WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 10:56 am GMT

PDB ID	:	4AZH
Title	:	Differential inhibition of the tandem GH20 catalytic modules in the pneumo-coccal exo-beta-D-N-acetylglucosaminidase, StrH
Authors	:	Pluvinage, B.; Stubbs, K.A.; Vocadlo, D.J.; Boraston, A.B.
Deposited on	:	2012-06-26
Resolution	:	2.22 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

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 2.22 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.
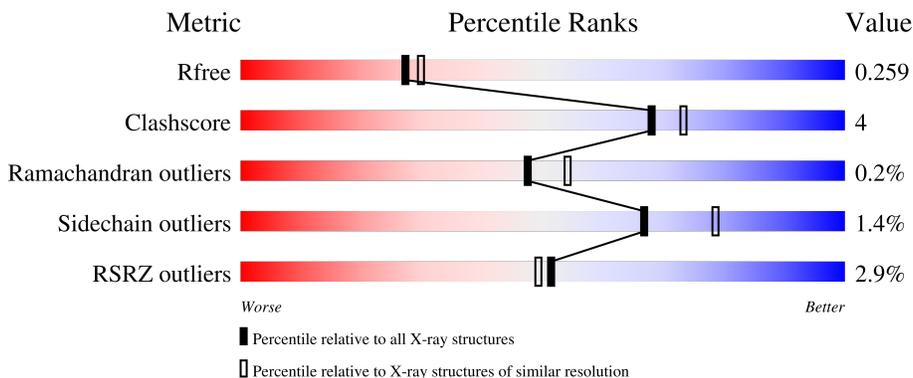
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 >=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 <=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	443	4% / 86% 9% 5%
1	B	443	3% / 82% 12% 5%
1	C	443	2% / 84% 9% 7%
1	D	443	2% / 85% 7% · 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 14690 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	1	4	0
			3361	2152	548	649	12			
1	B	419	Total	C	N	O	S	3	3	0
			3346	2144	545	645	12			
1	C	414	Total	C	N	O	S	0	3	0
			3302	2118	537	635	12			
1	D	411	Total	C	N	O	S	7	2	0
			3276	2100	534	630	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	622	ARG	-	expression tag	UNP P49610
A	623	GLY	-	expression tag	UNP P49610
A	624	SER	-	expression tag	UNP P49610
A	625	HIS	-	expression tag	UNP P49610
A	626	MET	-	expression tag	UNP P49610
B	622	ARG	-	expression tag	UNP P49610
B	623	GLY	-	expression tag	UNP P49610
B	624	SER	-	expression tag	UNP P49610
B	625	HIS	-	expression tag	UNP P49610
B	626	MET	-	expression tag	UNP P49610
C	622	ARG	-	expression tag	UNP P49610
C	623	GLY	-	expression tag	UNP P49610
C	624	SER	-	expression tag	UNP P49610
C	625	HIS	-	expression tag	UNP P49610
C	626	MET	-	expression tag	UNP P49610
D	622	ARG	-	expression tag	UNP P49610
D	623	GLY	-	expression tag	UNP P49610
D	624	SER	-	expression tag	UNP P49610
D	625	HIS	-	expression tag	UNP P49610
D	626	MET	-	expression tag	UNP P49610

- Molecule 2 is N-acetylglucosaminono-1,5-lactone (Z)-oxime (three-letter code: LOG) (formula: $C_8H_{14}N_2O_6$).
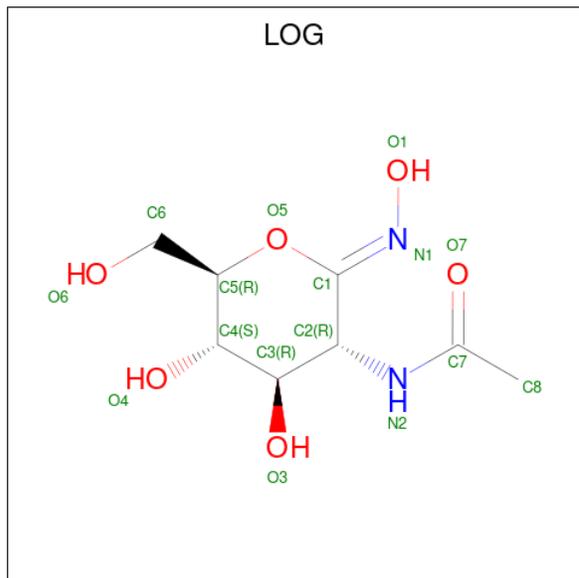
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	8	2	6		
2	B	1	Total	C	N	O	0	0
			16	8	2	6		
2	C	1	Total	C	N	O	0	0
			16	8	2	6		
2	D	1	Total	C	N	O	0	0
			16	8	2	6		

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

EDO

O2

OH

C1

C2

HO

O1
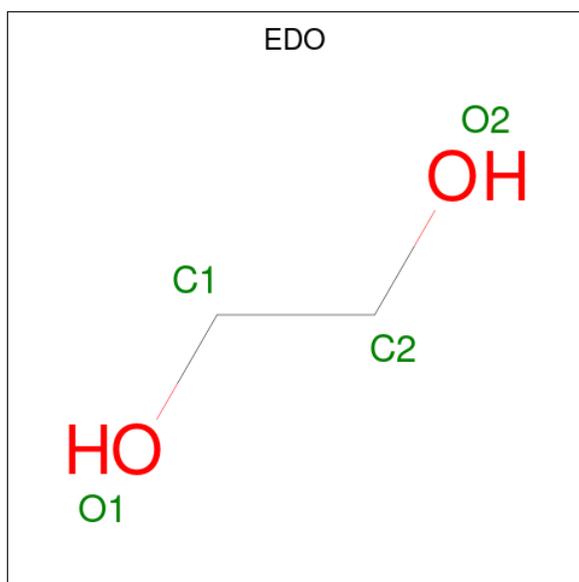
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	355	Total 355	O 355	0	0
4	B	310	Total 310	O 310	0	0
4	C	330	Total 330	O 330	0	0
4	D	298	Total 298	O 298	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: BETA-N-ACETYLHEXOSAMINIDASE
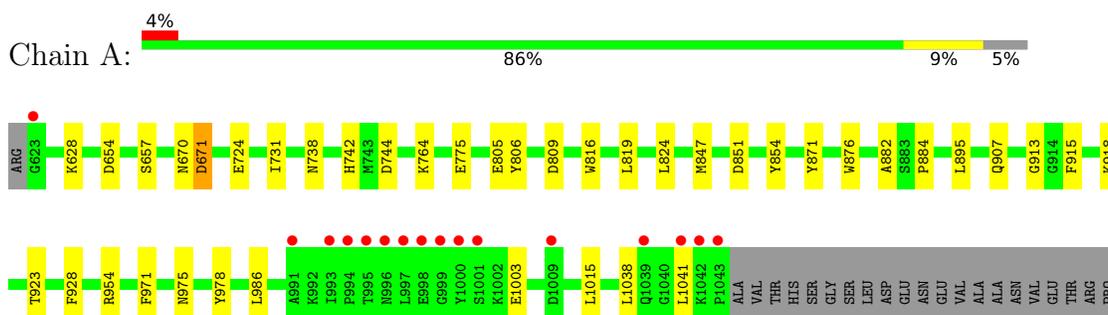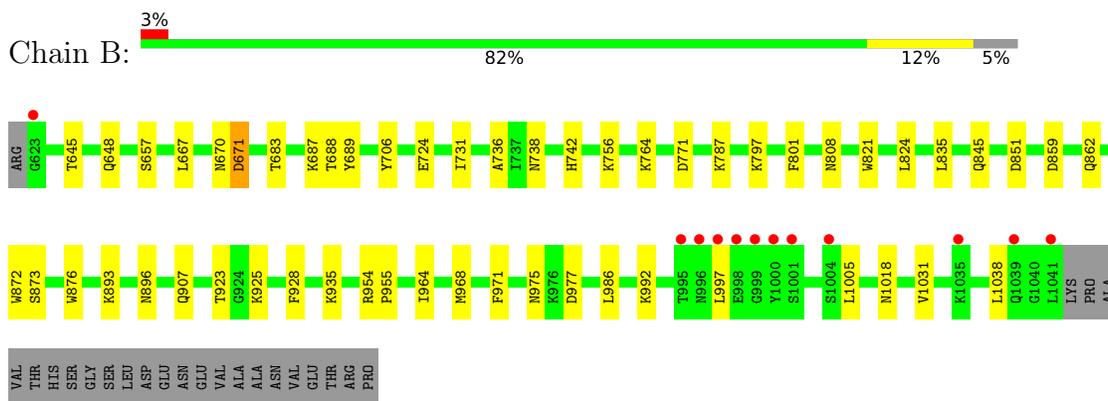
Chain A:

• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain B:

• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain C:

• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain D:

ARG GLY S624 K633 S636 G640 D654 E658 N670 D678 Q716 D744 M750 I755 D763 K767 K773 Y806 A807 N808 G815 W816 K820 W821 K827 D860 W876 K917 F928 S949 N975 K976 D977 N982

L986 A991 K992 I993 PRO THR ASN LEU GLU G999 Y1000 S1001 S1004 L1005 E1006 A1007 L1008 V1031 A1032 A1037 L1038 Q1039 GLY LEU LYS PRO ALA VAL THR HIS SER GLY SER LEU ASP GLU ASN GLU VAL ALA ALA ASN VAL GLU THR ARG PRO
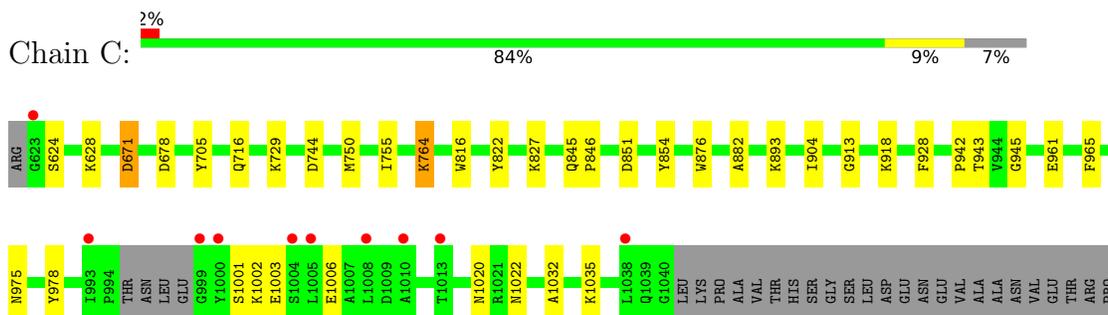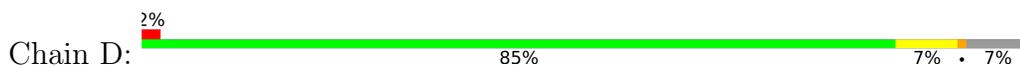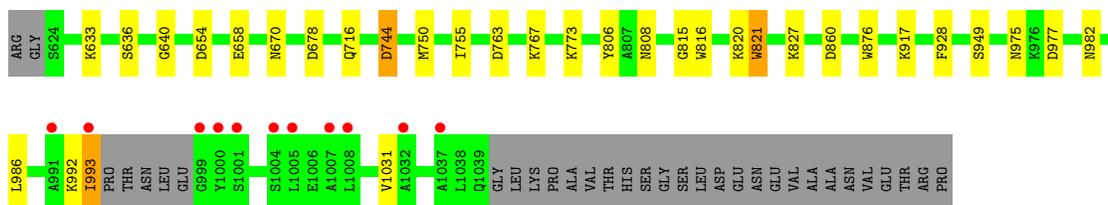
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.51Å 115.97Å 133.09Å 90.00° 99.85° 90.00°	Depositor
Resolution (Å)	43.71 – 2.22 43.71 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.71-2.22) 99.9 (43.71-2.22)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.259 0.197 , 0.259	Depositor DCC
R_{free} test set	4975 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14690	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2715e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: LOG, 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	0.67	2/3437 (0.1%)	0.71	0/4646
1	B	1.04	6/3424 (0.2%)	0.77	2/4627 (0.0%)
1	C	0.67	2/3379 (0.1%)	0.72	1/4565 (0.0%)
1	D	0.80	6/3352 (0.2%)	0.77	5/4528 (0.1%)
All	All	0.81	16/13592 (0.1%)	0.74	8/18366 (0.0%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	925	LYS	CE-NZ	-38.90	0.51	1.49
1	B	764	LYS	CE-NZ	-24.34	0.88	1.49
1	D	827	LYS	CE-NZ	-23.70	0.89	1.49
1	B	756	LYS	CE-NZ	-14.79	1.12	1.49
1	D	917	LYS	CG-CD	-13.40	1.06	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	925	LYS	CD-CE-NZ	17.56	152.08	111.70
1	D	827	LYS	CD-CE-NZ	14.53	145.11	111.70
1	B	764	LYS	CD-CE-NZ	13.97	143.84	111.70
1	D	917	LYS	CB-CG-CD	9.18	135.47	111.60
1	D	773	LYS	CD-CE-NZ	-7.88	93.57	111.70

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	3361	0	3259	23	0
1	B	3346	0	3265	33	0
1	C	3302	0	3218	26	0
1	D	3276	0	3187	14	0
2	A	16	0	14	2	0
2	B	16	0	14	0	0
2	C	16	0	14	0	0
2	D	16	0	14	0	0
3	A	16	0	24	2	0
3	B	8	0	12	5	0
3	C	24	0	36	2	0
4	A	355	0	0	5	0
4	B	310	0	0	9	0
4	C	330	0	0	6	0
4	D	298	0	0	1	0
All	All	14690	0	13057	99	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 4.

The worst 5 of 99 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:C:1003:GLU:HA	1:C:1006:GLU:HG2	1.36	1.07
1:C:943:THR:HG22	1:C:945:GLY:H	1.33	0.93
1:D:820:LYS:HE3	4:D:3138:HOH:O	1.72	0.89
1:B:787:LYS:HE3	4:B:3047:HOH:O	1.74	0.87
1:D:678:ASP:H	1:D:716:GLN:HE21	1.22	0.86

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	423/443 (96%)	407 (96%)	15 (4%)	1 (0%)	47	54
1	B	420/443 (95%)	400 (95%)	18 (4%)	2 (0%)	29	30
1	C	413/443 (93%)	393 (95%)	19 (5%)	1 (0%)	47	54
1	D	409/443 (92%)	389 (95%)	20 (5%)	0	100	100
All	All	1665/1772 (94%)	1589 (95%)	72 (4%)	4 (0%)	47	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671	ASP
1	B	896	ASN
1	B	671	ASP
1	C	671	ASP

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	344/364 (94%)	341 (99%)	3 (1%)	78	87
1	B	345/364 (95%)	339 (98%)	6 (2%)	60	73
1	C	339/364 (93%)	334 (98%)	5 (2%)	65	76
1	D	336/364 (92%)	330 (98%)	6 (2%)	59	71
All	All	1364/1456 (94%)	1344 (98%)	20 (2%)	67	76

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	633	LYS
1	D	860	ASP
1	D	993	ILE
1	D	977	ASP
1	B	851	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	761	HIS
1	D	808	ASN
1	D	975	ASN
1	B	742	HIS
1	B	670	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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
3	EDO	C	2044	-	3,3,3	0.39	0	2,2,2	0.49	0
2	LOG	C	2041	-	14,16,16	1.56	3 (21%)	14,22,22	1.38	3 (21%)
2	LOG	B	2042	-	14,16,16	1.29	2 (14%)	14,22,22	1.31	3 (21%)
3	EDO	A	2047	-	3,3,3	0.39	0	2,2,2	0.54	0
3	EDO	C	2043	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	C	2046	-	3,3,3	0.36	0	2,2,2	0.69	0
3	EDO	C	2045	-	3,3,3	0.39	0	2,2,2	0.50	0
3	EDO	C	2047	-	3,3,3	0.56	0	2,2,2	0.17	0
3	EDO	A	2046	-	3,3,3	0.51	0	2,2,2	0.74	0
3	EDO	A	2048	-	3,3,3	0.47	0	2,2,2	0.35	0
3	EDO	B	2043	-	3,3,3	0.40	0	2,2,2	0.38	0
3	EDO	B	2044	-	3,3,3	0.53	0	2,2,2	0.21	0
2	LOG	D	2040	-	14,16,16	1.63	1 (7%)	14,22,22	1.22	1 (7%)
3	EDO	C	2042	-	3,3,3	0.59	0	2,2,2	0.18	0
2	LOG	A	2044	-	14,16,16	1.83	3 (21%)	14,22,22	1.29	2 (14%)
3	EDO	A	2045	-	3,3,3	0.46	0	2,2,2	0.33	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	EDO	C	2044	-	-	0/1/1/1	-
2	LOG	C	2041	-	-	1/6/28/28	0/1/1/1
2	LOG	B	2042	-	-	2/6/28/28	0/1/1/1
3	EDO	A	2047	-	-	1/1/1/1	-
3	EDO	C	2043	-	-	1/1/1/1	-
3	EDO	C	2046	-	-	0/1/1/1	-
3	EDO	C	2045	-	-	1/1/1/1	-
3	EDO	C	2047	-	-	1/1/1/1	-
3	EDO	A	2046	-	-	0/1/1/1	-
3	EDO	A	2048	-	-	0/1/1/1	-
3	EDO	B	2043	-	-	1/1/1/1	-
3	EDO	B	2044	-	-	1/1/1/1	-
2	LOG	D	2040	-	-	1/6/28/28	0/1/1/1
3	EDO	C	2042	-	-	1/1/1/1	-
2	LOG	A	2044	-	-	1/6/28/28	0/1/1/1
3	EDO	A	2045	-	-	1/1/1/1	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2044	LOG	O5-C5	-5.17	1.39	1.46
2	D	2040	LOG	O5-C5	-4.98	1.39	1.46
2	C	2041	LOG	O5-C5	-3.70	1.41	1.46
2	C	2041	LOG	O5-C1	2.82	1.41	1.36
2	A	2044	LOG	O3-C3	2.80	1.49	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2040	LOG	O5-C1-C2	2.91	126.33	118.10
2	A	2044	LOG	O5-C1-C2	2.83	126.10	118.10
2	C	2041	LOG	O5-C1-C2	2.64	125.56	118.10
2	B	2042	LOG	O5-C1-C2	2.57	125.34	118.10
2	C	2041	LOG	C3-C4-C5	-2.51	105.76	110.24

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2045	EDO	O1-C1-C2-O2
3	B	2043	EDO	O1-C1-C2-O2
3	B	2044	EDO	O1-C1-C2-O2
3	C	2042	EDO	O1-C1-C2-O2
3	C	2043	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2047	EDO	1	0
3	C	2046	EDO	1	0
3	C	2045	EDO	1	0
3	B	2043	EDO	3	0
3	B	2044	EDO	2	0
2	A	2044	LOG	2	0
3	A	2045	EDO	2	0

5.7 Other polymers ⓘ

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, 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	421/443 (95%)	-0.33	16 (3%)	40	38	6, 13, 46, 94	12 (2%)
1	B	419/443 (94%)	-0.34	12 (2%)	51	49	9, 16, 44, 85	11 (2%)
1	C	414/443 (93%)	-0.38	10 (2%)	59	57	6, 13, 46, 84	15 (3%)
1	D	411/443 (92%)	-0.38	11 (2%)	54	52	9, 16, 46, 77	13 (3%)
All	All	1665/1772 (93%)	-0.36	49 (2%)	51	49	6, 14, 46, 94	51 (3%)

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	997	LEU	5.7
1	B	997	LEU	5.6
1	C	1004	SER	5.4
1	A	1043	PRO	4.9
1	D	1000	TYR	4.6

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 monosaccharides 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, 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	2048	4/4	0.62	0.35	81,84,87,91	0
3	EDO	C	2047	4/4	0.82	0.24	38,42,42,44	0
3	EDO	C	2044	4/4	0.88	0.22	31,32,33,34	0
3	EDO	C	2046	4/4	0.89	0.23	33,34,34,38	0
3	EDO	C	2042	4/4	0.90	0.13	23,23,25,26	0
3	EDO	C	2045	4/4	0.91	0.15	36,38,39,42	0
3	EDO	A	2047	4/4	0.92	0.14	31,33,35,35	0
3	EDO	A	2046	4/4	0.94	0.12	27,28,28,28	0
3	EDO	B	2043	4/4	0.95	0.19	23,24,25,25	0
3	EDO	A	2045	4/4	0.96	0.13	20,22,22,23	0
3	EDO	B	2044	4/4	0.96	0.14	23,23,25,26	0
2	LOG	D	2040	16/16	0.96	0.10	13,14,17,19	1
3	EDO	C	2043	4/4	0.96	0.11	27,28,28,29	0
2	LOG	B	2042	16/16	0.97	0.10	12,13,14,16	1
2	LOG	C	2041	16/16	0.97	0.12	10,10,12,14	1
2	LOG	A	2044	16/16	0.97	0.10	8,8,9,10	1

6.5 Other polymers ⓘ

There are no such residues in this entry.