



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:58 pm BST

PDB ID : 5Z5O  
Title : Structure of Pycnonodysostosis disease related I249T mutant of human cathepsin K  
Authors : Biswas, S.; Roy, S.  
Deposited on : 2018-01-19  
Resolution : 1.92 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

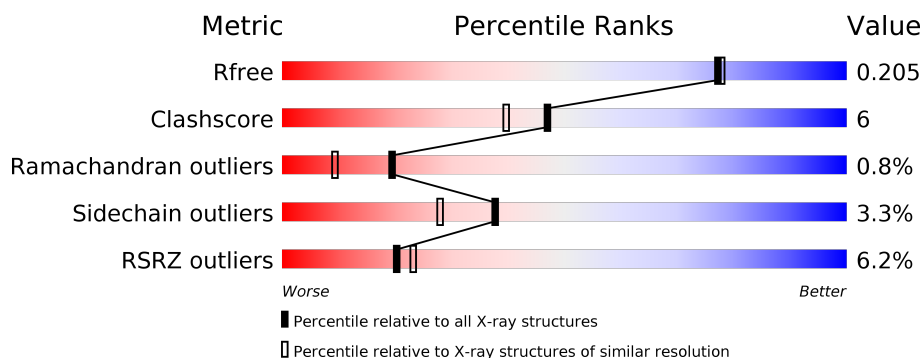
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	335	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>
2	B	94	<div> <div>10%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>18%</div> </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
3	GOL	A	404	-	-	X	-
3	GOL	A	406	-	-	-	X
4	EDO	A	420	-	-	-	X
4	EDO	B	103	-	-	-	X
6	PEG	A	426	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3527 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 Cathepsin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	3	0
			2470	1557	431	467	15			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P43235
A	-19	GLY	-	expression tag	UNP P43235
A	-18	SER	-	expression tag	UNP P43235
A	-17	SER	-	expression tag	UNP P43235
A	-16	HIS	-	expression tag	UNP P43235
A	-15	HIS	-	expression tag	UNP P43235
A	-14	HIS	-	expression tag	UNP P43235
A	-13	HIS	-	expression tag	UNP P43235
A	-12	HIS	-	expression tag	UNP P43235
A	-11	HIS	-	expression tag	UNP P43235
A	-10	SER	-	expression tag	UNP P43235
A	-9	SER	-	expression tag	UNP P43235
A	-8	GLY	-	expression tag	UNP P43235
A	-7	LEU	-	expression tag	UNP P43235
A	-6	VAL	-	expression tag	UNP P43235
A	-5	PRO	-	expression tag	UNP P43235
A	-4	ARG	-	expression tag	UNP P43235
A	-3	GLY	-	expression tag	UNP P43235
A	-2	SER	-	expression tag	UNP P43235
A	-1	HIS	-	expression tag	UNP P43235
A	0	MET	-	expression tag	UNP P43235
A	124	SER	CYS	engineered mutation	UNP P43235
A	234	THR	ILE	engineered mutation	UNP P43235

- Molecule 2 is a protein called Cathepsin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	77	Total	C	N	O	S	0	0	0
			639	406	111	120	2			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP P43235
B	-19	GLY	-	expression tag	UNP P43235
B	-18	SER	-	expression tag	UNP P43235
B	-17	SER	-	expression tag	UNP P43235
B	-16	HIS	-	expression tag	UNP P43235
B	-15	HIS	-	expression tag	UNP P43235
B	-14	HIS	-	expression tag	UNP P43235
B	-13	HIS	-	expression tag	UNP P43235
B	-12	HIS	-	expression tag	UNP P43235
B	-11	HIS	-	expression tag	UNP P43235
B	-10	SER	-	expression tag	UNP P43235
B	-9	SER	-	expression tag	UNP P43235
B	-8	GLY	-	expression tag	UNP P43235
B	-7	LEU	-	expression tag	UNP P43235
B	-6	VAL	-	expression tag	UNP P43235
B	-5	PRO	-	expression tag	UNP P43235
B	-4	ARG	-	expression tag	UNP P43235
B	-3	GLY	-	expression tag	UNP P43235
B	-2	SER	-	expression tag	UNP P43235
B	-1	HIS	-	expression tag	UNP P43235
B	0	MET	-	expression tag	UNP P43235

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



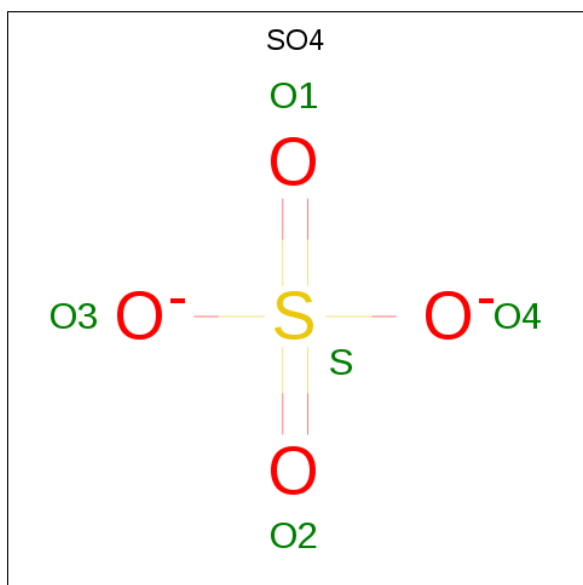
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).





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

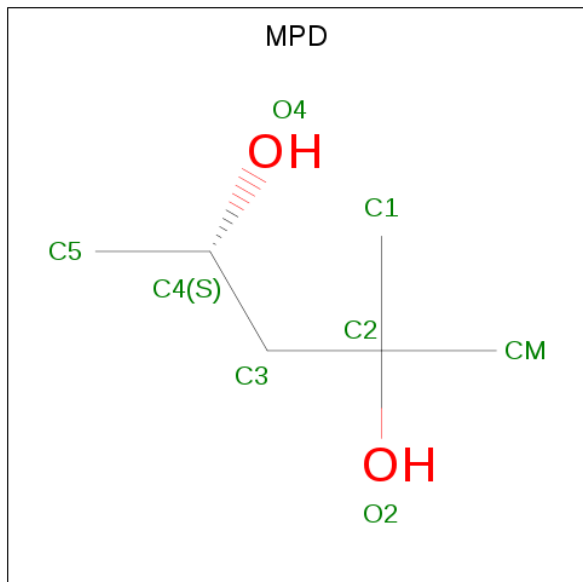
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			8	6	2		
9	B	1	Total	C	O	0	0
			8	6	2		
9	B	1	Total	C	O	0	0
			8	6	2		

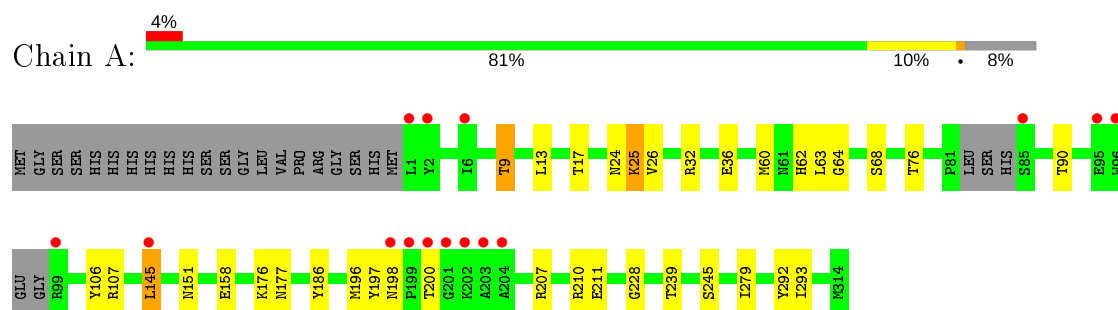
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	178	Total	O	0	0
			178	178		
10	B	28	Total	O	0	0
			28	28		

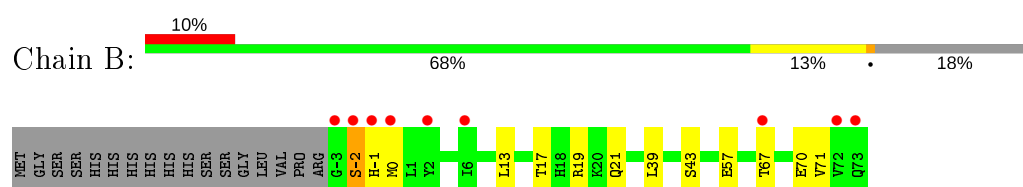
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: Cathepsin K



#### • Molecule 2: Cathepsin K



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.10Å 67.27Å 82.87Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	52.22 – 1.92 52.22 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.2 (52.22-1.92) 96.2 (52.22-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.92Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.162 , 0.204 0.171 , 0.205	Depositor DCC
$R_{free}$ test set	1995 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 75.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: GOL, MPD, CL, NA, EDO, SO4, PEG, SEB

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	0.56	0/2516	0.65	0/3393
2	B	0.42	0/654	0.55	0/885
All	All	0.53	0/3170	0.63	0/4278

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	2470	0	2416	34	0
2	B	639	0	617	5	0
3	A	42	0	54	4	0
3	B	6	0	8	0	0
4	A	52	0	78	2	0
4	B	12	0	18	0	0
5	A	5	0	0	0	0
5	B	20	0	0	0	0
6	A	42	0	60	7	0
6	B	7	0	10	2	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
9	B	24	0	42	0	0
10	A	178	0	0	6	0
10	B	28	0	0	6	0
All	All	3527	0	3303	41	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 6.

All (41) 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)
6:B:109:PEG:O2	10:B:201:HOH:O	1.98	0.81
2:B:43:SER:OG	10:B:203:HOH:O	2.02	0.77
2:B:57:GLU:OE1	10:B:202:HOH:O	2.02	0.76
1:A:13:LEU:O	1:A:17:THR:HG23	1.92	0.69
1:A:24:ASN:HB2	6:A:426:PEG:H31	1.79	0.65
1:A:158:GLU:OE1	10:A:501:HOH:O	2.15	0.65
1:A:68:SEB:CE	1:A:239:THR:OG1	2.49	0.60
1:A:245:SER:HA	3:A:404:GOL:H11	1.84	0.60
1:A:25:LYS:H	6:A:426:PEG:H31	1.70	0.56
1:A:62:HIS:HE1	10:A:612:HOH:O	1.90	0.53
1:A:68:SEB:HE2	1:A:239:THR:OG1	2.09	0.53
1:A:68:SEB:HE3	1:A:239:THR:OG1	2.08	0.52
2:B:13:LEU:O	2:B:17:THR:HG23	2.10	0.51
1:A:9:THR:HG22	10:A:509:HOH:O	2.10	0.50
1:A:245:SER:OG	3:A:404:GOL:H31	2.11	0.50
6:B:109:PEG:H32	10:B:217:HOH:O	2.11	0.49
1:A:196:MET:CE	1:A:197:TYR:CZ	2.96	0.49
1:A:25:LYS:CD	6:A:426:PEG:H32	2.43	0.48
1:A:177:ASN:HB2	10:A:557:HOH:O	2.15	0.47
1:A:32:ARG:NE	1:A:36:GLU:OE2	2.39	0.47
1:A:176:LYS:HE2	10:A:659:HOH:O	2.15	0.46
1:A:26:VAL:HG23	6:A:426:PEG:H12	1.98	0.46
1:A:107:ARG:HD3	1:A:292:TYR:CE2	2.51	0.45
1:A:25:LYS:H	6:A:426:PEG:C3	2.30	0.45
1:A:200:THR:HG21	10:A:651:HOH:O	2.17	0.44
1:A:279:ILE:HB	1:A:293:ILE:HG23	1.98	0.44
2:B:21:GLN:OE1	2:B:21:GLN:N	2.51	0.43
1:A:25:LYS:HB2	6:A:426:PEG:H11	2.00	0.43
1:A:25:LYS:HD2	6:A:426:PEG:H32	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:CG2	1:A:207:ARG:HG3	2.49	0.43
1:A:90:THR:O	1:A:210:ARG:HA	2.19	0.42
1:A:60:MET:SD	1:A:64:GLY:HA3	2.59	0.42
1:A:106:TYR:CZ	1:A:228:GLY:HA2	2.55	0.41
1:A:245:SER:OG	3:A:404:GOL:H12	2.21	0.41
1:A:211:GLU:OE1	4:A:420:EDO:H22	2.21	0.41
2:B:67:THR:OG1	2:B:70:GLU:HG3	2.20	0.41
1:A:76:THR:OG1	4:A:410:EDO:H21	2.20	0.41
1:A:17:THR:CG2	10:B:207:HOH:O	2.69	0.41
1:A:17:THR:HG21	10:B:207:HOH:O	2.22	0.40
1:A:245:SER:OG	3:A:404:GOL:C3	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/335 (91%)	295 (97%)	10 (3%)	0	100	100
2	B	75/94 (80%)	70 (93%)	2 (3%)	3 (4%)	3	0
All	All	380/429 (89%)	365 (96%)	12 (3%)	3 (1%)	19	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	0	MET
2	B	-2	SER
2	B	-1	HIS

### 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	264/283 (93%)	256 (97%)	8 (3%)	41	31
2	B	69/87 (79%)	65 (94%)	4 (6%)	20	10
All	All	333/370 (90%)	321 (96%)	12 (4%)	38	24

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	25	LYS
1	A	63	LEU
1	A	145[A]	LEU
1	A	145[B]	LEU
1	A	151	ASN
1	A	186	TYR
1	A	198	ASN
2	B	-2	SER
2	B	19	ARG
2	B	39	LEU
2	B	71	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	SEB	A	68	1	15,16,17	3.23	4 (26%)	15,21,23	1.47	1 (6%)

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
1	SEB	A	68	1	-	7/9/13/15	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	SEB	CE-SD	-10.35	1.68	1.78
1	A	68	SEB	OG-SD	5.06	1.71	1.56
1	A	68	SEB	OD2-SD	-2.40	1.37	1.44
1	A	68	SEB	OD1-SD	-2.25	1.38	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SEB	CB-OG-SD	4.91	129.77	119.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	SEB	CZ-CE-SD-OD2
1	A	68	SEB	CZ-CE-SD-OD1
1	A	68	SEB	CZ-CE-SD-OG
1	A	68	SEB	CB-OG-SD-CE
1	A	68	SEB	CB-OG-SD-OD1
1	A	68	SEB	SD-CE-CZ-CH2
1	A	68	SEB	CA-CB-OG-SD

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	68	SEB	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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	A	416	-	3,3,3	0.44	0	2,2,2	0.20	0
4	EDO	A	417	-	3,3,3	0.36	0	2,2,2	0.44	0
9	MPD	B	111	-	7,7,7	0.24	0	9,10,10	0.38	0
4	EDO	B	104	-	3,3,3	0.46	0	2,2,2	0.22	0
3	GOL	A	401	-	5,5,5	1.15	1 (20%)	5,5,5	0.85	0
6	PEG	A	423	-	6,6,6	0.54	0	5,5,5	0.36	0
4	EDO	A	418	-	3,3,3	0.35	0	2,2,2	0.83	0
4	EDO	A	411	-	3,3,3	0.43	0	2,2,2	0.19	0
4	EDO	A	415	-	3,3,3	0.54	0	2,2,2	0.05	0
4	EDO	A	413	-	3,3,3	0.55	0	2,2,2	0.31	0
6	PEG	A	427	-	6,6,6	0.47	0	5,5,5	0.36	0
9	MPD	B	110	-	7,7,7	0.30	0	9,10,10	0.50	0
4	EDO	A	410	-	3,3,3	0.54	0	2,2,2	0.09	0
9	MPD	B	112	-	7,7,7	0.30	0	9,10,10	0.36	0
3	GOL	A	405	-	5,5,5	1.15	0	5,5,5	0.94	0
4	EDO	B	103	-	3,3,3	0.43	0	2,2,2	0.17	0
6	PEG	A	422	-	6,6,6	0.52	0	5,5,5	0.33	0
6	PEG	A	425	-	6,6,6	0.48	0	5,5,5	0.82	0
4	EDO	A	412	-	3,3,3	0.43	0	2,2,2	0.39	0
3	GOL	A	406	-	5,5,5	1.02	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	420	-	3,3,3	0.41	0	2,2,2	0.29	0
6	PEG	A	426	-	6,6,6	0.50	0	5,5,5	0.75	0
5	SO4	B	108	-	4,4,4	0.11	0	6,6,6	0.16	0
4	EDO	A	414	-	3,3,3	0.45	0	2,2,2	0.34	0
6	PEG	A	424	-	6,6,6	0.50	0	5,5,5	0.40	0
6	PEG	B	109	-	6,6,6	0.49	0	5,5,5	0.47	0
4	EDO	A	419	-	3,3,3	0.62	0	2,2,2	0.27	0
5	SO4	A	421	-	4,4,4	0.16	0	6,6,6	0.09	0
3	GOL	A	402	-	5,5,5	0.81	0	5,5,5	1.08	0
3	GOL	B	101	-	5,5,5	0.90	0	5,5,5	1.03	0
4	EDO	A	409	-	3,3,3	0.48	0	2,2,2	0.26	0
4	EDO	A	408	-	3,3,3	0.47	0	2,2,2	0.56	0
5	SO4	B	107	-	4,4,4	0.14	0	6,6,6	0.13	0
3	GOL	A	404	-	5,5,5	1.27	0	5,5,5	1.09	1 (20%)
3	GOL	A	407	-	5,5,5	0.99	0	5,5,5	0.98	0
4	EDO	B	102	-	3,3,3	0.44	0	2,2,2	0.37	0
3	GOL	A	403	-	5,5,5	1.16	0	5,5,5	0.88	0
5	SO4	B	106	-	4,4,4	0.17	0	6,6,6	0.17	0
5	SO4	B	105	-	4,4,4	0.23	0	6,6,6	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
4	EDO	A	416	-	-	1/1/1/1	-
4	EDO	A	417	-	-	1/1/1/1	-
9	MPD	B	111	-	-	0/5/5/5	-
4	EDO	B	104	-	-	1/1/1/1	-
3	GOL	A	401	-	-	0/4/4/4	-
6	PEG	A	423	-	-	1/4/4/4	-
4	EDO	A	418	-	-	1/1/1/1	-
4	EDO	A	411	-	-	0/1/1/1	-
4	EDO	A	415	-	-	0/1/1/1	-
4	EDO	A	413	-	-	0/1/1/1	-
6	PEG	A	427	-	-	1/4/4/4	-
9	MPD	B	110	-	-	0/5/5/5	-
4	EDO	A	410	-	-	0/1/1/1	-
9	MPD	B	112	-	-	0/5/5/5	-
3	GOL	A	405	-	-	1/4/4/4	-
4	EDO	B	103	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	422	-	-	4/4/4/4	-
6	PEG	A	425	-	-	2/4/4/4	-
4	EDO	A	412	-	-	0/1/1/1	-
3	GOL	A	406	-	-	0/4/4/4	-
4	EDO	A	420	-	-	1/1/1/1	-
6	PEG	A	426	-	-	2/4/4/4	-
6	PEG	B	109	-	-	1/4/4/4	-
4	EDO	A	414	-	-	1/1/1/1	-
6	PEG	A	424	-	-	1/4/4/4	-
4	EDO	A	419	-	-	1/1/1/1	-
3	GOL	A	402	-	-	0/4/4/4	-
3	GOL	B	101	-	-	1/4/4/4	-
4	EDO	A	409	-	-	0/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
3	GOL	A	404	-	-	2/4/4/4	-
3	GOL	A	407	-	-	2/4/4/4	-
4	EDO	B	102	-	-	0/1/1/1	-
3	GOL	A	403	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GOL	O2-C2	-2.24	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	GOL	C3-C2-C1	-2.12	103.47	111.70

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	C1-C2-C3-O3
3	A	403	GOL	O1-C1-C2-C3
6	A	425	PEG	C4-C3-O2-C2
3	A	404	GOL	O2-C2-C3-O3
6	A	423	PEG	O2-C3-C4-O4
6	A	424	PEG	O2-C3-C4-O4
4	B	103	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-O2
6	A	422	PEG	C1-C2-O2-C3
4	A	417	EDO	O1-C1-C2-O2
6	B	109	PEG	C1-C2-O2-C3
6	A	422	PEG	O2-C3-C4-O4
6	A	425	PEG	C1-C2-O2-C3
6	A	427	PEG	O2-C3-C4-O4
6	A	422	PEG	O1-C1-C2-O2
4	A	420	EDO	O1-C1-C2-O2
6	A	426	PEG	C1-C2-O2-C3
3	A	405	GOL	O2-C2-C3-O3
4	A	416	EDO	O1-C1-C2-O2
4	B	104	EDO	O1-C1-C2-O2
3	A	407	GOL	O1-C1-C2-C3
3	A	407	GOL	O1-C1-C2-O2
6	A	422	PEG	C4-C3-O2-C2
4	A	414	EDO	O1-C1-C2-O2
6	A	426	PEG	O1-C1-C2-O2
3	B	101	GOL	O1-C1-C2-C3
4	A	418	EDO	O1-C1-C2-O2
4	A	419	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	410	EDO	1	0
4	A	420	EDO	1	0
6	A	426	PEG	7	0
6	B	109	PEG	2	0
3	A	404	GOL	4	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, 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	308/335 (91%)	0.15	15 (4%) 29 33	26, 40, 97, 195	0
2	B	77/94 (81%)	1.02	9 (11%) 4 5	35, 61, 146, 171	0
All	All	385/429 (89%)	0.32	24 (6%) 20 23	26, 43, 118, 195	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	-3	GLY	15.2
2	B	-1	HIS	9.0
2	B	0	MET	7.8
1	A	1	LEU	6.7
2	B	73	GLN	6.6
1	A	202	LYS	6.4
1	A	201	GLY	6.1
1	A	2	TYR	4.1
1	A	85	SER	3.7
2	B	-2	SER	3.7
1	A	203	ALA	3.4
2	B	72	VAL	3.4
2	B	2	TYR	3.3
1	A	200	THR	3.2
1	A	204	ALA	2.8
1	A	6	ILE	2.8
1	A	99	ARG	2.7
1	A	95	GLU	2.7
1	A	96	TRP	2.7
2	B	6	ILE	2.5
1	A	199	PRO	2.4
1	A	145[A]	LEU	2.3
1	A	198	ASN	2.2
2	B	67	THR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	SEB	A	68	16/17	0.90	0.18	35,198,249,286	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 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, 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
3	GOL	A	406	6/6	0.38	0.50	99,114,121,121	0
6	PEG	A	427	7/7	0.39	0.34	141,182,222,231	0
4	EDO	A	420	4/4	0.55	0.82	162,165,193,196	0
4	EDO	B	104	4/4	0.58	0.19	100,147,148,164	0
4	EDO	B	103	4/4	0.60	0.62	100,105,110,115	0
6	PEG	A	426	7/7	0.71	0.15	98,179,211,225	0
9	MPD	B	112	8/8	0.72	0.31	125,131,142,149	0
4	EDO	B	102	4/4	0.73	0.29	100,102,102,104	0
5	SO4	A	421	5/5	0.74	0.40	126,131,138,148	0
6	PEG	A	425	7/7	0.75	0.26	96,110,147,148	0
4	EDO	A	410	4/4	0.76	0.22	68,73,83,85	0
5	SO4	B	108	5/5	0.79	0.29	113,122,138,142	0
6	PEG	A	424	7/7	0.79	0.30	82,88,126,144	0
6	PEG	A	423	7/7	0.80	0.25	57,77,78,80	0
3	GOL	A	407	6/6	0.80	0.26	80,90,92,107	0
4	EDO	A	419	4/4	0.80	0.14	55,62,73,75	0
3	GOL	A	405	6/6	0.81	0.13	63,66,85,103	0
4	EDO	A	415	4/4	0.84	0.25	63,66,89,90	0
4	EDO	A	408	4/4	0.84	0.18	64,73,75,77	0
6	PEG	A	422	7/7	0.85	0.25	64,88,95,108	0
8	NA	A	429	1/1	0.85	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	101	6/6	0.86	0.30	72,82,90,92	0
4	EDO	A	417	4/4	0.87	0.20	89,89,92,100	0
4	EDO	A	418	4/4	0.87	0.19	62,68,73,89	0
4	EDO	A	413	4/4	0.88	0.12	59,67,81,86	0
6	PEG	B	109	7/7	0.88	0.10	60,75,77,81	0
4	EDO	A	416	4/4	0.90	0.27	69,72,82,90	0
3	GOL	A	404	6/6	0.90	0.23	49,92,114,124	0
4	EDO	A	411	4/4	0.91	0.15	51,59,60,70	0
4	EDO	A	409	4/4	0.92	0.27	66,66,77,86	0
7	CL	A	428	1/1	0.92	0.14	84,84,84,84	0
3	GOL	A	403	6/6	0.92	0.23	49,77,96,116	0
5	SO4	B	106	5/5	0.92	0.13	89,109,119,131	0
5	SO4	B	107	5/5	0.93	0.26	101,122,127,128	0
9	MPD	B	111	8/8	0.94	0.14	60,68,76,78	0
3	GOL	A	401	6/6	0.95	0.10	38,60,63,63	0
3	GOL	A	402	6/6	0.95	0.14	48,56,58,63	0
4	EDO	A	414	4/4	0.95	0.29	65,69,73,76	0
5	SO4	B	105	5/5	0.96	0.13	60,62,84,116	0
4	EDO	A	412	4/4	0.97	0.13	72,72,76,79	0
9	MPD	B	110	8/8	0.97	0.23	56,72,81,81	0

## 6.5 Other polymers

There are no such residues in this entry.