wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 11:15 AM EDT

PDB ID	:	4K1P
Title	:	Structure of the NheA component of the Nhe toxin from Bacillus cereus
Authors	:	Ganash, M.; Phung, D.; Artymiuk, P.J.
Deposited on	:	2013-04-05
Resolution	:	2.05 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
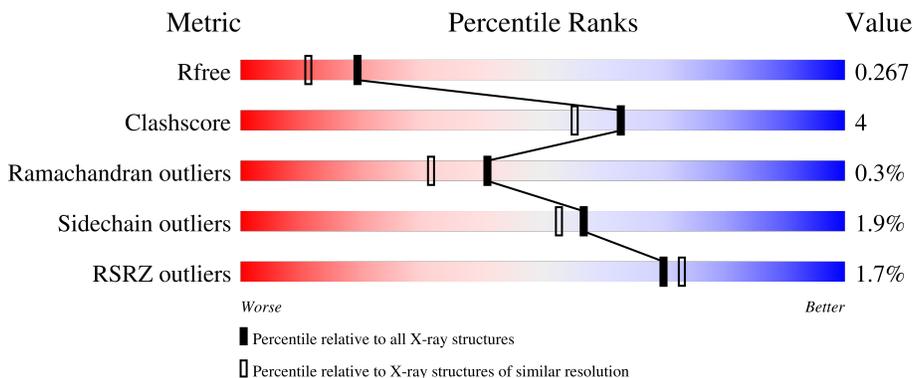
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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

Mol	Chain	Length	Quality of chain
1	A	360	85% 9% 6%
1	B	360	86% 10% •
1	C	360	82% 9% • 8%
1	D	360	85% 11% •
1	E	360	80% 9% 10%

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Mol	Chain	Length	Quality of chain
1	F	360	2% 81% 9% 10%
1	G	360	% 80% 10% 10%
1	H	360	% 82% 11% 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 22614 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 NheA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2689	1685	458	539	7			
1	B	346	Total	C	N	O	S	0	0	0
			2740	1721	466	546	7			
1	C	330	Total	C	N	O	S	0	0	3
			2570	1614	438	511	7			
1	D	346	Total	C	N	O	S	0	0	0
			2743	1723	466	547	7			
1	E	325	Total	C	N	O	S	0	0	0
			2562	1607	442	506	7			
1	F	325	Total	C	N	O	S	0	0	0
			2581	1622	435	517	7			
1	G	325	Total	C	N	O	S	0	0	1
			2552	1598	439	508	7			
1	H	336	Total	C	N	O	S	0	0	0
			2646	1662	455	522	7			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
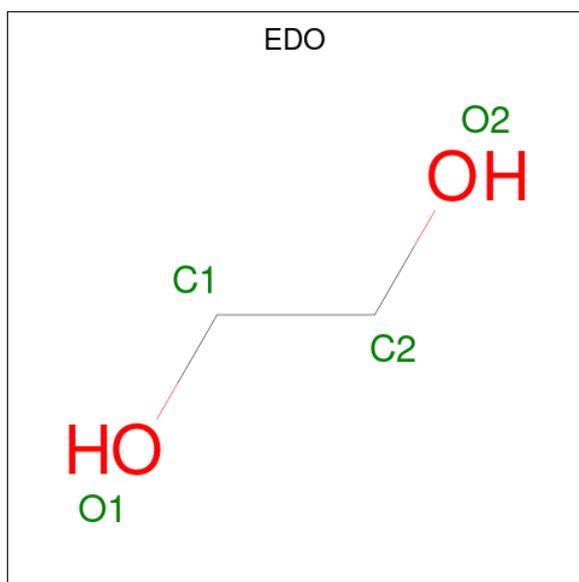
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	E	1	Total 3	C 2	O 1	0	0
2	G	1	Total 4	C 2	O 2	0	0

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
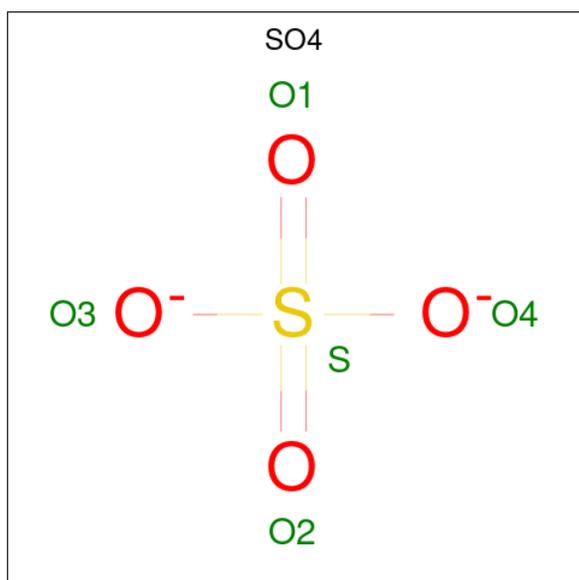
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total 217	O 217	0	0
4	B	184	Total 184	O 184	0	0
4	C	226	Total 226	O 226	0	0
4	D	213	Total 213	O 213	0	0
4	E	166	Total 166	O 166	0	0
4	F	205	Total 205	O 205	0	0
4	G	155	Total 155	O 155	0	0
4	H	141	Total 141	O 141	0	0

3 Residue-property plots ⓘ

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: NheA
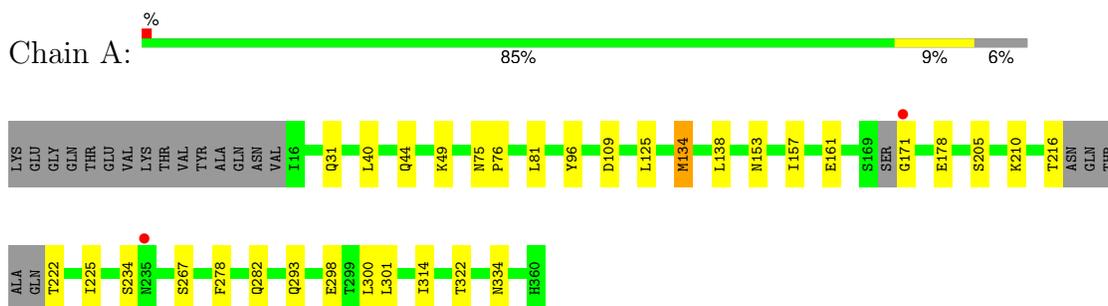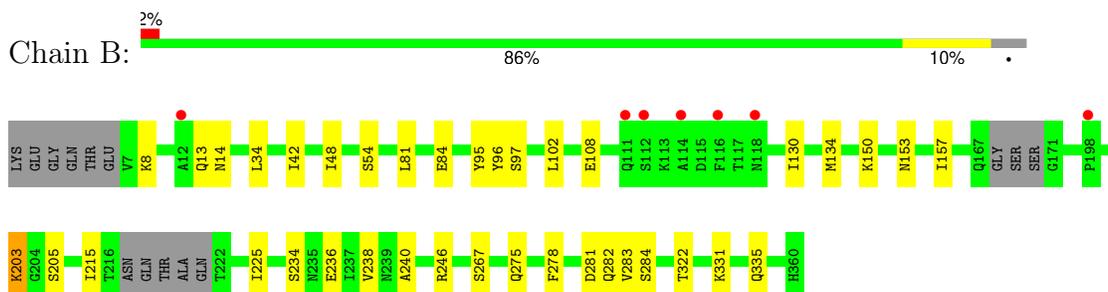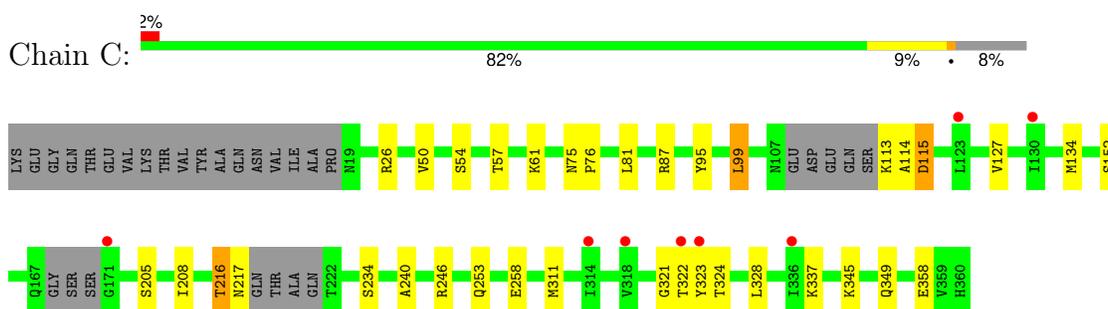
Chain A:

• Molecule 1: NheA

Chain B:

• Molecule 1: NheA

Chain C:

• Molecule 1: NheA

Chain D:

• Molecule 1: NheA

Chain E:

• Molecule 1: NheA

Chain F:

• Molecule 1: NheA

Chain G:

• Molecule 1: NheA

Chain H:
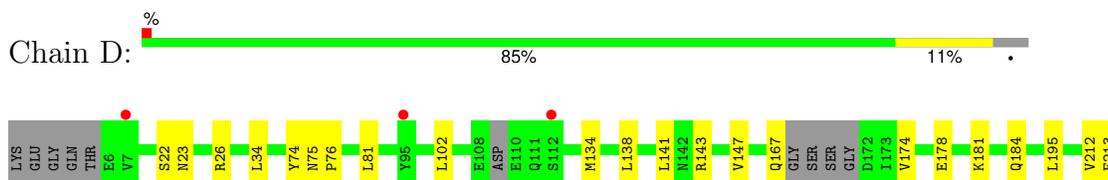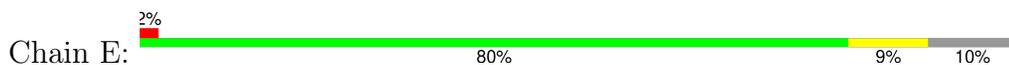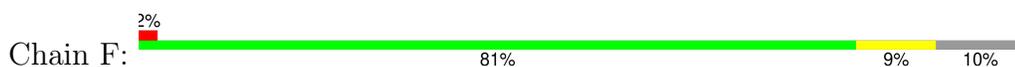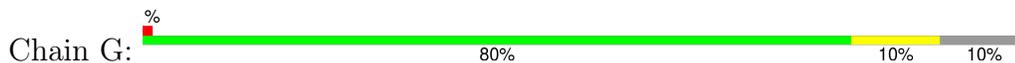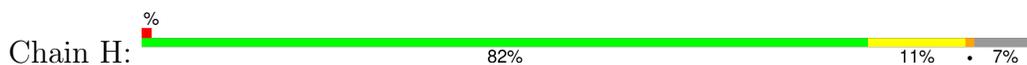
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	309.01Å 58.24Å 173.00Å 90.00° 110.61° 90.00°	Depositor
Resolution (Å)	49.90 – 2.05 49.85 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.90-2.05) 98.5 (49.85-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.262 0.214 , 0.267	Depositor DCC
R_{free} test set	8966 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.0	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22614	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8571e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SO4

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	0.35	0/2717	0.48	0/3669
1	B	0.32	0/2770	0.45	0/3745
1	C	0.34	0/2590	0.48	0/3491
1	D	0.34	0/2768	0.50	0/3739
1	E	0.32	0/2583	0.46	0/3482
1	F	0.35	0/2603	0.47	0/3510
1	G	0.33	0/2576	0.46	0/3476
1	H	0.29	0/2674	0.43	0/3612
All	All	0.33	0/21281	0.47	0/28724

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 ⓘ

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	2689	0	2684	31	1
1	B	2740	0	2734	22	0
1	C	2570	0	2529	18	0
1	D	2743	0	2721	31	1
1	E	2562	0	2543	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2581	0	2562	22	0
1	G	2552	0	2522	23	0
1	H	2646	0	2637	22	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	D	4	0	6	0	0
2	E	3	0	3	1	0
2	G	4	0	6	0	0
3	B	5	0	0	0	0
4	A	217	0	0	4	0
4	B	184	0	0	2	1
4	C	226	0	0	3	1
4	D	213	0	0	1	0
4	E	166	0	0	2	0
4	F	205	0	0	4	0
4	G	155	0	0	2	0
4	H	141	0	0	2	0
All	All	22614	0	20959	180	2

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.

The worst 5 of 180 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA2	1:D:212:VAL:CG2	1.81	1.08
1:C:323:TYR:CD1	1:C:323:TYR:CD2	2.44	0.99
1:A:134:MET:HE1	1:A:300:LEU:HG	1.54	0.90
1:A:171:GLY:HA2	1:D:212:VAL:HG21	1.60	0.82
1:A:314:ILE:CB	1:A:314:ILE:CD1	2.60	0.79

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:NZ	1:D:178:GLU:OE2[1_545]	2.12	0.08
4:B:573:HOH:O	4:C:580:HOH:O[3_545]	2.16	0.04

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	333/360 (92%)	328 (98%)	5 (2%)	0	100	100
1	B	340/360 (94%)	333 (98%)	6 (2%)	1 (0%)	41	31
1	C	317/360 (88%)	306 (96%)	8 (2%)	3 (1%)	17	8
1	D	337/360 (94%)	332 (98%)	5 (2%)	0	100	100
1	E	315/360 (88%)	305 (97%)	8 (2%)	2 (1%)	25	15
1	F	315/360 (88%)	313 (99%)	2 (1%)	0	100	100
1	G	315/360 (88%)	309 (98%)	5 (2%)	1 (0%)	41	31
1	H	330/360 (92%)	322 (98%)	6 (2%)	2 (1%)	25	15
All	All	2602/2880 (90%)	2548 (98%)	45 (2%)	9 (0%)	41	31

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	108	GLU
1	C	114	ALA
1	C	115	ASP
1	C	322	THR
1	E	112	SER

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	302/329 (92%)	298 (99%)	4 (1%)	69	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	306/329 (93%)	302 (99%)	4 (1%)	69	67
1	C	281/329 (85%)	273 (97%)	8 (3%)	43	37
1	D	304/329 (92%)	300 (99%)	4 (1%)	69	67
1	E	283/329 (86%)	276 (98%)	7 (2%)	47	40
1	F	288/329 (88%)	284 (99%)	4 (1%)	67	65
1	G	283/329 (86%)	276 (98%)	7 (2%)	47	40
1	H	296/329 (90%)	289 (98%)	7 (2%)	49	42
All	All	2343/2632 (89%)	2298 (98%)	45 (2%)	57	53

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	324	THR
1	G	205	SER
1	F	331	LYS
1	G	26	ARG
1	G	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	C	235	ASN
1	C	239	ASN
1	E	58	ASN
1	H	211	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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	EDO	E	401	-	2,2,3	0.51	0	1,1,2	0.29	0
2	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	G	401	-	3,3,3	0.40	0	2,2,2	0.45	0
3	SO4	B	401	-	4,4,4	0.43	0	6,6,6	0.14	0
2	EDO	A	401	-	3,3,3	0.33	0	2,2,2	0.56	0
2	EDO	D	401	-	3,3,3	0.45	0	2,2,2	0.31	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	401	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	G	401	-	-	0/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	EDO	1	0
2	B	402	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	339/360 (94%)	-0.22	2 (0%)	89	91	14, 27, 49, 63	0
1	B	346/360 (96%)	-0.14	7 (2%)	65	69	16, 30, 53, 66	0
1	C	330/360 (91%)	-0.12	8 (2%)	59	63	14, 28, 51, 72	0
1	D	346/360 (96%)	-0.21	4 (1%)	79	81	14, 27, 50, 67	0
1	E	325/360 (90%)	-0.02	9 (2%)	53	58	15, 31, 59, 74	0
1	F	325/360 (90%)	-0.05	6 (1%)	68	71	14, 30, 56, 75	0
1	G	325/360 (90%)	-0.02	5 (1%)	73	76	15, 33, 60, 73	0
1	H	336/360 (93%)	-0.09	4 (1%)	79	81	19, 35, 59, 71	0
All	All	2672/2880 (92%)	-0.11	45 (1%)	70	73	14, 30, 56, 75	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	323	TYR	5.4
1	C	318	VAL	4.7
1	F	324	THR	3.7
1	C	323	TYR	3.6
1	B	116	PHE	3.3

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 monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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
2	EDO	E	401	3/4	0.82	0.26	37,37,46,53	0
2	EDO	G	401	4/4	0.87	0.17	36,37,54,55	0
2	EDO	B	402	4/4	0.90	0.14	37,44,55,65	0
2	EDO	D	401	4/4	0.91	0.13	42,47,51,64	0
2	EDO	A	401	4/4	0.93	0.17	30,30,52,56	0
3	SO4	B	401	5/5	0.94	0.15	49,51,66,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.