



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 21, 2025 – 03:43 PM EST

PDB ID : 8F9X  
Title : Cyclase-Phosphotriesterase from Ruegeria pomeroyi DSS-3  
Authors : Frkic, R.L.; Ji, D.; Jackson, C.J.  
Deposited on : 2022-11-24  
Resolution : 2.32 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>.

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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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

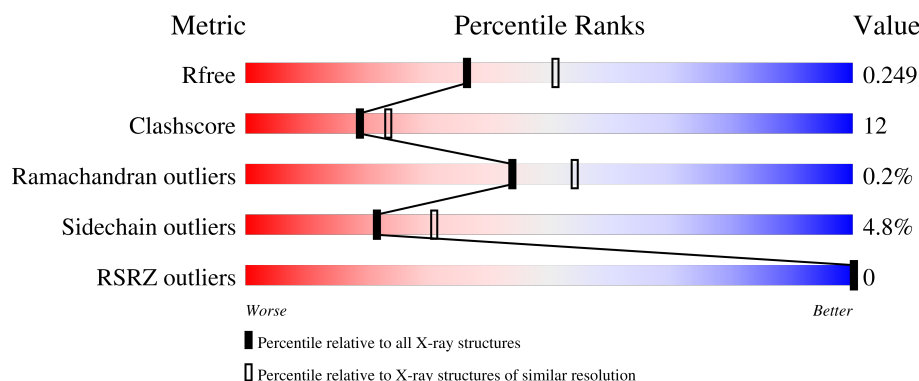
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	230	 76% 22% .
1	B	230	 82% 16% ..
1	C	230	 74% 23% ..
1	D	230	 70% 26% ..
1	E	230	 70% 27% ..

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Mol	Chain	Length	Quality of chain
1	F	230	<div><div></div><div>74%23%..</div></div>
1	G	230	<div><div></div><div>71%26%..</div></div>
1	H	230	<div><div></div><div>65%30%..</div></div>
1	I	230	<div><div></div><div>75%21%..</div></div>
1	J	230	<div><div></div><div>78%22%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17432 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 Cyclase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1708	1076	296	326	10			
1	B	228	Total	C	N	O	S	0	0	0
			1695	1068	294	324	9			
1	C	226	Total	C	N	O	S	0	0	0
			1683	1060	292	322	9			
1	D	225	Total	C	N	O	S	0	0	0
			1679	1058	291	321	9			
1	E	227	Total	C	N	O	S	0	0	0
			1691	1066	293	323	9			
1	F	225	Total	C	N	O	S	0	0	0
			1679	1058	291	321	9			
1	G	228	Total	C	N	O	S	0	0	0
			1695	1068	294	324	9			
1	H	228	Total	C	N	O	S	0	0	0
			1695	1068	294	324	9			
1	I	227	Total	C	N	O	S	0	0	0
			1691	1066	293	323	9			
1	J	230	Total	C	N	O	S	0	0	0
			1708	1076	296	326	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	MET	-	initiating methionine	UNP Q5LVE1
B	43	MET	-	initiating methionine	UNP Q5LVE1
C	43	MET	-	initiating methionine	UNP Q5LVE1
D	43	MET	-	initiating methionine	UNP Q5LVE1
E	43	MET	-	initiating methionine	UNP Q5LVE1
F	43	MET	-	initiating methionine	UNP Q5LVE1
G	43	MET	-	initiating methionine	UNP Q5LVE1
H	43	MET	-	initiating methionine	UNP Q5LVE1
I	43	MET	-	initiating methionine	UNP Q5LVE1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	43	MET	-	initiating methionine	UNP Q5LVE1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 3	Zn 3	0	1
2	B	3	Total 3	Zn 3	0	0
2	C	2	Total 3	Zn 3	0	1
2	D	2	Total 3	Zn 3	0	1
2	E	2	Total 3	Zn 3	0	1
2	F	2	Total 3	Zn 3	0	1
2	G	3	Total 3	Zn 3	0	0
2	H	3	Total 3	Zn 3	0	0
2	I	3	Total 3	Zn 3	0	0
2	J	3	Total 3	Zn 3	0	0

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



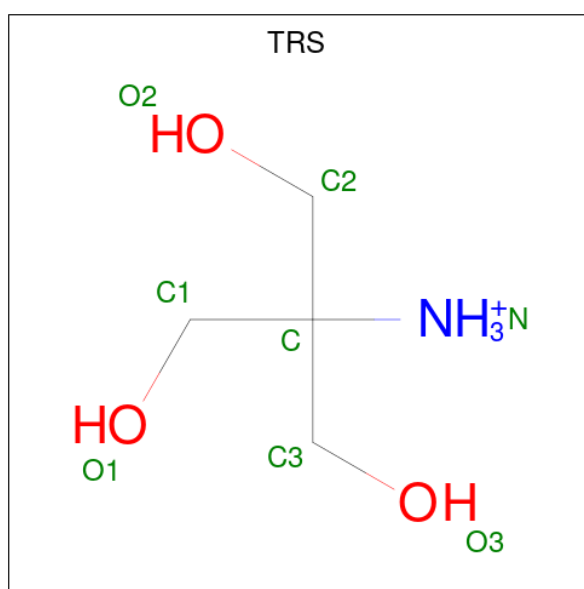
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	D	1	Total	C	N	O	0	0
			8	4	1	3		
5	E	1	Total	C	N	O	0	0
			8	4	1	3		
5	H	1	Total	C	N	O	0	0
			8	4	1	3		
5	I	1	Total	C	N	O	0	0
			8	4	1	3		

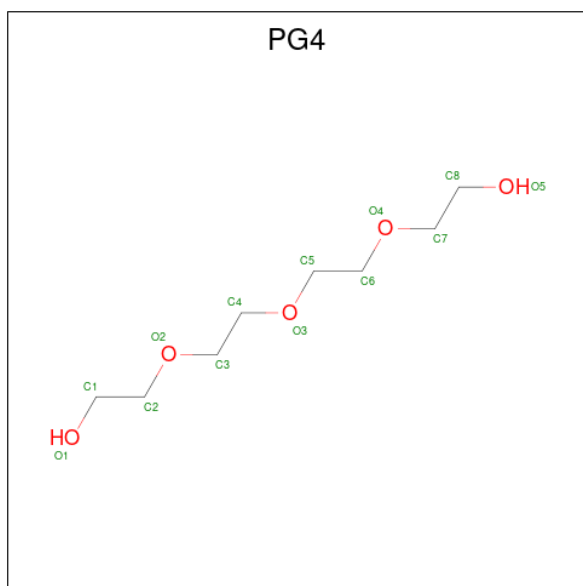
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		
7	B	25	Total	O	0	0
			25	25		
7	C	18	Total	O	0	0
			18	18		
7	D	14	Total	O	0	0
			14	14		
7	E	9	Total	O	0	0
			9	9		
7	F	14	Total	O	0	0
			14	14		
7	G	19	Total	O	0	0
			19	19		

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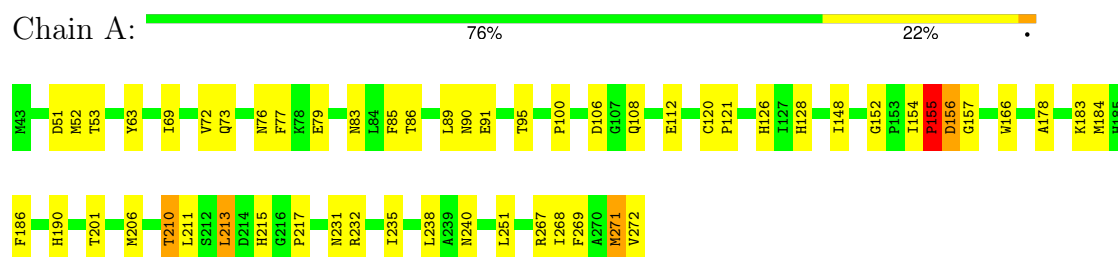
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	8	Total 8	O 8	0	0
7	I	11	Total 11	O 11	0	0
7	J	11	Total 11	O 11	0	0

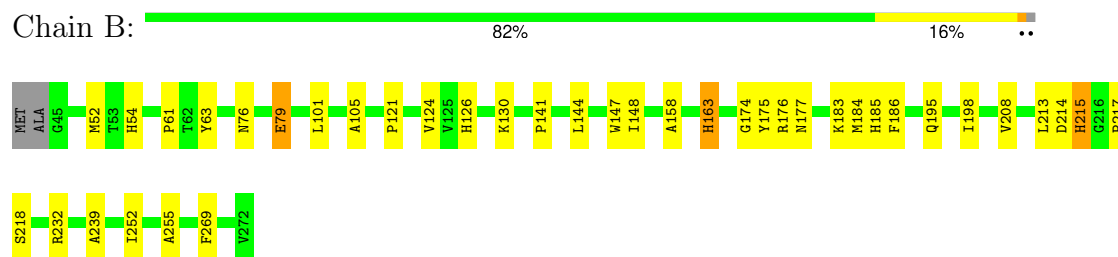
### 3 Residue-property plots

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.

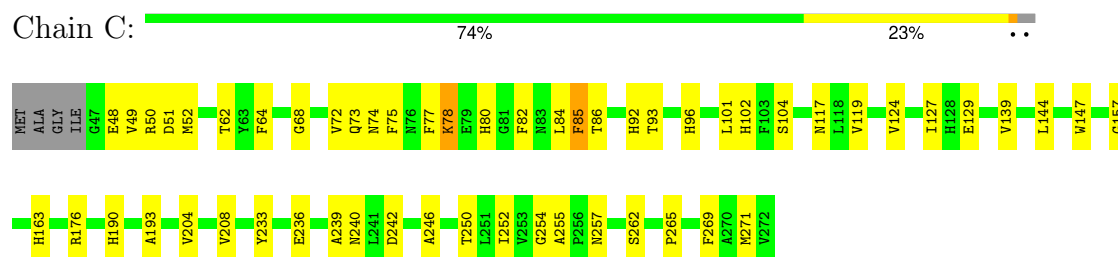
#### • Molecule 1: Cyclase family protein



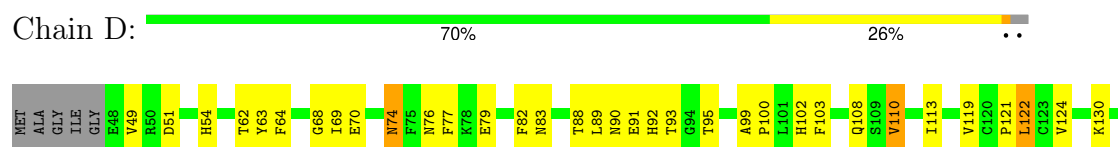
#### • Molecule 1: Cyclase family protein



#### • Molecule 1: Cyclase family protein

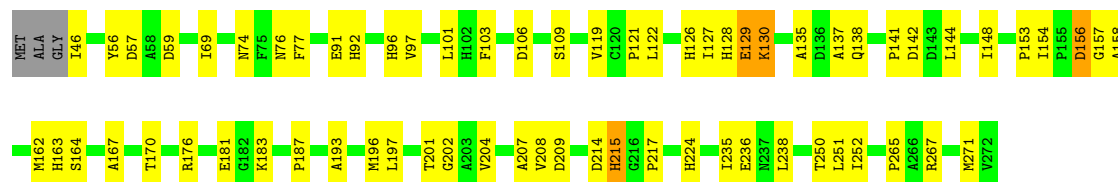


#### • Molecule 1: Cyclase family protein

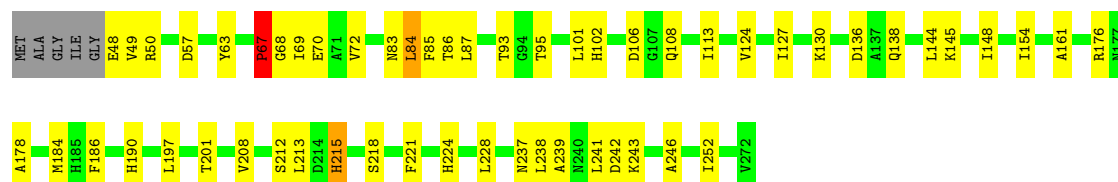




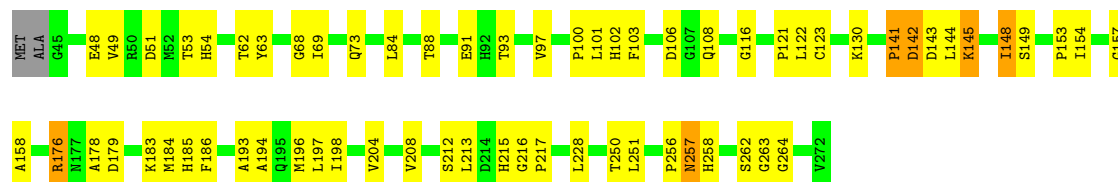
- Molecule 1: Cyclase family protein



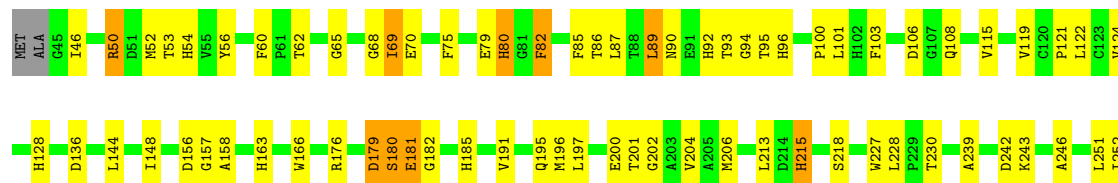
- Molecule 1: Cyclase family protein



- Molecule 1: Cyclase family protein

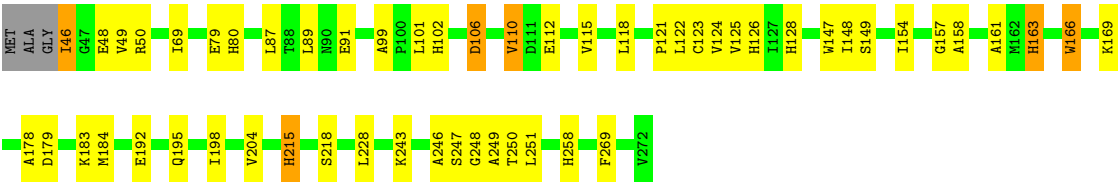


- Molecule 1: Cyclase family protein

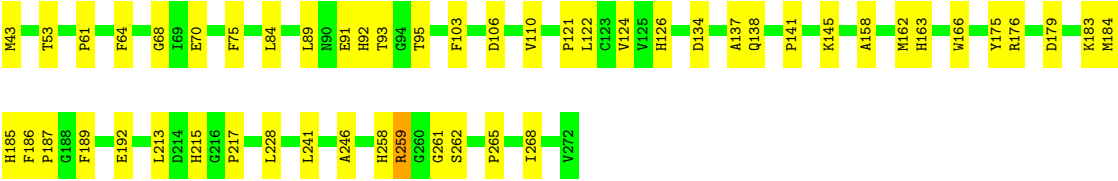


- Molecule 1: Cyclase family protein





● Molecule 1: Cyclase family protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.08Å 68.08Å 446.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.04 – 2.32 34.04 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.04-2.32) 99.9 (34.04-2.32)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.219 , 0.253 0.216 , 0.249	Depositor DCC
$R_{free}$ test set	5012 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l 0.477 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
Reported twinning fraction	0.499 for H, K, L 0.501 for K, H, -L	Depositor
Outliers	0 of 100157 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	17432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, PG4, EDO, ZN, TRS

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	0.26	0/1757	0.47	0/2396
1	B	0.26	0/1744	0.47	0/2379
1	C	0.25	0/1732	0.44	0/2363
1	D	0.27	0/1728	0.47	0/2358
1	E	0.28	0/1740	0.48	0/2374
1	F	0.28	0/1728	0.49	0/2358
1	G	0.31	0/1744	0.50	0/2379
1	H	0.28	0/1744	0.49	0/2379
1	I	0.28	0/1740	0.49	0/2374
1	J	0.25	0/1757	0.45	0/2396
All	All	0.27	0/17414	0.47	0/23756

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	1708	0	1603	35	0
1	B	1695	0	1589	28	0
1	C	1683	0	1575	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1679	0	1572	53	0
1	E	1691	0	1586	41	0
1	F	1679	0	1572	39	0
1	G	1695	0	1589	48	0
1	H	1695	0	1589	57	0
1	I	1691	0	1586	35	0
1	J	1708	0	1603	32	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	28	0	38	3	0
3	B	14	0	19	1	0
3	C	14	0	19	2	0
3	D	14	0	19	0	0
3	F	28	0	38	8	0
3	G	28	0	38	4	0
3	H	14	0	19	1	0
3	I	28	0	38	3	0
3	J	28	0	38	5	0
4	A	8	0	12	0	0
4	C	12	0	18	0	0
4	D	4	0	6	0	0
4	E	12	0	18	0	0
4	F	12	0	18	0	0
4	G	4	0	6	0	0
4	H	12	0	18	0	0
4	I	8	0	12	0	0
4	J	4	0	6	0	0
5	B	8	0	12	0	0
5	D	8	0	12	1	0
5	E	8	0	12	0	0
5	H	8	0	12	0	0
5	I	8	0	12	0	0
5	J	8	0	12	0	0
6	C	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	16	0	0	0	0
7	B	25	0	0	0	0
7	C	18	0	0	0	0
7	D	14	0	0	0	0
7	E	9	0	0	0	0
7	F	14	0	0	0	0
7	G	19	0	0	1	0
7	H	8	0	0	0	0
7	I	11	0	0	0	0
7	J	11	0	0	0	0
All	All	17432	0	16334	394	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 394 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:G:148:ILE:HD13	1:G:153:PRO:HA	1.47	0.95
1:G:148:ILE:HD11	1:G:154:ILE:HG12	1.55	0.86
1:C:84:LEU:HD13	1:D:90:ASN:OD1	1.80	0.81
1:I:166:TRP:CE2	1:I:169:LYS:HE2	2.19	0.78
1:G:68:GLY:HA3	1:G:93:THR:HG21	1.66	0.77

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	228/230 (99%)	212 (93%)	14 (6%)	2 (1%)	14	17
1	B	226/230 (98%)	209 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	224/230 (97%)	208 (93%)	16 (7%)	0	100	100
1	D	223/230 (97%)	209 (94%)	14 (6%)	0	100	100
1	E	225/230 (98%)	198 (88%)	27 (12%)	0	100	100
1	F	223/230 (97%)	204 (92%)	18 (8%)	1 (0%)	30	37
1	G	226/230 (98%)	209 (92%)	16 (7%)	1 (0%)	30	37
1	H	226/230 (98%)	213 (94%)	13 (6%)	0	100	100
1	I	225/230 (98%)	213 (95%)	12 (5%)	0	100	100
1	J	228/230 (99%)	207 (91%)	21 (9%)	0	100	100
All	All	2254/2300 (98%)	2082 (92%)	168 (8%)	4 (0%)	44	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ASP
1	G	48	GLU
1	A	155	PRO
1	F	67	PRO

### 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	172/172 (100%)	165 (96%)	7 (4%)	26	38
1	B	171/172 (99%)	167 (98%)	4 (2%)	45	62
1	C	170/172 (99%)	163 (96%)	7 (4%)	26	38
1	D	170/172 (99%)	166 (98%)	4 (2%)	44	60
1	E	171/172 (99%)	158 (92%)	13 (8%)	11	14
1	F	170/172 (99%)	162 (95%)	8 (5%)	22	32
1	G	171/172 (99%)	160 (94%)	11 (6%)	14	20
1	H	171/172 (99%)	158 (92%)	13 (8%)	11	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	171/172 (99%)	162 (95%)	9 (5%)	19	27
1	J	172/172 (100%)	166 (96%)	6 (4%)	31	44
All	All	1709/1720 (99%)	1627 (95%)	82 (5%)	21	31

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	80	HIS
1	I	149	SER
1	H	86	THR
1	H	181	GLU
1	I	250	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	163	HIS
1	G	258	HIS
1	I	215	HIS
1	I	90	ASN
1	D	92	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 30 are monoatomic - leaving 40 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	EDO	E	306	-	3,3,3	0.42	0	2,2,2	0.37	0
4	EDO	F	307	-	3,3,3	0.43	0	2,2,2	0.37	0
3	BTB	A	303	-	13,13,13	0.88	0	7,16,16	0.70	0
4	EDO	E	305	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	I	307	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	G	306	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	H	306	-	3,3,3	0.43	0	2,2,2	0.38	0
3	BTB	B	305	-	13,13,13	0.90	0	7,16,16	0.63	0
4	EDO	H	308	-	3,3,3	0.43	0	2,2,2	0.39	0
3	BTB	J	306	-	13,13,13	0.89	0	7,16,16	0.73	0
5	TRS	D	303	-	7,7,7	0.35	0	9,9,9	0.35	0
3	BTB	J	305	-	13,13,13	0.86	0	7,16,16	0.66	0
4	EDO	C	306	-	3,3,3	0.42	0	2,2,2	0.38	0
3	BTB	D	304	-	13,13,13	0.88	0	7,16,16	0.75	0
3	BTB	F	303	-	13,13,13	0.63	0	7,16,16	0.20	0
4	EDO	D	305	-	3,3,3	0.42	0	2,2,2	0.37	0
5	TRS	J	304	-	7,7,7	0.35	0	9,9,9	0.37	0
3	BTB	G	305	-	13,13,13	0.85	0	7,16,16	0.75	0
4	EDO	E	304	-	3,3,3	0.42	0	2,2,2	0.39	0
5	TRS	B	304	-	7,7,7	0.34	0	9,9,9	0.33	0
5	TRS	E	303	-	7,7,7	0.34	0	9,9,9	0.34	0
6	PG4	C	307	-	12,12,12	0.10	0	11,11,11	0.67	0
5	TRS	H	304	-	7,7,7	0.34	0	9,9,9	0.36	0
4	EDO	C	305	-	3,3,3	0.42	0	2,2,2	0.39	0
5	TRS	I	304	-	7,7,7	0.35	0	9,9,9	0.34	0
4	EDO	J	307	-	3,3,3	0.43	0	2,2,2	0.38	0
3	BTB	F	304	-	13,13,13	0.87	0	7,16,16	0.68	0
3	BTB	G	304	-	13,13,13	0.87	0	7,16,16	0.69	0
4	EDO	H	307	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	F	306	-	3,3,3	0.42	0	2,2,2	0.39	0
3	BTB	C	303	-	13,13,13	0.88	0	7,16,16	0.69	0
4	EDO	F	305	-	3,3,3	0.42	0	2,2,2	0.39	0
3	BTB	H	305	-	13,13,13	0.86	0	7,16,16	0.73	0
3	BTB	A	304	-	13,13,13	0.88	0	7,16,16	0.68	0
3	BTB	I	305	-	13,13,13	0.86	0	7,16,16	0.74	0
4	EDO	A	305	-	3,3,3	0.42	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	I	306	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	A	306	-	3,3,3	0.43	0	2,2,2	0.37	0
3	BTB	I	308	-	13,13,13	0.87	0	7,16,16	0.77	0
4	EDO	C	304	-	3,3,3	0.42	0	2,2,2	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	306	-	-	0/1/1/1	-
4	EDO	F	307	-	-	0/1/1/1	-
3	BTB	A	303	-	-	10/21/21/21	-
4	EDO	E	305	-	-	0/1/1/1	-
4	EDO	I	307	-	-	0/1/1/1	-
4	EDO	G	306	-	-	0/1/1/1	-
4	EDO	H	306	-	-	0/1/1/1	-
3	BTB	B	305	-	-	12/21/21/21	-
4	EDO	H	308	-	-	0/1/1/1	-
3	BTB	J	306	-	-	12/21/21/21	-
5	TRS	D	303	-	-	0/9/9/9	-
3	BTB	J	305	-	-	7/21/21/21	-
4	EDO	C	306	-	-	0/1/1/1	-
3	BTB	D	304	-	-	10/21/21/21	-
3	BTB	F	303	-	-	1/21/21/21	-
4	EDO	D	305	-	-	0/1/1/1	-
5	TRS	J	304	-	-	2/9/9/9	-
3	BTB	G	305	-	-	7/21/21/21	-
4	EDO	E	304	-	-	0/1/1/1	-
5	TRS	B	304	-	-	0/9/9/9	-
5	TRS	E	303	-	-	0/9/9/9	-
6	PG4	C	307	-	-	7/10/10/10	-
5	TRS	H	304	-	-	0/9/9/9	-
4	EDO	C	305	-	-	0/1/1/1	-
5	TRS	I	304	-	-	0/9/9/9	-
4	EDO	J	307	-	-	0/1/1/1	-
3	BTB	F	304	-	-	11/21/21/21	-
3	BTB	G	304	-	-	10/21/21/21	-
4	EDO	H	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	306	-	-	0/1/1/1	-
3	BTB	C	303	-	-	11/21/21/21	-
4	EDO	F	305	-	-	0/1/1/1	-
3	BTB	H	305	-	-	2/21/21/21	-
3	BTB	A	304	-	-	9/21/21/21	-
3	BTB	I	305	-	-	7/21/21/21	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	I	306	-	-	0/1/1/1	-
4	EDO	A	306	-	-	0/1/1/1	-
3	BTB	I	308	-	-	3/21/21/21	-
4	EDO	C	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	BTB	C1-C2-C4-O4
3	A	303	BTB	C3-C2-C4-O4
3	A	303	BTB	N-C2-C4-O4
3	A	303	BTB	C1-C2-N-C7
3	A	303	BTB	C3-C2-N-C7

There are no ring outliers.

13 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	BTB	1	0
3	J	306	BTB	2	0
5	D	303	TRS	1	0
3	J	305	BTB	3	0
3	F	303	BTB	6	0
3	G	305	BTB	1	0
3	F	304	BTB	2	0
3	G	304	BTB	3	0
3	C	303	BTB	2	0
3	H	305	BTB	1	0
3	A	304	BTB	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	305	BTB	2	0
3	I	308	BTB	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 [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	230/230 (100%)	-1.34	0 100 100	38, 47, 61, 145	0
1	B	228/230 (99%)	-1.33	0 100 100	36, 51, 71, 99	0
1	C	226/230 (98%)	-1.36	0 100 100	41, 54, 75, 90	0
1	D	225/230 (97%)	-1.31	0 100 100	46, 57, 73, 93	0
1	E	227/230 (98%)	-1.23	0 100 100	43, 61, 89, 108	0
1	F	225/230 (97%)	-1.31	0 100 100	41, 55, 75, 87	0
1	G	228/230 (99%)	-1.34	0 100 100	39, 52, 69, 102	0
1	H	228/230 (99%)	-1.27	0 100 100	41, 55, 83, 131	0
1	I	227/230 (98%)	-1.36	0 100 100	32, 54, 71, 100	0
1	J	230/230 (100%)	-1.35	0 100 100	36, 52, 68, 94	0
All	All	2274/2300 (98%)	-1.32	0 100 100	32, 54, 76, 145	0

There are no RSRZ outliers to report.

### 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(Å <sup>2</sup> )	Q<0.9
4	EDO	G	306	4/4	0.94	0.11	74,81,83,84	0
4	EDO	E	305	4/4	0.96	0.04	91,97,99,101	0
4	EDO	D	305	4/4	0.96	0.06	56,56,59,59	0
4	EDO	I	307	4/4	0.96	0.08	47,53,54,55	0
5	TRS	E	303	8/8	0.96	0.05	66,72,77,78	0
4	EDO	F	305	4/4	0.97	0.09	51,52,54,55	0
4	EDO	F	306	4/4	0.97	0.06	50,52,53,55	0
4	EDO	F	307	4/4	0.97	0.07	44,45,45,51	0
4	EDO	C	306	4/4	0.97	0.05	52,57,58,60	0
4	EDO	H	307	4/4	0.97	0.04	100,100,101,102	0
3	BTB	A	303	14/14	0.97	0.04	53,62,66,66	0
5	TRS	D	303	8/8	0.97	0.04	72,78,80,81	0
4	EDO	C	305	4/4	0.97	0.05	69,69,70,73	0
5	TRS	J	304	8/8	0.97	0.05	57,64,70,71	0
3	BTB	G	305	14/14	0.98	0.04	45,49,53,55	0
4	EDO	E	306	4/4	0.98	0.09	82,86,87,94	0
3	BTB	I	305	14/14	0.98	0.04	49,53,56,57	0
3	BTB	I	308	14/14	0.98	0.04	56,61,62,62	0
3	BTB	J	306	14/14	0.98	0.04	57,63,69,70	0
4	EDO	A	305	4/4	0.98	0.06	58,61,62,62	0
4	EDO	C	304	4/4	0.98	0.04	61,65,68,71	0
3	BTB	A	304	14/14	0.98	0.04	43,46,55,56	0
4	EDO	J	307	4/4	0.98	0.05	44,48,53,54	0
5	TRS	B	304	8/8	0.98	0.03	53,57,60,64	0
3	BTB	B	305	14/14	0.98	0.04	54,59,61,61	0
3	BTB	D	304	14/14	0.98	0.03	48,52,54,59	0
5	TRS	H	304	8/8	0.98	0.04	54,57,60,60	0
4	EDO	E	304	4/4	0.98	0.06	48,48,51,51	0
6	PG4	C	307	13/13	0.98	0.04	57,59,63,63	0
4	EDO	H	306	4/4	0.99	0.04	54,55,56,59	0
3	BTB	H	305	14/14	0.99	0.04	61,65,73,75	0
4	EDO	H	308	4/4	0.99	0.05	46,47,49,52	0
4	EDO	I	306	4/4	0.99	0.04	43,46,46,49	0
3	BTB	C	303	14/14	0.99	0.03	50,53,57,61	0
2	ZN	A	301[B]	1/1	0.99	0.04	38,38,38,38	1
3	BTB	J	305	14/14	0.99	0.03	47,50,55,56	0
3	BTB	F	303	14/14	0.99	0.04	58,64,65,66	0
3	BTB	F	304	14/14	0.99	0.04	64,67,70,70	0
4	EDO	A	306	4/4	0.99	0.05	41,43,44,45	0
5	TRS	I	304	8/8	0.99	0.02	48,51,52,52	0
3	BTB	G	304	14/14	0.99	0.03	54,56,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	301[A]	1/1	0.99	0.04	39,39,39,39	1
2	ZN	E	302	1/1	1.00	0.02	95,95,95,95	0
2	ZN	F	301[A]	1/1	1.00	0.04	42,42,42,42	1
2	ZN	F	301[B]	1/1	1.00	0.04	46,46,46,46	1
2	ZN	F	302	1/1	1.00	0.01	46,46,46,46	0
2	ZN	G	301	1/1	1.00	0.01	48,48,48,48	0
2	ZN	G	302	1/1	1.00	0.01	52,52,52,52	0
2	ZN	G	303	1/1	1.00	0.01	49,49,49,49	0
2	ZN	H	301	1/1	1.00	0.02	45,45,45,45	0
2	ZN	H	302	1/1	1.00	0.01	51,51,51,51	0
2	ZN	H	303	1/1	1.00	0.01	62,62,62,62	0
2	ZN	I	301	1/1	1.00	0.02	45,45,45,45	0
2	ZN	I	302	1/1	1.00	0.01	31,31,31,31	0
2	ZN	I	303	1/1	1.00	0.01	68,68,68,68	0
2	ZN	J	301	1/1	1.00	0.01	36,36,36,36	0
2	ZN	J	302	1/1	1.00	0.01	39,39,39,39	0
2	ZN	J	303	1/1	1.00	0.01	53,53,53,53	0
2	ZN	A	302	1/1	1.00	0.01	56,56,56,56	0
2	ZN	B	301	1/1	1.00	0.01	38,38,38,38	0
2	ZN	B	302	1/1	1.00	0.01	38,38,38,38	0
2	ZN	B	303	1/1	1.00	0.01	52,52,52,52	0
2	ZN	C	301[A]	1/1	1.00	0.03	39,39,39,39	1
2	ZN	C	301[B]	1/1	1.00	0.03	43,43,43,43	1
2	ZN	C	302	1/1	1.00	0.02	68,68,68,68	0
2	ZN	D	301[A]	1/1	1.00	0.04	53,53,53,53	1
2	ZN	D	301[B]	1/1	1.00	0.04	50,50,50,50	1
2	ZN	D	302	1/1	1.00	0.01	70,70,70,70	0
2	ZN	E	301[A]	1/1	1.00	0.02	46,46,46,46	1
2	ZN	E	301[B]	1/1	1.00	0.02	47,47,47,47	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.