



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:48 PM GMT

PDB ID : 3ZST  
Title : GLGE ISOFORM 1 FROM STREPTOMYCES COELICOLOR WITH  
ALPHA-CYCLODEXTRIN BOUND  
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C.J.; Field, R.A.; Chater, K.F.; Lawson, D.M.; Bornemann, S.  
Deposited on : 2011-06-30  
Resolution : 2.30 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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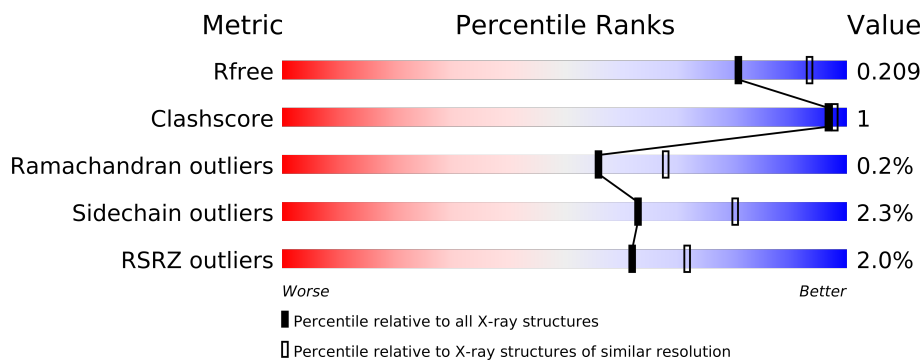
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	695	
1	B	695	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACX	A	700	-	X
2	ACX	B	700	-	X
3	EDO	A	750	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11175 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 PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISO-FORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	5	0
			5157	3260	937	950	10			
1	B	649	Total	C	N	O	S	0	5	0
			5151	3257	936	948	10			

There are 40 discrepancies between the modelled and reference sequences:

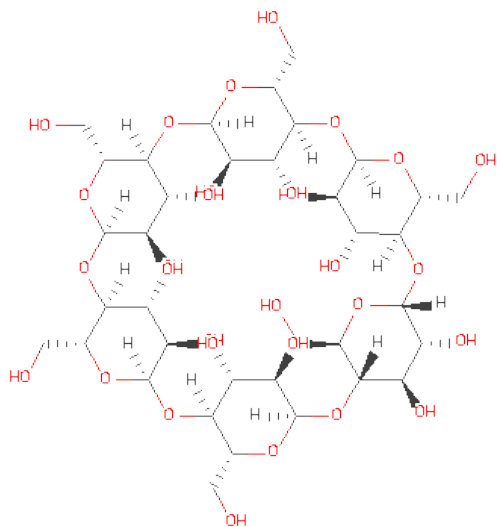
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
A	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
A	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
A	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
A	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
A	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
B	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2

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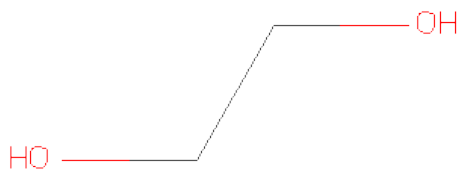
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
B	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
B	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
B	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2

- Molecule 2 is SUGAR (ALPHA-CYCLODEXTRIN (CYCLOHEXA-AMYLOSE)) (three-letter code: ACX) (formula:  $C_{36}H_{60}O_{30}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			66	36	30		
2	B	1	Total	C	O	0	0
			66	36	30		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 4 is water.

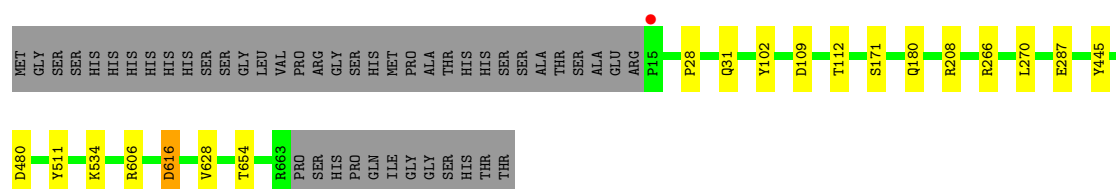
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	488	Total	O	0	0
			488	488		
4	B	243	Total	O	0	0
			243	243		

### 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.

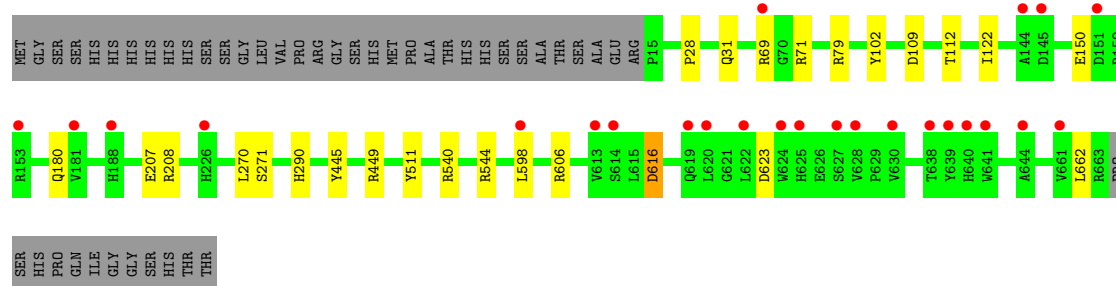
#### • Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISOFORM 1

Chain A: 



#### • Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A GLGE ISOFORM 1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.24Å 113.24Å 314.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.54 – 2.30 56.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (106.54-2.30) 93.4 (56.10-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.16 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.173 , 0.201 0.181 , 0.209	Depositor DCC
$R_{free}$ test set	4301 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 85748 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.80	1/5324 (0.0%)	0.78	4/7280 (0.1%)
1	B	0.71	0/5319	0.73	1/7275 (0.0%)
All	All	0.75	1/10643 (0.0%)	0.76	5/14555 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	GLU	CD-OE1	5.36	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	208	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	606	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	266[A]	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	266[B]	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5157	0	0	4	0
1	B	5151	0	0	6	0
2	A	66	0	60	1	0
2	B	66	0	60	2	0
3	A	4	0	6	0	0
4	A	488	0	0	0	0
4	B	243	0	0	2	0
All	All	11175	0	126	10	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 1.

All (10) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:445:TYR:CE1	2:B:700:ACX:H1A	2.51	0.46
1:A:480:ASP:OD1	1:A:534:LYS:NZ	2.50	0.44
1:A:445:TYR:CE1	2:A:700:ACX:H1E	2.53	0.44
1:B:28:PRO:O	1:B:102:TYR:OH	2.35	0.44
1:B:449:ARG:NH2	2:B:700:ACX:O2A	2.52	0.43
1:B:109:ASP:OD2	1:B:112:THR:OG1	2.37	0.42
1:A:28:PRO:O	1:A:102:TYR:OH	2.38	0.42
1:B:290:HIS:N	4:B:2143:HOH:O	2.52	0.42
1:B:540:ARG:NH1	4:B:2110:HOH:O	2.53	0.41
1:A:109:ASP:OD2	1:A:112:THR:OG1	2.39	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	652/695 (94%)	640 (98%)	11 (2%)	1 (0%)	56	68
1	B	652/695 (94%)	641 (98%)	10 (2%)	1 (0%)	56	68
All	All	1304/1390 (94%)	1281 (98%)	21 (2%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	616	ASP
1	A	616	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	539/575 (94%)	531 (98%)	8 (2%)	76	89
1	B	538/575 (94%)	520 (97%)	18 (3%)	50	66
All	All	1077/1150 (94%)	1051 (98%)	26 (2%)	63	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	171	SER
1	A	180	GLN
1	A	270	LEU
1	A	511	TYR
1	A	616	ASP
1	A	628	VAL
1	A	654	THR
1	B	31	GLN
1	B	69	ARG
1	B	71	ARG
1	B	79	ARG
1	B	122	ILE
1	B	150	GLU
1	B	180	GLN
1	B	207	GLU
1	B	270	LEU
1	B	271	SER
1	B	511	TYR
1	B	544	ARG
1	B	598	LEU
1	B	606[A]	ARG

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Mol	Chain	Res	Type
1	B	606[B]	ARG
1	B	616	ASP
1	B	623	ASP
1	B	662	LEU

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 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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACX	A	700	-	72,72,72	1.23	6 (8%)	108,108,108	1.59	25 (23%)
3	EDO	A	750	-	3,3,3	0.84	0	2,2,2	0.16	0
2	ACX	B	700	-	72,72,72	1.34	8 (11%)	108,108,108	1.43	16 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACX	A	700	-	-	0/36/156/156	0/0/7/7
3	EDO	A	750	-	-	0/1/1/1	0/0/0/0
2	ACX	B	700	-	-	0/36/156/156	0/0/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	ACX	O5A-C1A	3.64	1.51	1.41
2	A	700	ACX	O5E-C1E	3.17	1.50	1.41
2	B	700	ACX	O5E-C1E	3.01	1.49	1.41
2	B	700	ACX	O1E-C1E	2.64	1.48	1.41
2	A	700	ACX	O5A-C1A	2.58	1.48	1.41
2	B	700	ACX	C4C-C5C	2.56	1.60	1.52
2	A	700	ACX	O1E-C1E	2.50	1.48	1.41
2	B	700	ACX	O5E-C5E	2.42	1.50	1.44
2	A	700	ACX	O2E-C2E	2.30	1.48	1.43
2	A	700	ACX	O1E-C4F	2.12	1.49	1.43
2	B	700	ACX	O5C-C1C	2.11	1.47	1.41
2	B	700	ACX	O5B-C1B	2.08	1.47	1.41
2	A	700	ACX	C4A-C5A	2.04	1.58	1.52
2	B	700	ACX	O1B-C1B	2.03	1.47	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACX	O5C-C5C-C4C	4.62	119.35	109.70
2	A	700	ACX	O1A-C4B-C3B	-4.30	96.14	107.16
2	B	700	ACX	O1A-C1A-C2A	-4.09	98.32	108.12
2	B	700	ACX	O5E-C5E-C4E	4.06	118.18	109.70
2	A	700	ACX	C6F-C5F-C4F	-3.55	103.26	113.25
2	B	700	ACX	O5D-C5D-C6D	3.54	115.03	106.34
2	A	700	ACX	O5D-C5D-C4D	3.20	116.39	109.70
2	A	700	ACX	O5E-C1E-C2E	3.06	116.59	110.31
2	B	700	ACX	C1D-O5D-C5D	-3.06	107.78	113.73
2	A	700	ACX	C3A-C4A-C5A	2.95	117.49	110.85
2	A	700	ACX	C2E-C3E-C4E	2.94	116.00	109.61
2	A	700	ACX	O1C-C1C-C2C	2.88	115.04	108.12
2	B	700	ACX	C3A-C4A-C5A	2.84	117.23	110.85
2	A	700	ACX	O5A-C5A-C6A	2.82	113.28	106.34
2	A	700	ACX	O5F-C5F-C4F	-2.73	104.00	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACX	O5F-C1F-C2F	-2.70	104.77	110.31
2	B	700	ACX	O1E-C1E-O5E	2.64	117.27	110.69
2	A	700	ACX	O5D-C1D-C2D	2.62	115.69	110.31
2	B	700	ACX	O1A-C1A-O5A	2.59	117.14	110.69
2	A	700	ACX	O1A-C1A-O5A	-2.58	104.25	110.69
2	A	700	ACX	C3D-C4D-C5D	2.55	116.58	110.85
2	A	700	ACX	C1D-O1D-C4E	-2.53	111.53	117.99
2	B	700	ACX	C1E-O5E-C5E	2.50	118.59	113.73
2	A	700	ACX	O5A-C1A-C2A	2.48	115.40	110.31
2	A	700	ACX	C1E-C2E-C3E	-2.48	105.17	110.00
2	A	700	ACX	C6C-C5C-C4C	-2.45	106.35	113.25
2	B	700	ACX	O5B-C5B-C4B	-2.41	104.67	109.70
2	A	700	ACX	C1C-O5C-C5C	2.40	118.39	113.73
2	B	700	ACX	O5B-C5B-C6B	2.32	112.04	106.34
2	A	700	ACX	O1B-C4C-C3C	2.27	113.00	107.16
2	B	700	ACX	O5A-C5A-C6A	2.27	111.93	106.34
2	B	700	ACX	O5A-C1A-C2A	2.25	114.93	110.31
2	A	700	ACX	O5B-C5B-C4B	2.25	114.41	109.70
2	A	700	ACX	C3E-C4E-C5E	2.22	115.83	110.85
2	A	700	ACX	C3B-C4B-C5B	2.21	115.81	110.85
2	A	700	ACX	O1C-C1C-O5C	-2.14	105.35	110.69
2	B	700	ACX	O1C-C1C-C2C	2.12	113.20	108.12
2	A	700	ACX	O1E-C1E-C2E	-2.11	103.07	108.12
2	B	700	ACX	C2F-C3F-C4F	2.10	114.18	109.61
2	B	700	ACX	O5C-C5C-C6C	2.06	111.40	106.34
2	B	700	ACX	O5F-C5F-C4F	2.06	114.00	109.70

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, 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	649/695 (93%)	-0.47	1 (0%) 93 97	26, 36, 64, 103	0
1	B	649/695 (93%)	-0.06	25 (3%) 37 48	36, 53, 86, 121	0
All	All	1298/1390 (93%)	-0.27	26 (2%) 62 72	26, 46, 78, 121	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	TRP	4.0
1	B	144	ALA	3.9
1	B	661	VAL	3.8
1	B	628	VAL	3.4
1	B	627	SER	3.4
1	B	625	HIS	3.4
1	B	622	LEU	3.2
1	B	598	LEU	3.1
1	B	639	TYR	3.0
1	B	145	ASP	3.0
1	B	644	ALA	2.9
1	B	640	HIS	2.8
1	B	226	HIS	2.7
1	B	620	LEU	2.7
1	B	630	VAL	2.7
1	B	613	VAL	2.7
1	B	181	VAL	2.5
1	B	638	THR	2.3
1	B	151	ASP	2.3
1	B	614	SER	2.2
1	B	624	TRP	2.2
1	A	15	PRO	2.1
1	B	153	ARG	2.1
1	B	619	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	69	ARG	2.0
1	B	188	HIS	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACX	B	700	66/66	0.28	12.84	60,81,108,118	0
2	ACX	A	700	66/66	0.17	3.28	46,70,100,102	0
3	EDO	A	750	4/4	0.14	3.21	42,46,52,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.