



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:01 PM GMT

PDB ID : 4E0T
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

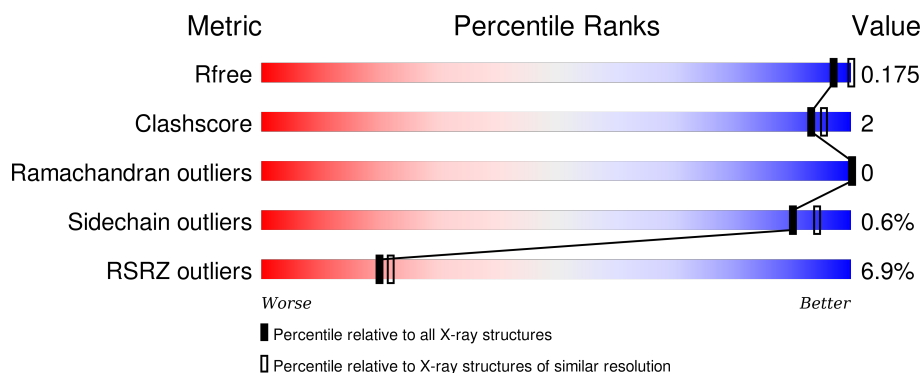
1 Overall quality at a glance

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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>91%</div> <div>5%</div> </div>
1	B	428	<div> <div>9%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	C	428	<div> <div>6%</div> <div>89%</div> <div>5%</div> <div>5%</div> </div>
1	D	428	<div> <div>6%</div> <div>91%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	602	-	-	-	X
2	EDO	A	603	-	-	-	X
2	EDO	A	604	-	-	-	X
2	EDO	B	501	-	-	-	X
2	EDO	B	502	-	-	-	X
2	EDO	B	504	-	-	-	X
2	EDO	B	509	-	-	-	X
2	EDO	C	705	-	-	-	X
2	EDO	C	709	-	-	-	X
2	EDO	C	710	-	-	-	X
2	EDO	D	501	-	-	-	X
2	EDO	D	502	-	-	-	X
2	EDO	D	507	-	-	-	X
5	NA	B	508	-	-	-	X

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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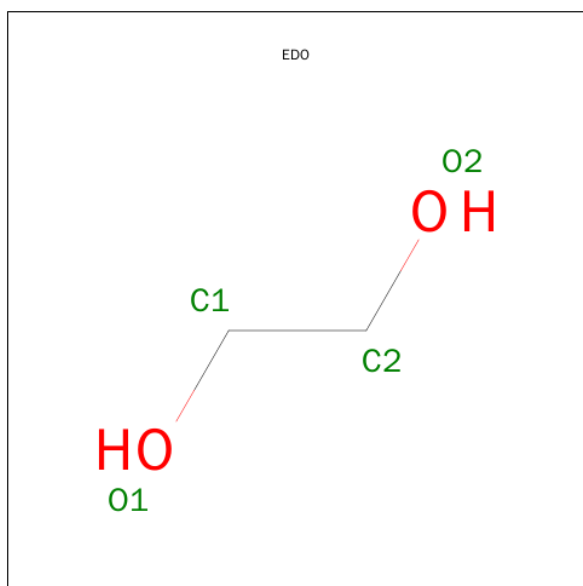
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	EXPRESSION TAG	UNP D1D8L6
B	19	SER	-	EXPRESSION TAG	UNP D1D8L6
B	20	SER	-	EXPRESSION TAG	UNP D1D8L6
B	21	GLY	-	EXPRESSION TAG	UNP D1D8L6
B	22	LEU	-	EXPRESSION TAG	UNP D1D8L6
B	23	VAL	-	EXPRESSION TAG	UNP D1D8L6
B	24	PRO	-	EXPRESSION TAG	UNP D1D8L6
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 (three-letter code: EDO) (formula: C₂H₆O₂).



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 (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

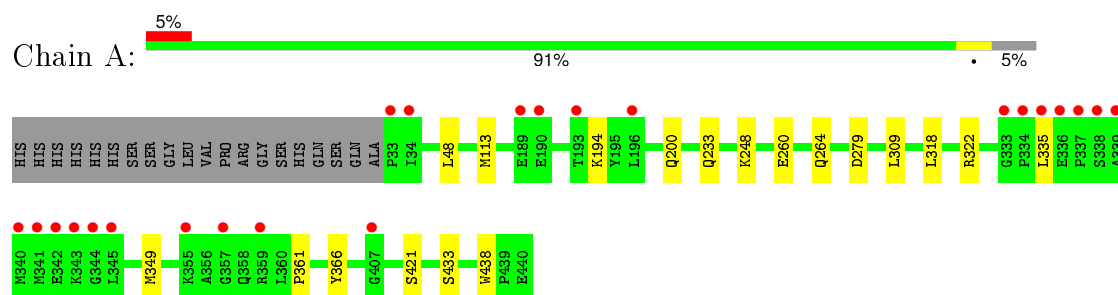
- Molecule 6 is water.

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

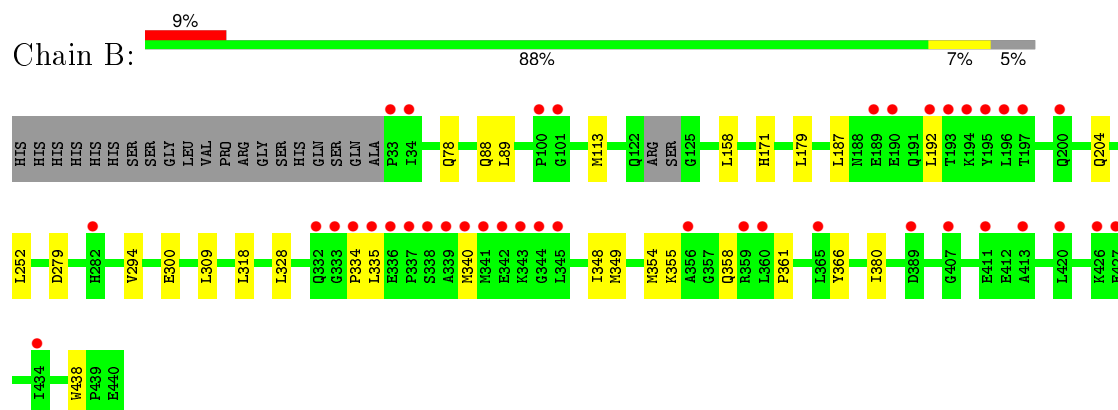
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

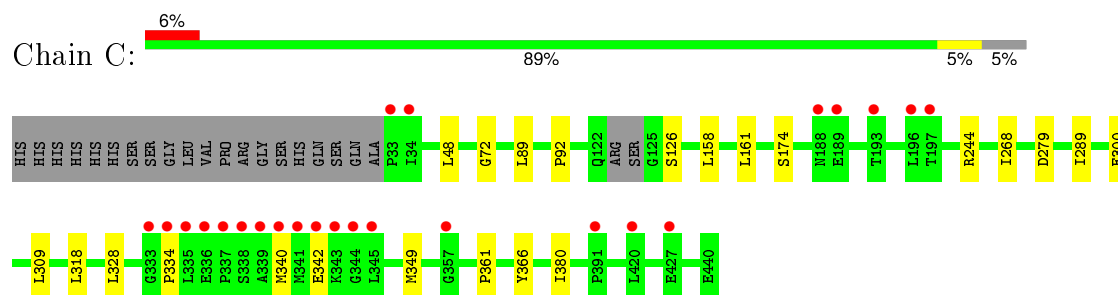
- Molecule 1: Cyclic dipeptide N-prenyltransferase



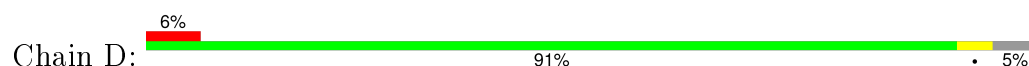
- Molecule 1: Cyclic dipeptide N-prenyltransferase

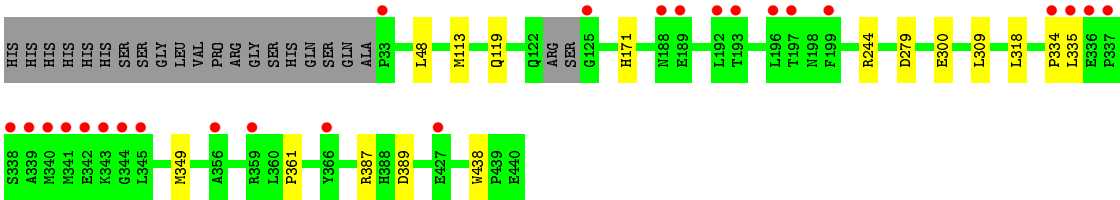


- Molecule 1: Cyclic dipeptide N-prenyltransferase



- 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	BUSTER 2.10.0	Depositor
R, R_{free}	0.166 , 0.193 0.172 , 0.175	Depositor DCC
R_{free} test set	5432 reflections (5.26%)	DCC
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 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 108641 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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, PEG, EDO, CL

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	0.53	0/3364	0.65	0/4566
1	B	0.50	0/3333	0.64	0/4526
1	C	0.49	0/3329	0.62	0/4522
1	D	0.52	0/3342	0.64	0/4538
All	All	0.51	0/13368	0.64	0/18152

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	3271	0	3231	12	0
1	B	3241	0	3183	16	0
1	C	3237	0	3171	13	0
1	D	3249	0	3193	10	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	1	0
3	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	49	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 (49) 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:C:244:ARG:HD2	6:C:911:HOH:O	2.00	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
1:B:294:VAL:HG13	1:B:348:ILE:HG23	1.88	0.55
1:C:89:LEU:HD21	1:C:158:LEU:HA	1.91	0.52
1:C:48:LEU:O	2:C:703:EDO:H12	2.09	0.52
1:B:309:LEU:HD21	1:B:361:PRO:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:349:MET:HE3	2:D:501:EDO:H22	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:D:113:MET:HG3	1:D:438:TRP:CD1	2.54	0.43
1:A:349:MET:HB2	1:A:366:TYR:HB2	1.99	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:248:LYS:HD2	6:A:931:HOH:O	2.18	0.42
1:A:194:LYS:HG2	1:A:200:GLN:HG3	2.00	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:B:328:LEU:HA	1:B:380:ILE:HD13	2.03	0.41
1:A:318:LEU:O	1:A:322[A]:ARG:HG3	2.20	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 ⓘ

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	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 ⓘ

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%)	347 (100%)	1 (0%)	94	97
1	B	342/367 (93%)	340 (99%)	2 (1%)	90	94
1	C	343/367 (94%)	341 (99%)	2 (1%)	90	94
1	D	345/367 (94%)	342 (99%)	3 (1%)	84	91
All	All	1378/1468 (94%)	1370 (99%)	8 (1%)	90	94

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

Mol	Chain	Res	Type
1	A	335	LEU
1	B	78	GLN
1	B	335	LEU
1	C	174	SER
1	C	342	GLU
1	D	334	PRO
1	D	335	LEU
1	D	389	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	HIS
1	B	88	GLN
1	B	204	GLN
1	C	57	HIS
1	C	78	GLN
1	C	122	GLN
1	D	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	601	-	3,3,3	0.66	0	2,2,2	0.35	0
2	EDO	A	602	-	3,3,3	0.62	0	2,2,2	0.40	0
2	EDO	A	603	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	A	604	-	3,3,3	0.61	0	2,2,2	0.45	0
3	PEG	A	605	-	6,6,6	0.28	0	5,5,5	0.09	0
2	EDO	A	610	-	3,3,3	0.58	0	2,2,2	0.44	0
2	EDO	B	501	-	3,3,3	0.68	0	2,2,2	0.23	0
2	EDO	B	502	-	3,3,3	0.69	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	503	-	3,3,3	0.63	0	2,2,2	0.40	0
2	EDO	B	504	-	3,3,3	0.65	0	2,2,2	0.37	0
2	EDO	B	509	-	3,3,3	0.82	0	2,2,2	0.06	0
2	EDO	C	702	-	3,3,3	0.62	0	2,2,2	0.75	0
2	EDO	C	703	-	3,3,3	0.41	0	2,2,2	0.65	0
2	EDO	C	704	-	3,3,3	0.49	0	2,2,2	0.68	0
2	EDO	C	705	-	3,3,3	0.53	0	2,2,2	0.42	0
2	EDO	C	709	-	3,3,3	0.51	0	2,2,2	0.36	0
2	EDO	C	710	-	3,3,3	0.80	0	2,2,2	0.23	0
2	EDO	D	501	-	3,3,3	0.52	0	2,2,2	0.44	0
2	EDO	D	502	-	3,3,3	0.64	0	2,2,2	0.47	0
2	EDO	D	507	-	3,3,3	0.69	0	2,2,2	0.27	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	A	601	-	-	0/1/1/1	0/0/0/0
2	EDO	A	602	-	-	0/1/1/1	0/0/0/0
2	EDO	A	603	-	-	0/1/1/1	0/0/0/0
2	EDO	A	604	-	-	0/1/1/1	0/0/0/0
3	PEG	A	605	-	-	0/4/4/4	0/0/0/0
2	EDO	A	610	-	-	0/1/1/1	0/0/0/0
2	EDO	B	501	-	-	0/1/1/1	0/0/0/0
2	EDO	B	502	-	-	0/1/1/1	0/0/0/0
2	EDO	B	503	-	-	0/1/1/1	0/0/0/0
2	EDO	B	504	-	-	0/1/1/1	0/0/0/0
2	EDO	B	509	-	-	0/1/1/1	0/0/0/0
2	EDO	C	702	-	-	0/1/1/1	0/0/0/0
2	EDO	C	703	-	-	0/1/1/1	0/0/0/0
2	EDO	C	704	-	-	0/1/1/1	0/0/0/0
2	EDO	C	705	-	-	0/1/1/1	0/0/0/0
2	EDO	C	709	-	-	0/1/1/1	0/0/0/0
2	EDO	C	710	-	-	0/1/1/1	0/0/0/0
2	EDO	D	501	-	-	0/1/1/1	0/0/0/0
2	EDO	D	502	-	-	0/1/1/1	0/0/0/0
2	EDO	D	507	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 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	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

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%)	-0.12	23 (5%) 28 31	24, 42, 83, 114	0
1	B	406/428 (94%)	0.19	40 (9%) 9 10	28, 57, 101, 143	0
1	C	406/428 (94%)	0.05	24 (5%) 26 28	27, 53, 94, 138	0
1	D	406/428 (94%)	-0.06	25 (6%) 24 26	23, 42, 76, 125	0
All	All	1626/1712 (94%)	0.02	112 (6%) 20 22	23, 47, 92, 143	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	PRO	9.4
1	D	335	LEU	8.8
1	C	344	GLY	8.5
1	D	337	PRO	7.5
1	C	335	LEU	7.4
1	C	337	PRO	7.3
1	B	335	LEU	7.3
1	C	340	MET	7.1
1	B	334	PRO	7.1
1	B	338	SER	7.0
1	B	337	PRO	6.9
1	C	338	SER	6.8
1	C	33	PRO	6.6
1	C	341	MET	6.6
1	D	334	PRO	6.5
1	B	339	ALA	6.4
1	D	338	SER	6.4
1	A	338	SER	6.2
1	B	340	MET	6.2
1	D	199	PHE	6.1
1	A	335	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	336	GLU	6.0
1	B	193	THR	5.7
1	A	337	PRO	5.7
1	C	339	ALA	5.7
1	D	340	MET	5.6
1	D	336	GLU	5.4
1	D	339	ALA	5.1
1	C	342	GLU	5.1
1	A	339	ALA	5.0
1	C	193	THR	4.9
1	A	33	PRO	4.9
1	A	334	PRO	4.9
1	D	342	GLU	4.7
1	D	341	MET	4.6
1	B	333	GLY	4.6
1	A	342	GLU	4.4
1	B	345	LEU	4.4
1	D	33	PRO	4.4
1	B	192	LEU	4.3
1	A	340	MET	4.3
1	B	341	MET	4.2
1	A	345	LEU	4.0
1	C	345	LEU	4.0
1	B	33	PRO	4.0
1	C	343	LYS	3.9
1	A	359	ARG	3.9
1	A	336	GLU	3.8
1	B	196	LEU	3.7
1	B	342	GLU	3.7
1	C	196	LEU	3.6
1	A	341	MET	3.6
1	A	193	THR	3.6
1	C	336	GLU	3.6
1	B	101	GLY	3.6
1	A	196	LEU	3.5
1	B	190	GLU	3.4
1	B	195	TYR	3.4
1	B	420	LEU	3.3
1	D	196	LEU	3.2
1	D	345	LEU	3.1
1	A	344	GLY	3.1
1	B	332	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	34	ILE	3.0
1	B	100	PRO	3.0
1	C	333	GLY	3.0
1	D	189	GLU	3.0
1	B	356	ALA	2.9
1	B	197	THR	2.8
1	B	360	LEU	2.8
1	D	193	THR	2.8
1	C	34	ILE	2.8
1	B	344	GLY	2.8
1	A	357	GLY	2.7
1	C	188	ASN	2.7
1	D	192	LEU	2.6
1	A	189	GLU	2.6
1	C	189	GLU	2.6
1	D	343	LYS	2.6
1	C	391	PRO	2.6
1	D	197	THR	2.6
1	A	407	GLY	2.5
1	A	34	ILE	2.5
1	D	188	ASN	2.5
1	B	343	LYS	2.4
1	A	190	GLU	2.4
1	C	357	GLY	2.4
1	A	343	LYS	2.4
1	B	426	LYS	2.4
1	C	420	LEU	2.4
1	D	344	GLY	2.3
1	B	359	ARG	2.3
1	B	189	GLU	2.3
1	B	389	ASP	2.3
1	A	355	LYS	2.3
1	D	359	ARG	2.3
1	D	356	ALA	2.3
1	B	411	GLU	2.2
1	B	365	LEU	2.2
1	B	427	GLU	2.2
1	B	194	LYS	2.2
1	B	413	ALA	2.2
1	B	407	GLY	2.1
1	B	200	GLN	2.1
1	D	427	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLY	2.1
1	B	282	HIS	2.1
1	C	427	GLU	2.1
1	D	366	TYR	2.1
1	A	333	GLY	2.0
1	C	197	THR	2.0
1	B	434	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	C	705	4/4	0.95	0.39	15.72	61,61,62,64	0
2	EDO	B	504	4/4	0.94	0.56	14.85	63,63,67,71	0
2	EDO	B	509	4/4	0.85	0.57	14.05	72,74,76,77	0
2	EDO	A	604	4/4	0.88	0.47	12.31	54,56,61,66	0
2	EDO	D	501	4/4	0.89	0.46	6.95	54,54,56,56	0
2	EDO	C	710	4/4	0.92	0.22	5.78	57,58,59,60	0
2	EDO	D	502	4/4	0.87	0.21	3.90	58,62,66,70	0
2	EDO	B	501	4/4	0.94	0.12	3.61	46,50,56,61	0
2	EDO	C	709	4/4	0.96	0.18	3.06	40,47,53,57	0
2	EDO	D	507	4/4	0.84	0.13	2.95	55,57,57,58	0
5	NA	B	508	1/1	0.97	0.23	2.77	63,63,63,63	0
2	EDO	A	602	4/4	0.98	0.20	2.31	51,57,60,62	0
2	EDO	A	603	4/4	0.95	0.15	2.18	55,56,57,58	0
2	EDO	B	502	4/4	0.97	0.13	2.08	50,51,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	EDO	C	704	4/4	0.96	0.14	1.74	59,59,59,60	0
2	EDO	A	610	4/4	0.94	0.12	1.71	54,58,61,64	0
5	NA	D	506	1/1	0.99	0.18	1.47	34,34,34,34	0
2	EDO	C	703	4/4	0.96	0.14	1.13	38,43,50,56	0
2	EDO	B	503	4/4	0.97	0.14	1.05	50,50,50,52	0
2	EDO	A	601	4/4	0.97	0.13	0.60	51,53,54,54	0
2	EDO	C	702	4/4	0.95	0.12	0.41	34,40,41,46	0
5	NA	C	708	1/1	0.97	0.11	-0.66	57,57,57,57	0
4	CL	A	607	1/1	0.94	0.10	-0.82	71,71,71,71	0
4	CL	B	506	1/1	0.89	0.09	-1.03	80,80,80,80	0
4	CL	C	701	1/1	0.96	0.07	-1.43	64,64,64,64	0
4	CL	D	505	1/1	0.97	0.07	-1.65	70,70,70,70	0
4	CL	A	606	1/1	0.96	0.10	-1.69	67,67,67,67	0
5	NA	A	609	1/1	0.99	0.08	-1.83	40,40,40,40	0
4	CL	D	504	1/1	0.98	0.09	-3.09	61,61,61,61	0
4	CL	C	706	1/1	0.94	0.08	-3.75	72,72,72,72	0
4	CL	B	505	1/1	0.99	0.05	-8.16	71,71,71,71	0
4	CL	D	503	1/1	0.98	0.05	-	51,51,51,51	0
3	PEG	A	605	7/7	0.88	0.14	-	77,78,79,79	0
4	CL	A	608	1/1	0.99	0.16	-	55,55,55,55	0
4	CL	B	507	1/1	0.97	0.14	-	56,56,56,56	0
4	CL	C	707	1/1	0.99	0.09	-	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.