



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2017 – 07:59 PM EDT

PDB ID : 3K8L  
Title : Crystal structure of SusG-D498N mutant with maltoheptaose  
Authors : Koropatkin, N.M.; Smith, T.J.  
Deposited on : unknown  
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

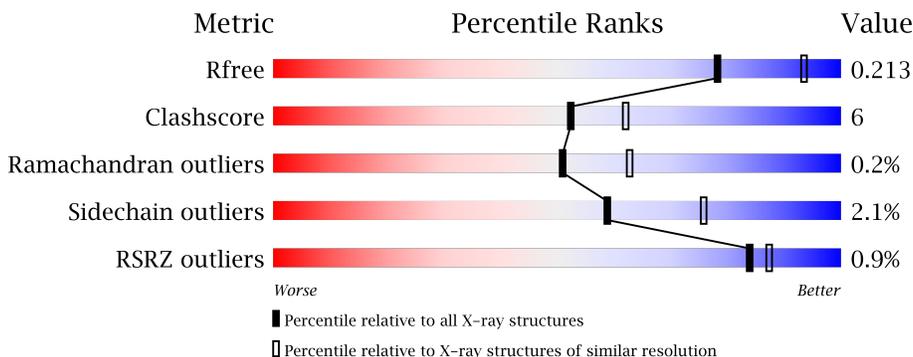
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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. 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	669	 85% 12% . .
1	B	669	 82% 14% . .

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
4	CEY	A	730	-	-	-	X
4	CEY	B	830	-	-	-	X
4	CEY	B	840	-	-	-	X
5	GLC	A	740	-	-	-	X
7	EDO	A	900	-	-	-	X
7	EDO	A	930	-	-	-	X
7	EDO	B	920	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11264 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 Alpha-amylase, susG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	649	5169	3288	836	1029	16	0	0	0
1	B	646	5146	3277	832	1021	16	0	0	0

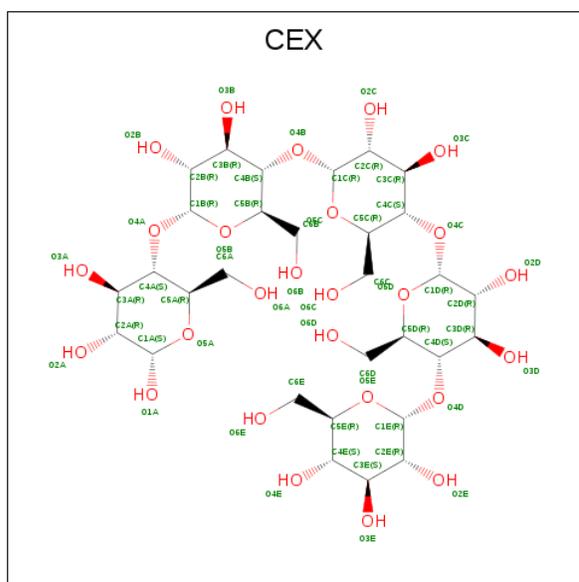
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ASN	ASP	ENGINEERED	UNP Q8A1G3
B	498	ASN	ASP	ENGINEERED	UNP Q8A1G3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

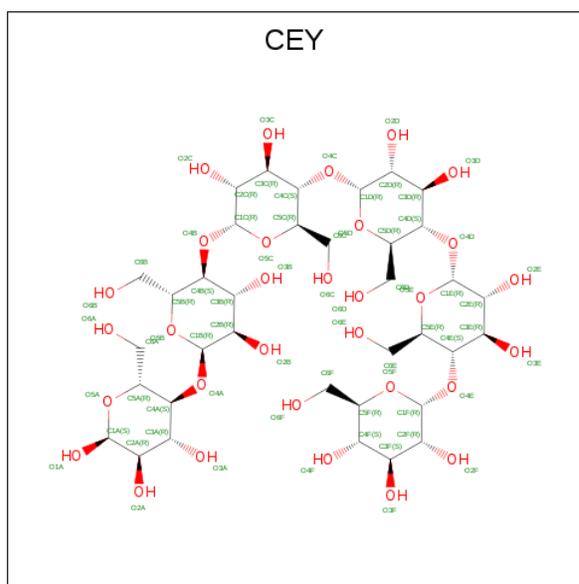
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Ca 2	0	0
2	A	2	Total 2	Ca 2	0	0

- Molecule 3 is alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (three-letter code: CEX) (formula: C<sub>30</sub>H<sub>52</sub>O<sub>26</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	1	0
			56	30	26		
3	B	1	Total	C	O	0	0
			56	30	26		

- Molecule 4 is alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranosyl-(1->4)-alpha-D-glucopyranose (three-letter code: CEY) (formula: C<sub>36</sub>H<sub>62</sub>O<sub>31</sub>).



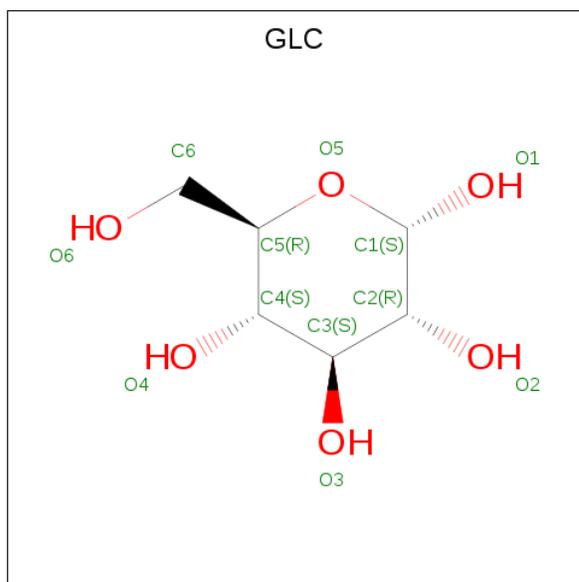
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	C	O	0	0
			67	36	31		

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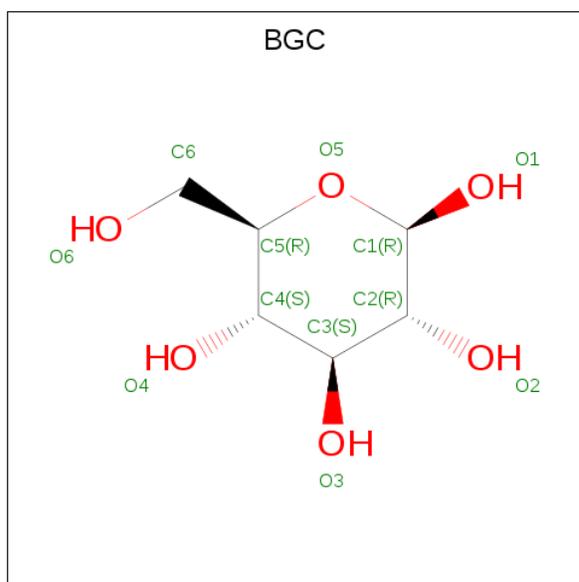
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			67	36	31		
4	B	1	Total	C	O	0	0
			67	36	31		

- Molecule 5 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



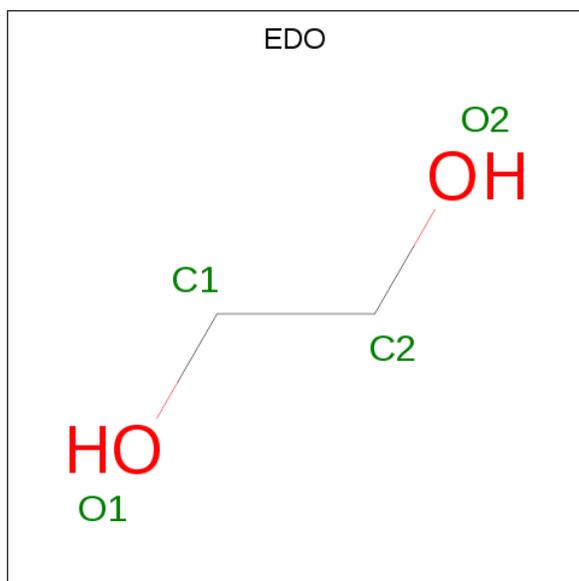
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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

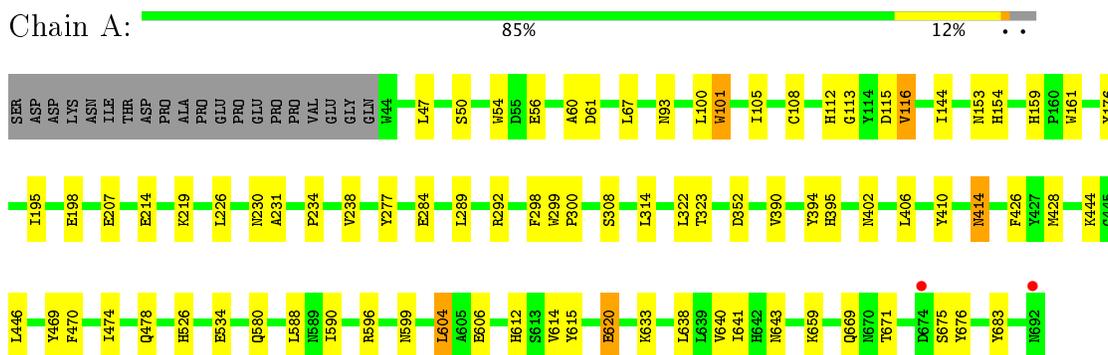
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	342	Total	O	0	0
			342	342		
8	B	196	Total	O	0	0
			196	196		

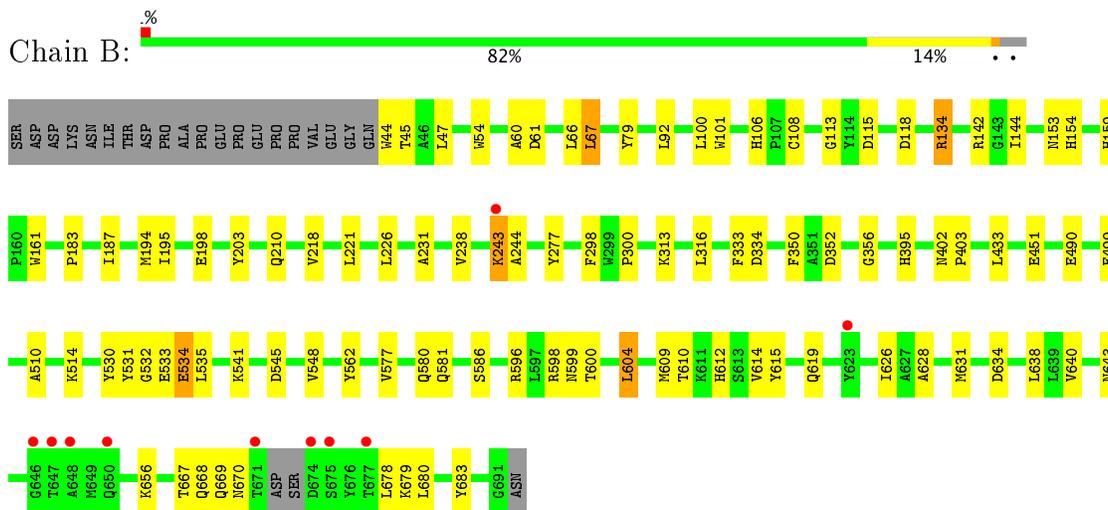
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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: Alpha-amylase, susG



- Molecule 1: Alpha-amylase, susG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.04Å 128.04Å 130.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 45.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.30) 92.2 (45.69-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.184 , 0.216 0.183 , 0.213	Depositor DCC
$R_{free}$ test set	8826 reflections (11.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h,-l,-k 0.005 for -h,l,k 0.006 for l,-k,h 0.019 for -l,-k,-h 0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: BGC, CA, GLC, EDO, CEY, CEX

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	0.35	0/5308	0.60	0/7214
1	B	0.33	0/5284	0.56	0/7181
All	All	0.34	0/10592	0.58	0/14395

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	5169	0	4872	55	0
1	B	5146	0	4856	71	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	56	0	52	1	0
3	B	56	0	52	1	0
4	A	67	0	62	2	0
4	B	134	0	124	2	0
5	A	66	0	55	1	0
6	A	12	0	11	0	0
7	A	12	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	6	1	0
8	A	342	0	0	3	0
8	B	196	0	0	2	0
All	All	11264	0	10108	131	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.

The worst 5 of 131 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:TYR:H	1:A:402:ASN:HD21	1.04	0.93
1:B:159:HIS:HD2	1:B:161:TRP:H	1.16	0.92
1:A:159:HIS:HD2	1:A:161:TRP:H	1.14	0.92
1:A:153:ASN:HD22	1:A:154:HIS:HD2	1.16	0.88
1:B:153:ASN:HD22	1:B:154:HIS:HD2	1.19	0.88

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	647/669 (97%)	621 (96%)	25 (4%)	1 (0%)	51 63
1	B	642/669 (96%)	603 (94%)	38 (6%)	1 (0%)	51 63
All	All	1289/1338 (96%)	1224 (95%)	63 (5%)	2 (0%)	51 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ALA

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Mol	Chain	Res	Type
1	B	231	ALA

### 5.3.2 Protein sidechains [i](#)

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	550/568 (97%)	536 (98%)	14 (2%)	53 70
1	B	547/568 (96%)	538 (98%)	9 (2%)	68 82
All	All	1097/1136 (97%)	1074 (98%)	23 (2%)	59 76

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	GLU
1	A	604	LEU
1	B	604	LEU
1	A	590	ILE
1	A	620	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	580	GLN
1	A	608	ASN
1	B	599	ASN
1	A	581	GLN
1	A	589	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
3	CEX	A	720	-	60,60,60	1.02	4 (6%)	89,89,89	0.88	1 (1%)
4	CEY	A	730	-	72,72,72	1.06	6 (8%)	107,107,107	0.88	2 (1%)
5	GLC	A	740	5	11,11,12	1.23	1 (9%)	13,15,17	0.71	0
5	GLC	A	741	5	11,11,12	1.52	2 (18%)	13,15,17	1.14	2 (15%)
5	GLC	A	742	5	11,11,12	1.33	3 (27%)	13,15,17	0.72	0
5	GLC	A	743	5	11,11,12	1.22	1 (9%)	13,15,17	1.12	0
5	GLC	A	744	5	11,11,12	1.16	0	13,15,17	0.70	0
5	GLC	A	745	5,6	11,11,12	0.89	0	13,15,17	0.87	0
6	BGC	A	746	5	12,12,12	0.96	0	17,17,17	0.83	0
7	EDO	A	900	-	3,3,3	0.72	0	2,2,2	0.38	0
7	EDO	A	910	-	3,3,3	0.65	0	2,2,2	0.40	0
7	EDO	A	930	-	3,3,3	0.74	0	2,2,2	0.37	0
3	CEX	B	820	-	60,60,60	1.03	3 (5%)	89,89,89	0.87	3 (3%)
4	CEY	B	830	-	72,72,72	1.23	8 (11%)	107,107,107	0.93	3 (2%)
4	CEY	B	840	-	72,72,72	1.11	4 (5%)	107,107,107	0.99	3 (2%)
7	EDO	B	920	-	3,3,3	0.76	0	2,2,2	0.34	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
3	CEX	A	720	-	-	0/26/126/126	0/5/5/5
4	CEY	A	730	-	-	0/32/152/152	0/6/6/6
5	GLC	A	740	5	-	0/2/19/22	0/1/1/1
5	GLC	A	741	5	-	0/2/19/22	0/1/1/1
5	GLC	A	742	5	-	0/2/19/22	0/1/1/1
5	GLC	A	743	5	-	0/2/19/22	0/1/1/1
5	GLC	A	744	5	-	0/2/19/22	0/1/1/1
5	GLC	A	745	5,6	-	0/2/19/22	0/1/1/1
6	BGC	A	746	5	-	0/2/22/22	0/1/1/1
7	EDO	A	900	-	-	0/1/1/1	0/0/0/0
7	EDO	A	910	-	-	0/1/1/1	0/0/0/0
7	EDO	A	930	-	-	0/1/1/1	0/0/0/0
3	CEX	B	820	-	-	0/26/126/126	0/5/5/5
4	CEY	B	830	-	-	0/32/152/152	0/6/6/6
4	CEY	B	840	-	-	0/32/152/152	0/6/6/6
7	EDO	B	920	-	-	0/1/1/1	0/0/0/0

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	830	CEY	O5A-C1A	2.00	1.46	1.43
4	A	730	CEY	O5C-C1C	2.05	1.46	1.41
4	A	730	CEY	O5E-C1E	2.06	1.46	1.41
4	A	730	CEY	O5F-C1F	2.07	1.47	1.41
4	B	840	CEY	O5E-C1E	2.08	1.47	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	840	CEY	C1B-O4A-C4A	-4.51	107.00	118.00
4	B	840	CEY	C1C-O4B-C4B	-3.71	108.96	118.00
4	A	730	CEY	C1F-O4E-C4E	-3.34	109.86	118.00
4	B	830	CEY	C1F-O4E-C4E	-3.34	109.86	118.00
4	B	840	CEY	C1F-O4E-C4E	-3.15	110.32	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	720	CEX	1	0
4	A	730	CEY	2	0
5	A	743	GLC	1	0
5	A	744	GLC	1	0
7	A	900	EDO	1	0
7	A	930	EDO	1	0
3	B	820	CEX	1	0
4	B	840	CEY	2	0
7	B	920	EDO	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	649/669 (97%)	-0.48	2 (0%) 93 96	15, 26, 44, 67	0
1	B	646/669 (96%)	-0.18	10 (1%) 74 78	20, 37, 54, 69	0
All	All	1295/1338 (96%)	-0.33	12 (0%) 84 87	15, 31, 52, 69	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	675	SER	3.4
1	A	692	ASN	3.4
1	B	674	ASP	3.2
1	B	677	THR	2.9
1	B	646	GLY	2.7

### 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	A	930	4/4	0.89	0.22	13.48	53,57,57,59	0
7	EDO	B	920	4/4	0.84	0.24	9.19	53,53,54,55	0
7	EDO	A	900	4/4	0.92	0.18	5.13	45,46,47,49	0
4	CEY	A	730	67/67	0.91	0.14	4.79	30,50,65,68	0
5	GLC	A	740	11/12	0.78	0.20	4.23	47,51,52,53	0
4	CEY	B	830	67/67	0.80	0.21	2.86	51,63,75,76	0
4	CEY	B	840	67/67	0.83	0.19	2.23	32,47,70,72	0
7	EDO	A	910	4/4	0.93	0.14	1.05	41,42,43,43	0
2	CA	A	700	1/1	0.98	0.10	1.03	31,31,31,31	0
3	CEX	A	720	56/56	0.90	0.13	0.55	27,41,65,66	1
5	GLC	A	743	11/12	0.94	0.14	0.52	21,23,25,26	0
3	CEX	B	820	56/56	0.93	0.14	0.44	22,43,70,71	0
5	GLC	A	742	11/12	0.95	0.14	0.43	22,23,29,34	0
5	GLC	A	744	11/12	0.96	0.14	0.40	24,27,29,35	0
2	CA	B	800	1/1	0.97	0.09	-0.85	37,37,37,37	0
2	CA	B	810	1/1	0.99	0.08	-2.11	29,29,29,29	0
2	CA	A	710	1/1	0.99	0.07	-3.81	16,16,16,16	0
6	BGC	A	746	12/12	0.84	0.19	-	48,58,60,61	0
5	GLC	A	745	11/12	0.96	0.12	-	35,40,43,45	0
5	GLC	A	741	11/12	0.82	0.16	-	40,43,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.