B	505	1/1	0.98	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	608	1/1	0.98	0.23	55,55,55,55	0
4	CL	C	707	1/1	0.98	0.13	51,51,51,51	0
4	CL	D	503	1/1	0.98	0.12	51,51,51,51	0
4	CL	D	504	1/1	0.98	0.19	61,61,61,61	0
4	CL	B	507	1/1	0.98	0.22	56,56,56,56	0
5	NA	B	508	1/1	0.98	0.09	63,63,63,63	0
5	NA	C	708	1/1	0.98	0.04	57,57,57,57	0
5	NA	A	609	1/1	0.99	0.03	40,40,40,40	0
5	NA	D	506	1/1	0.99	0.04	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.