



Full wwPDB X-ray Structure Validation Report

Oct 2, 2014 – 05:41 PM EDT

PDB ID : 4UTR
Title : Crystal structure of zebrafish Sirtuin 5 in complex with glutarylated CPS1-peptide
Authors : Pannek, M.; Gertz, M.; Steegborn, C.
Deposited on : 2014-07-22
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

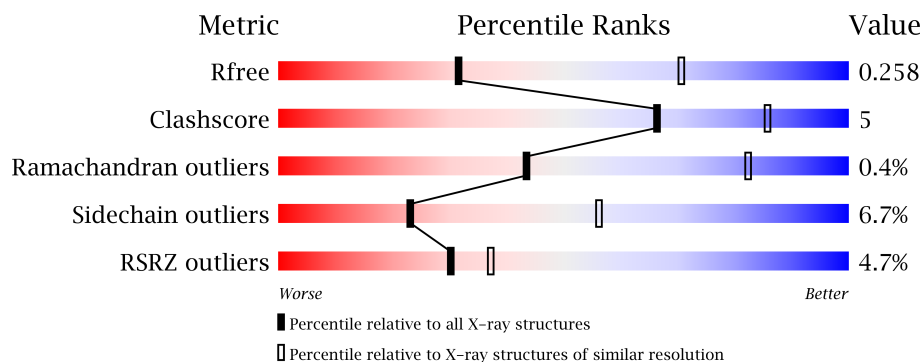
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance




The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	275	
1	B	275	
2	C	9	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4206 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	2	0
			2051	1293	371	372	15			
1	B	257	Total	C	N	O	S	0	1	0
			2003	1265	361	362	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP Q6DHI5
A	25	ILE	-	EXPRESSION TAG	UNP Q6DHI5
A	26	ASP	-	EXPRESSION TAG	UNP Q6DHI5
A	27	PRO	-	EXPRESSION TAG	UNP Q6DHI5
A	28	PHE	-	EXPRESSION TAG	UNP Q6DHI5
A	29	THR	-	EXPRESSION TAG	UNP Q6DHI5
B	24	GLY	-	EXPRESSION TAG	UNP Q6DHI5
B	25	ILE	-	EXPRESSION TAG	UNP Q6DHI5
B	26	ASP	-	EXPRESSION TAG	UNP Q6DHI5
B	27	PRO	-	EXPRESSION TAG	UNP Q6DHI5
B	28	PHE	-	EXPRESSION TAG	UNP Q6DHI5
B	29	THR	-	EXPRESSION TAG	UNP Q6DHI5

- Molecule 2 is a protein called GLUTARYL-CPS1 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			68	47	9	12			

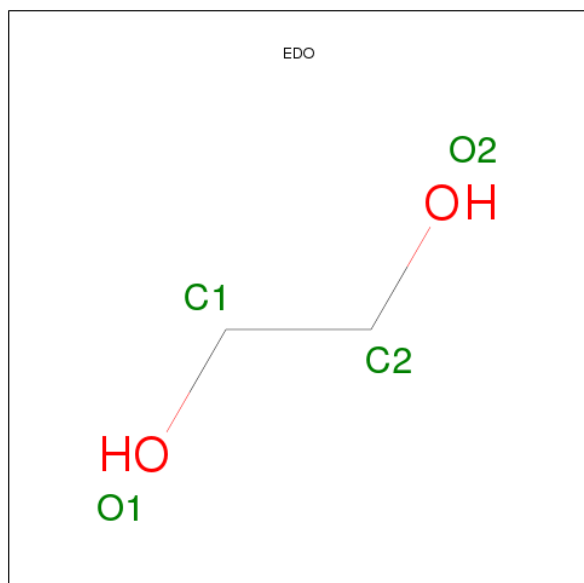
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	BEZ	-	BENZOYLATION	UNP Q5R209

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

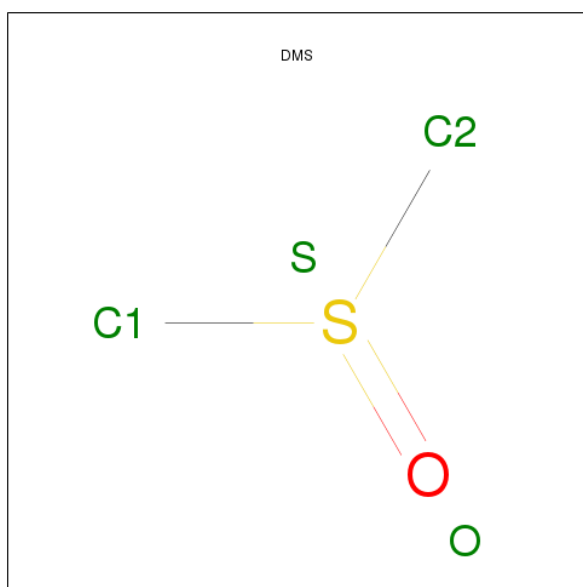
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).

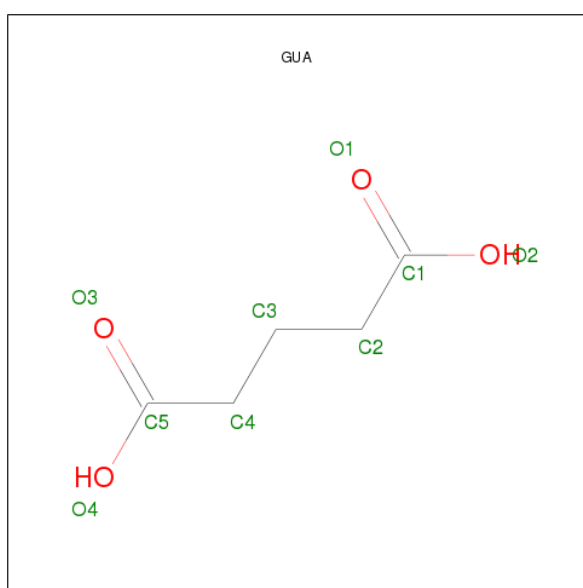


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is GLUTARIC ACID (three-letter code: GUA) (formula: C₅H₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			8	5	3		

- Molecule 8 is water.

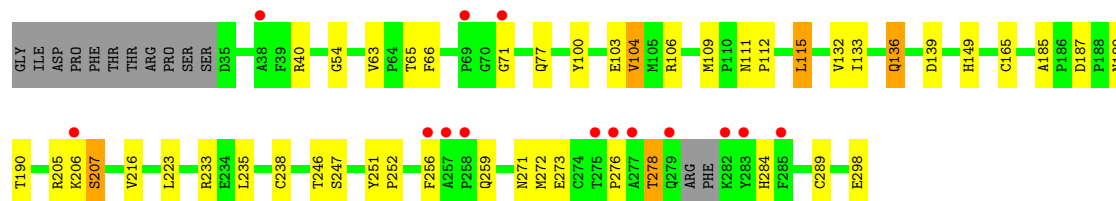
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	18	Total	O	0	0
			18	18		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

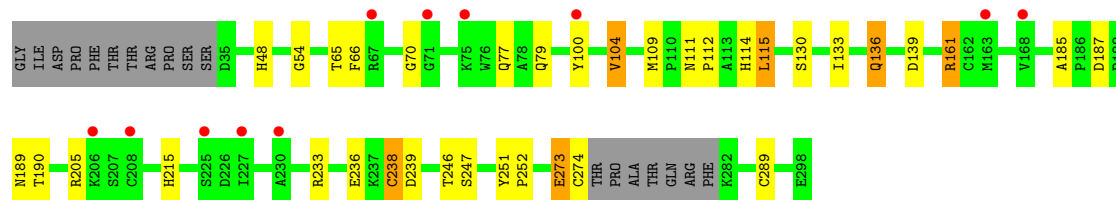
- Molecule 1: NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL

Chain A: 



- Molecule 1: NAD-DEPENDENT PROTEIN DEACYLASE SIRTUIN-5, MITOCHONDRIAL

Chain B: 



- Molecule 2: GLUTARYL-CPS1 PEPTIDE

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.22Å 87.22Å 314.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.53 – 2.90 75.53 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.53-2.90) 99.9 (75.53-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.213 , 0.262 0.217 , 0.258	Depositor DCC
R_{free} test set	830 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 16592 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4206	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: GUA, NA, ZN, EDO, BEZ, DMS

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	0.68	0/2106	0.88	3/2855 (0.1%)
1	B	0.66	0/2059	0.90	2/2789 (0.1%)
2	C	0.81	0/60	1.04	1/79 (1.3%)
All	All	0.67	0/4225	0.89	6/5723 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	LYS	CG-CD-CE	-5.62	95.06	111.90
1	B	161	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	115	LEU	CA-CB-CG	-5.57	102.48	115.30
1	B	115	LEU	CA-CB-CG	-5.30	103.11	115.30
1	A	63	VAL	CB-CA-C	-5.23	101.46	111.40
1	A	206	LYS	N-CA-C	-5.15	97.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	THR	Peptide
1	B	70	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2051	0	2007	24	0
1	B	2003	0	1968	21	0
2	C	68	0	66	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
5	B	4	0	6	0	0
6	B	1	0	0	0	0
7	C	8	0	0	0	0
8	A	39	0	0	1	0
8	B	18	0	0	0	0
All	All	4206	0	4065	42	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (42) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:132:VAL:HG12	1:A:149[B]:HIS:CD2	2.21	0.75
1:A:235:LEU:HD13	1:A:256:PHE:HB3	1.72	0.71
1:B:100:TYR:O	1:B:104:VAL:HG13	1.96	0.66
1:A:100:TYR:O	1:A:104:VAL:HG13	1.98	0.64
1:B:111:ASN:H	1:B:114:HIS:HD2	1.44	0.64
1:A:54:GLY:HA2	1:A:136:GLN:HG2	1.83	0.60
1:A:233:ARG:HD3	8:A:2037:HOH:O	2.01	0.60
1:A:115:LEU:HD11	1:B:115:LEU:HD11	1.82	0.60
1:A:71:GLY:O	1:A:77:GLN:HG2	2.03	0.57
1:A:165:CYS:SG	1:A:205:ARG:NH1	2.77	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:115:LEU:HB3	1:B:109:MET:HE2	1.89	0.54
1:A:103:GLU:OE1	1:A:106:ARG:NH1	2.41	0.53
1:B:111:ASN:H	1:B:114:HIS:CD2	2.26	0.53
1:B:65:THR:O	1:B:66:PHE:HB2	2.08	0.53
1:A:111:ASN:HB2	1:A:112:PRO:CD	2.39	0.52
1:A:251:TYR:CD2	1:A:252:PRO:HA	2.45	0.52
1:A:40:ARG:NH2	1:A:298:GLU:OXT	2.42	0.52
1:A:132:VAL:HG12	1:A:149[B]:HIS:CG	2.46	0.51
1:A:65:THR:O	1:A:66:PHE:HB2	2.11	0.50
1:B:251:TYR:CD1	1:B:252:PRO:HA	2.47	0.50
1:B:111:ASN:HB2	1:B:112:PRO:CD	2.41	0.50
1:A:235:LEU:CD1	1:A:256:PHE:HB3	2.42	0.48
1:B:54:GLY:HA2	1:B:136:GLN:HG2	1.95	0.48
1:A:185:ALA:HB3	1:A:190:THR:HG21	1.94	0.48
1:A:111:ASN:HB2	1:A:112:PRO:HD2	1.95	0.47
1:B:273:GLU:O	1:B:274:CYS:HB2	2.13	0.47
1:A:246:THR:OG1	1:A:247:SER:N	2.47	0.47
1:A:251:TYR:CD1	1:A:251:TYR:C	2.88	0.47
1:A:109:MET:HE2	1:B:115:LEU:HB3	1.96	0.46
1:B:185:ALA:HB3	1:B:190:THR:HG21	1.97	0.46
1:B:239:ASP:OD1	1:B:239:ASP:N	2.47	0.46
1:B:233:ARG:O	1:B:236:GLU:HG2	2.15	0.45
1:B:246:THR:OG1	1:B:247:SER:N	2.49	0.45
1:B:133:ILE:HD12	1:B:133:ILE:N	2.32	0.44
1:B:111:ASN:HB2	1:B:112:PRO:HD2	1.99	0.44
1:A:251:TYR:HB2	2:C:6:TYR:CE2	2.53	0.43
1:A:133:ILE:HD12	1:A:133:ILE:N	2.33	0.43
1:B:48[B]:HIS:HB3	1:B:238:CYS:HA	2.02	0.42
1:A:271:ASN:OD1	1:A:284:HIS:HE1	2.02	0.42
1:B:161:ARG:HH11	1:B:215:HIS:CE1	2.38	0.41
1:B:65:THR:O	1:B:66:PHE:CB	2.68	0.41
1:B:48[A]:HIS:HB2	1:B:238:CYS:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/275 (94%)	250 (96%)	8 (3%)	2 (1%)	27	68
1	B	254/275 (92%)	246 (97%)	8 (3%)	0	100	100
2	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	521/559 (93%)	502 (96%)	17 (3%)	2 (0%)	43	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	SER
1	A	276	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	219/229 (96%)	205 (94%)	14 (6%)	25	59
1	B	214/229 (93%)	202 (94%)	12 (6%)	30	66
2	C	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	439/464 (95%)	410 (93%)	29 (7%)	23	57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	136	GLN
1	A	139	ASP
1	A	187	ASP
1	A	189	ASN
1	A	207	SER
1	A	216	VAL
1	A	223	LEU
1	A	238	CYS
1	A	259	GLN

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Mol	Chain	Res	Type
1	A	272	MET
1	A	273	GLU
1	A	278	THR
1	A	289	CYS
1	B	77	GLN
1	B	79	GLN
1	B	104	VAL
1	B	130	SER
1	B	136	GLN
1	B	139	ASP
1	B	187	ASP
1	B	189	ASN
1	B	205	ARG
1	B	238	CYS
1	B	273	GLU
1	B	289	CYS
2	C	3	LEU
2	C	4	LYS
2	C	8	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	136	GLN
1	A	284	HIS
1	B	42	HIS
1	B	79	GLN
1	B	99	HIS
1	B	114	HIS
1	B	136	GLN
1	B	284	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	1301	-	3,3,3	0.62	0	2,2,2	0.60	0
4	EDO	A	1302	-	3,3,3	0.34	0	2,2,2	0.88	0
4	EDO	B	1300	-	3,3,3	0.60	0	2,2,2	0.24	0
5	DMS	B	1301	-	3,3,3	0.49	0	3,3,3	0.98	0
7	GUA	C	1299	2	7,7,8	7.12	2 (28%)	5,7,9	1.39	1 (20%)

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	1301	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1302	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1300	-	-	0/1/1/1	0/0/0/0
5	DMS	B	1301	-	-	0/0/0/0	0/0/0/0
7	GUA	C	1299	2	-	0/4/5/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1299	GUA	O3-C5	18.47	1.24	1.11
7	C	1299	GUA	C2-C1	2.45	1.56	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	C	1299	GUA	C3-C2-C1	-2.38	108.18	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	262/275 (95%)	0.45	14 (5%)	25 31	32, 52, 89, 126	0
1	B	257/275 (93%)	0.43	11 (4%)	34 40	34, 60, 105, 126	0
2	C	9/9 (100%)	0.02	0	100 100	44, 52, 67, 74	0
All	All	528/559 (94%)	0.43	25 (4%)	30 37	32, 55, 99, 126	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	6.4
1	A	279	GLN	6.3
1	A	275	THR	6.1
1	A	277	ALA	3.8
1	A	276	PRO	3.8
1	A	282	LYS	3.5
1	B	67	ARG	3.1
1	A	69	PRO	2.9
1	A	256	PHE	2.9
1	B	168	VAL	2.8
1	A	257	ALA	2.8
1	B	227	ILE	2.7
1	B	230	ALA	2.7
1	A	258	PRO	2.6
1	B	163	MET	2.6
1	A	38	ALA	2.5
1	A	283	TYR	2.5
1	B	206	LYS	2.5
1	B	75	LYS	2.3
1	A	206	LYS	2.2
1	B	100	TYR	2.2
1	B	208	CYS	2.1
1	A	285	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	2.1
1	B	225	SER	2.0

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	GUA	C	1299	8/9	0.28	1.93	44,53,65,67	0
4	EDO	B	1300	4/4	0.23	0.46	54,54,59,67	0
5	DMS	B	1301	4/4	0.20	0.21	47,49,52,54	0
3	ZN	A	1300	1/1	0.14	-0.46	44,44,44,44	0
4	EDO	A	1301	4/4	0.18	-0.52	52,55,56,60	0
4	EDO	A	1302	4/4	0.19	-0.66	56,57,57,57	0
6	NA	B	1302	1/1	0.17	-1.84	60,60,60,60	1
3	ZN	B	1299	1/1	0.07	-3.84	86,86,86,86	0

6.5 Other polymers

There are no such residues in this entry.