



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 07:45 am BST

PDB ID : 5NEL  
Title : Crystal structure of the polysaccharide deacetylase Bc1974 from *Bacillus cereus* in complex with ThiametG  
Authors : Andreou, A.; Giastas, P.; Eliopoulos, E.E.  
Deposited on : 2017-03-10  
Resolution : 2.73 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
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

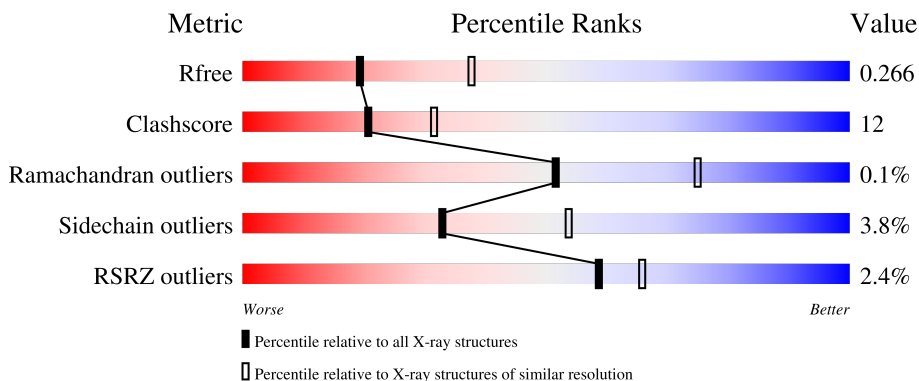
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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  $\geq 3$ , 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	247	<div> <div>2%</div> <div>63% 19% 17%</div> </div>
1	B	247	<div> <div>%</div> <div>55% 27% 17%</div> </div>
1	C	247	<div> <div>5%</div> <div>66% 17% 17%</div> </div>
1	D	247	<div> <div></div> <div>58% 24% 17%</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
7	CIT	D	303	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6692 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 Peptidoglycan N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1620	1037	276	300	7			
1	B	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			
1	C	205	Total	C	N	O	S	0	0	0
			1640	1051	280	302	7			
1	D	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

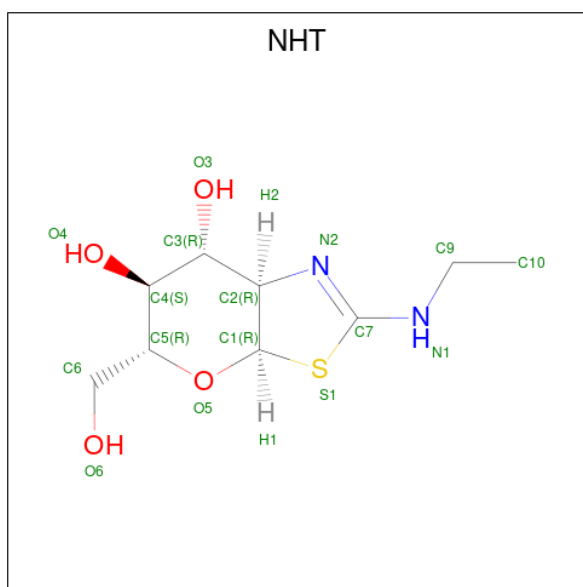
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 4 is (3AR,5R,6S,7R,7AR)-2-(ETHYLAMINO)-5-(HYDROXYMETHYL)-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D][1,3]THIAZOLE-6,7-DIOL (three-letter code: NHT) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>2</sub>O<sub>4</sub>S).



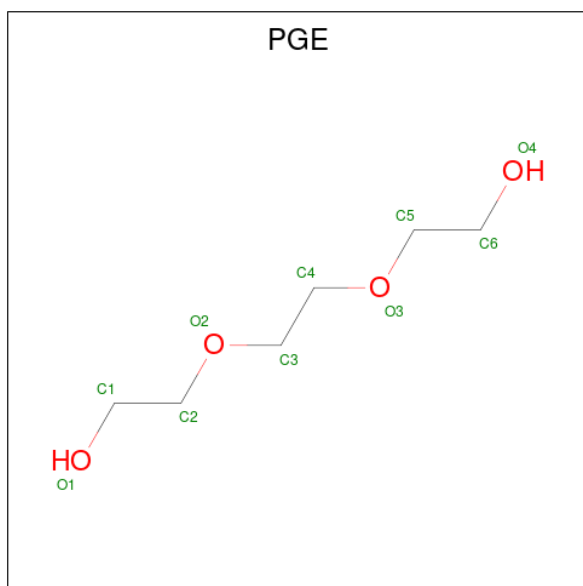
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			16	9	2	4	1		

*Continued on next page...*

Continued from previous page...

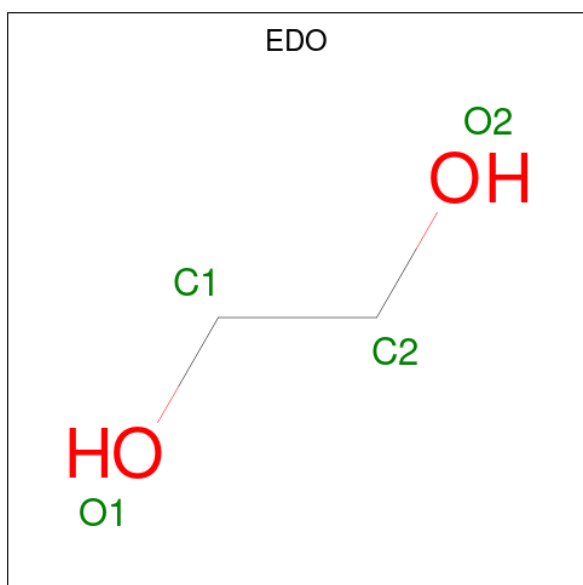
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			16	9	2	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



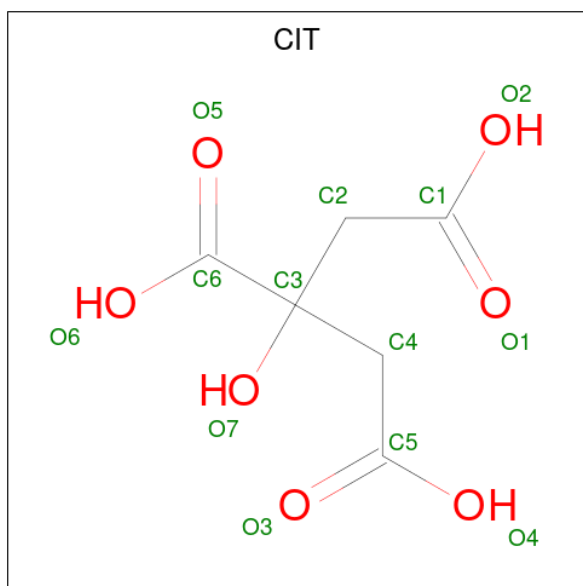
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	6	7		

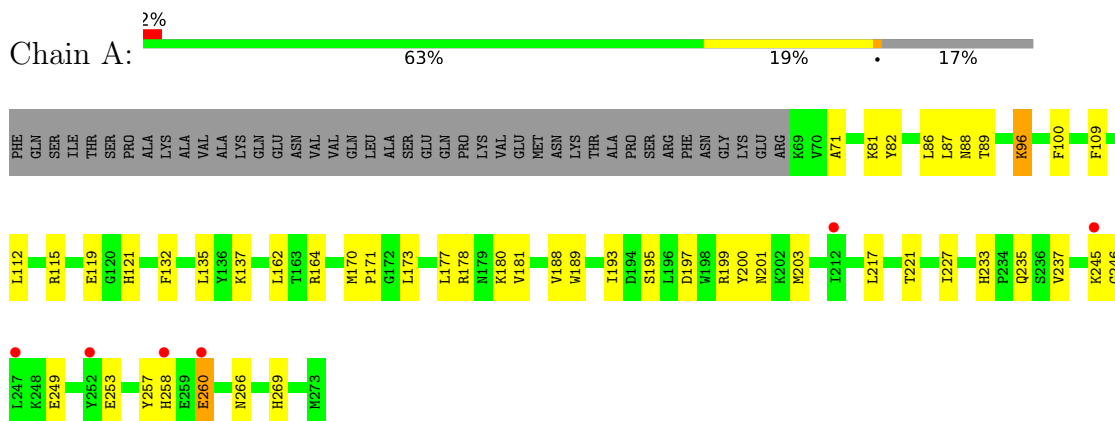
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	15	Total	O	0	0
			15	15		
8	B	19	Total	O	0	0
			19	19		
8	C	14	Total	O	0	0
			14	14		
8	D	11	Total	O	0	0
			11	11		

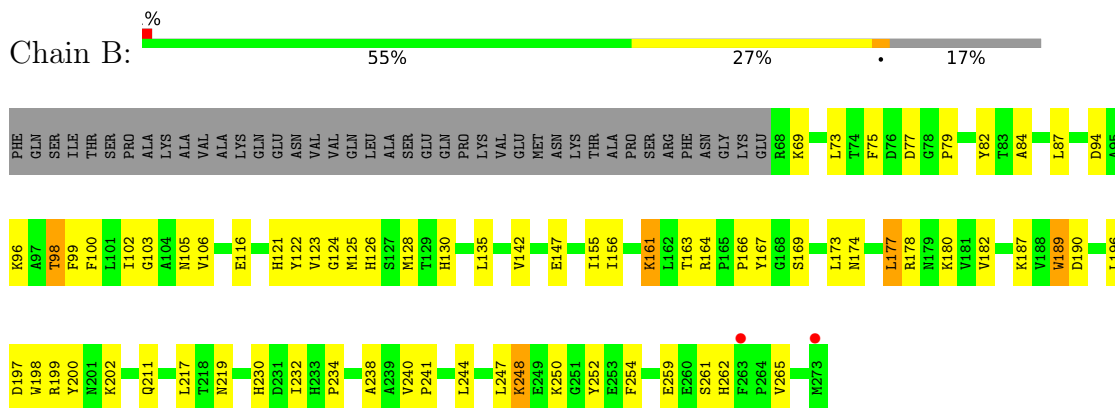
### 3 Residue-property plots

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.

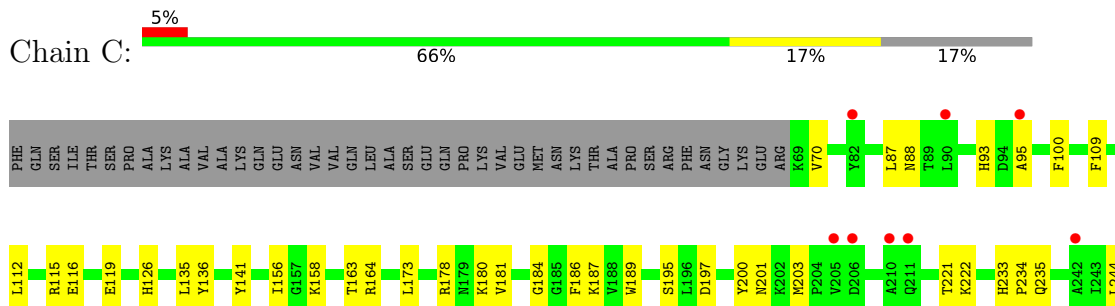
• Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase



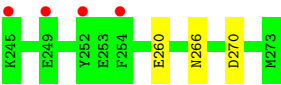
• Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase



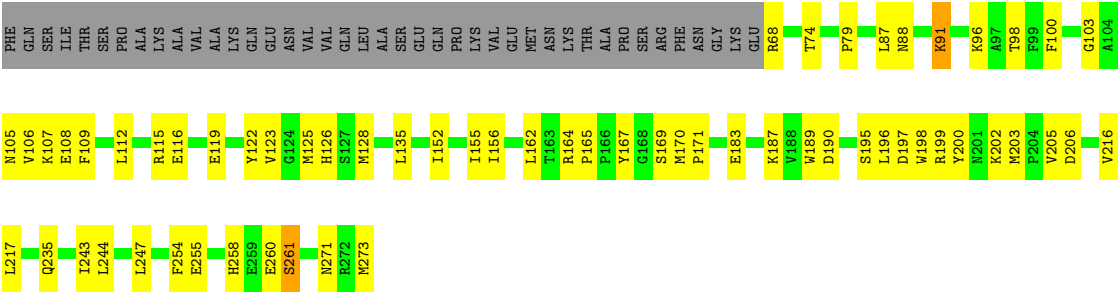
• Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase







● Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.44Å 117.97Å 98.20Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	48.34 – 2.73 48.34 – 2.73	Depositor EDS
% Data completeness (in resolution range)	89.7 (48.34-2.73) 90.5 (48.34-2.73)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.205 , 0.266 0.208 , 0.266	Depositor DCC
$R_{free}$ test set	1322 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CIT, ACT, EDO, NHT, PGE, ZN

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	0.43	0/1665	0.58	0/2260
1	B	0.47	0/1696	0.58	0/2295
1	C	0.42	0/1685	0.57	0/2281
1	D	0.45	0/1696	0.59	0/2295
All	All	0.44	0/6742	0.58	0/9131

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	1620	0	1550	34	0
1	B	1651	0	1611	56	0
1	C	1640	0	1598	29	0
1	D	1651	0	1611	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	0	3	1	0
4	B	16	0	14	1	0
4	D	16	0	14	1	0
5	B	10	0	14	5	0
6	B	4	0	6	0	0
7	D	13	0	5	3	0
8	A	15	0	0	0	0
8	B	19	0	0	2	0
8	C	14	0	0	3	0
8	D	11	0	0	2	0
All	All	6692	0	6429	160	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 12.

The worst 5 of 160 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:170:MET:HG2	7:D:303:CIT:H42	1.64	0.78
1:B:232:ILE:O	8:B:401:HOH:O	2.03	0.76
1:D:258:HIS:HB2	1:D:261:SER:HB2	1.68	0.76
1:B:202:LYS:HE3	1:D:199:ARG:HH22	1.50	0.75
1:A:132:PHE:HE2	1:A:137:LYS:HE3	1.51	0.75

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	203/247 (82%)	194 (96%)	9 (4%)	0	100	100
1	B	204/247 (83%)	188 (92%)	15 (7%)	1 (0%)	29	48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	203/247 (82%)	195 (96%)	8 (4%)	0	100	100
1	D	204/247 (83%)	188 (92%)	16 (8%)	0	100	100
All	All	814/988 (82%)	765 (94%)	48 (6%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	ASP

### 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	167/208 (80%)	161 (96%)	6 (4%)	35	55
1	B	173/208 (83%)	164 (95%)	9 (5%)	23	39
1	C	172/208 (83%)	170 (99%)	2 (1%)	71	83
1	D	173/208 (83%)	164 (95%)	9 (5%)	23	39
All	All	685/832 (82%)	659 (96%)	26 (4%)	33	54

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	261	SER
1	D	91	LYS
1	D	261	SER
1	C	189	TRP
1	D	106	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	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 ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	NHT	B	302	2	15,17,17	4.64	6 (40%)	14,24,24	1.53	3 (21%)
6	EDO	B	304	-	3,3,3	0.51	0	2,2,2	0.19	0
3	ACT	C	302	2	3,3,3	0.79	0	3,3,3	1.54	0
4	NHT	D	302	2	15,17,17	4.41	6 (40%)	14,24,24	1.31	3 (21%)
5	PGE	B	303	-	9,9,9	0.40	0	8,8,8	0.56	0
3	ACT	A	302	2	3,3,3	0.78	0	3,3,3	1.57	0
7	CIT	D	303	-	12,12,12	1.08	0	17,17,17	2.00	6 (35%)

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	NHT	B	302	2	-	1/5/33/33	0/2/2/2
6	EDO	B	304	-	-	0/1/1/1	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NHT	D	302	2	-	2/5/33/33	0/2/2/2
5	PGE	B	303	-	-	3/7/7/7	-
7	CIT	D	303	-	-	12/16/16/16	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	302	NHT	C2-N2	12.31	1.61	1.47
4	D	302	NHT	C2-N2	11.51	1.60	1.47
4	B	302	NHT	C7-N2	9.83	1.52	1.29
4	D	302	NHT	C7-N2	9.41	1.51	1.29
4	B	302	NHT	O5-C1	5.08	1.50	1.42

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	303	CIT	O6-C6-C3	4.26	120.45	113.05
4	B	302	NHT	N1-C7-N2	3.91	129.37	124.26
7	D	303	CIT	O2-C1-C2	2.94	123.80	114.35
7	D	303	CIT	O7-C3-C6	2.90	112.93	108.86
4	B	302	NHT	O5-C5-C6	2.74	113.25	106.44

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	303	CIT	C1-C2-C3-O7
7	D	303	CIT	C1-C2-C3-C6
7	D	303	CIT	C2-C3-C4-C5
7	D	303	CIT	O7-C3-C4-C5
7	D	303	CIT	C6-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	NHT	1	0
3	C	302	ACT	1	0
4	D	302	NHT	1	0
5	B	303	PGE	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	303	CIT	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	205/247 (82%)	0.28	6 (2%) 51 58	40, 67, 106, 127	0
1	B	206/247 (83%)	0.22	2 (0%) 82 86	43, 65, 96, 110	0
1	C	205/247 (82%)	0.44	12 (5%) 22 25	43, 76, 120, 153	0
1	D	206/247 (83%)	0.17	0 100 100	39, 60, 85, 105	0
All	All	822/988 (83%)	0.27	20 (2%) 59 66	39, 66, 107, 153	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	GLU	3.8
1	A	252	TYR	3.2
1	A	258	HIS	3.2
1	C	210	ALA	3.0
1	C	211	GLN	2.8

### 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 monosaccharides 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, 95<sup>th</sup> 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
7	CIT	D	303	13/13	0.81	0.27	63,77,87,91	0
4	NHT	D	302	16/16	0.86	0.26	43,82,102,165	16
6	EDO	B	304	4/4	0.87	0.32	56,59,62,63	0
4	NHT	B	302	16/16	0.91	0.23	44,90,124,139	0
5	PGE	B	303	10/10	0.92	0.34	81,81,85,85	0
3	ACT	A	302	4/4	0.92	0.18	75,89,89,96	0
3	ACT	C	302	4/4	0.92	0.17	73,76,79,81	0
2	ZN	C	301	1/1	0.95	0.13	65,65,65,65	0
2	ZN	A	301	1/1	0.97	0.18	63,63,63,63	0
2	ZN	D	301	1/1	0.98	0.25	72,72,72,72	0
2	ZN	B	301	1/1	0.99	0.19	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.