WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2024 – 10:15 pm BST

PDB ID	:	8RU4
Title	:	Crystal structure of Human Catenin Beta-1 in complex with stitched peptide inhibitor
Authors	:	Yeste Vazquez, A.; Klintrot, C.I.R.; Grossmann, T.N.; Hennig, S.
Deposited on	:	2024-01-30
Resolution	:	2.13 Å(reported)

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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.13 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		16.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
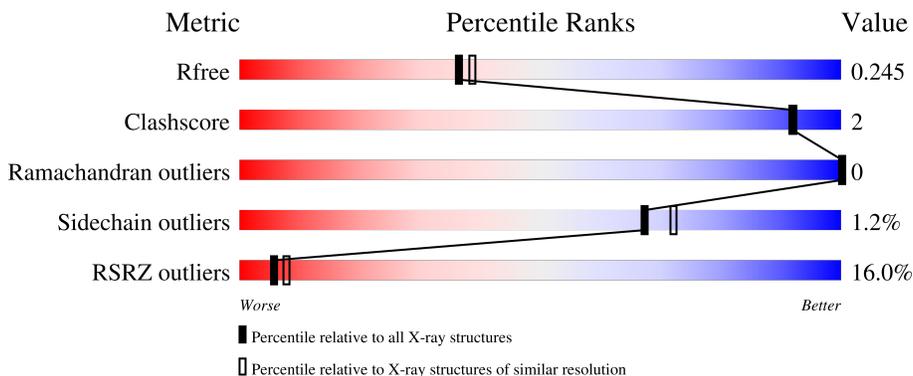
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3336 (2.16-2.12)
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)
RSRZ outliers	164620	3337 (2.16-2.12)

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	523	14% / 92%
1	B	523	16% / 92%
2	C	13	23% / 77% / 23%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 8174 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 Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total 3818	C 2400	N 693	O 699	S 26	0	1	0
1	B	503	Total 3801	C 2391	N 686	O 698	S 26	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	expression tag	UNP P35222
A	144	PRO	-	expression tag	UNP P35222
B	143	GLY	-	expression tag	UNP P35222
B	144	PRO	-	expression tag	UNP P35222

- Molecule 2 is a protein called Axin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total 108	C 76	N 18	O 14	0	0	1

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ACE	-	acetylation	UNP O15169
C	2	MH8	SER	engineered mutation	UNP O15169
C	6	B5I	GLU	engineered mutation	UNP O15169
C	8	LEU	VAL	engineered mutation	UNP O15169
C	9	MH8	GLN	engineered mutation	UNP O15169
C	12	TRP	LEU	engineered mutation	UNP O15169
C	13	NH2	-	amidation	UNP O15169

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).

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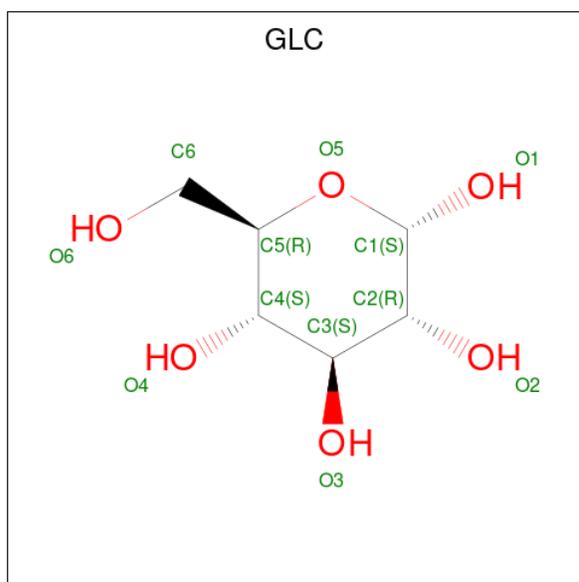
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 6	O 6	0	0
3	A	1	Total 12	C 6	O 6	0	0
3	A	1	Total 12	C 6	O 6	0	0
3	B	1	Total 12	C 6	O 6	0	0
3	B	1	Total 12	C 6	O 6	0	0
3	B	1	Total 12	C 6	O 6	0	0
3	B	1	Total 12	C 6	O 6	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

TRS
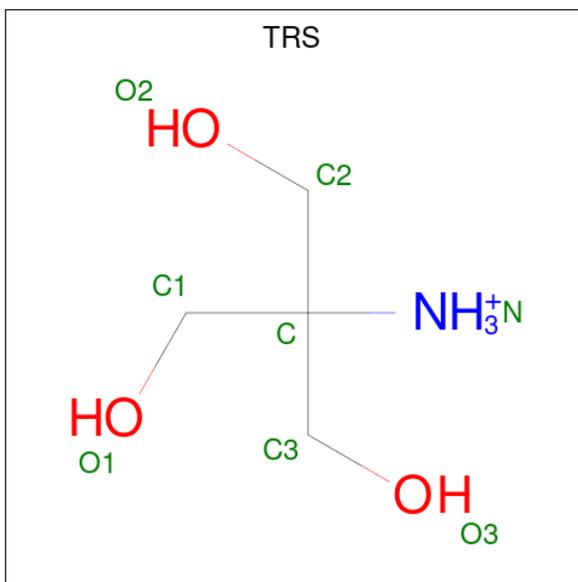
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 8	C 4	N 1	O 3	0	0
4	A	1	Total 8	C 4	N 1	O 3	0	0
4	B	1	Total 8	C 4	N 1	O 3	0	0
4	B	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	140	Total 140	O 140	0	0
7	B	184	Total 184	O 184	0	0
7	C	4	Total 4	O 4	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: Catenin beta-1

Chain A:

- Molecule 1: Catenin beta-1

Chain B:

- Molecule 2: Axin-1

Chain C:
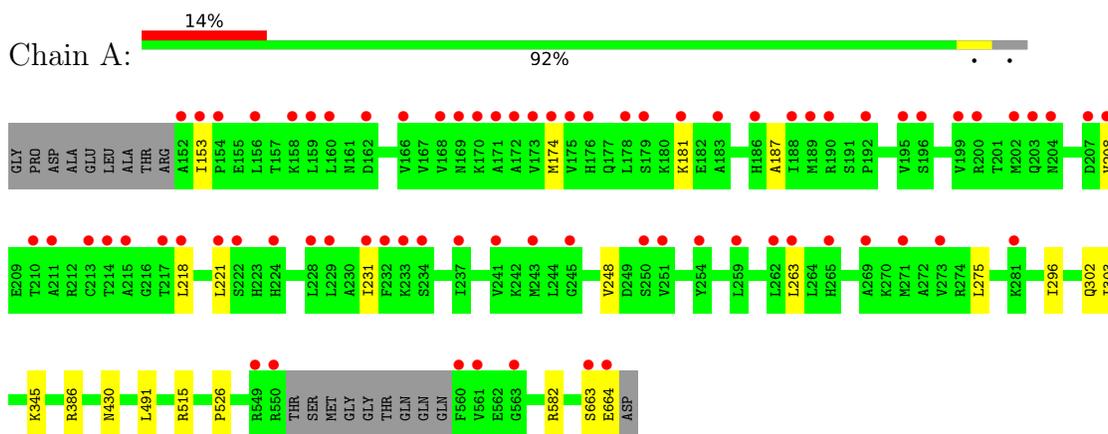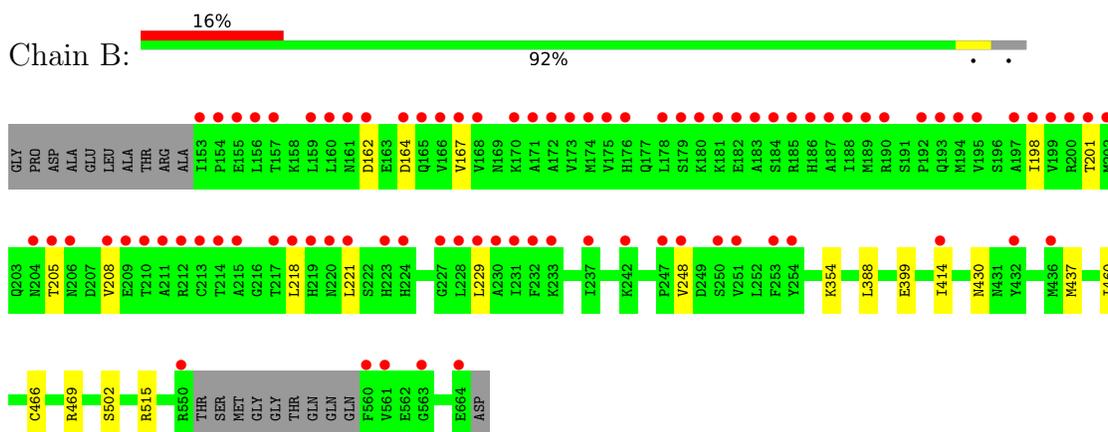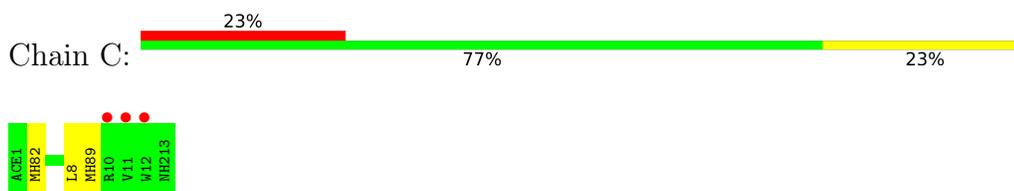
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.57Å 103.62Å 187.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.96 – 2.13 93.96 – 2.13	Depositor EDS
% Data completeness (in resolution range)	72.1 (93.96-2.13) 71.6 (93.96-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.201 , 0.240 0.208 , 0.245	Depositor DCC
R_{free} test set	2502 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8174	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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 67.96 % 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 4.7247e-06. 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 $< |L| >$, $< L^2 >$ 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: CL, MH8, NH2, ACE, CSO, NA, TRS, B5I, GLC

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	0.29	0/3863	0.55	0/5245
1	B	0.29	0/3847	0.54	0/5227
2	C	0.37	0/74	0.59	0/97
All	All	0.29	0/7784	0.55	0/10569

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	3818	0	3943	12	0
1	B	3801	0	3891	11	0
2	C	108	0	101	2	0
3	A	36	0	36	4	0
3	B	48	0	48	0	0
4	A	16	0	24	0	0
4	B	16	0	24	1	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	140	0	0	1	0
7	B	184	0	0	0	0
7	C	4	0	0	0	0
All	All	8174	0	8067	24	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 2.

The worst 5 of 24 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:218:LEU:HD22	1:A:231:ILE:HG12	1.78	0.66
1:B:164:ASP:HB3	1:B:167:VAL:HB	1.80	0.63
1:A:296:ILE:HD11	2:C:8:LEU:HD23	1.86	0.57
1:A:582:ARG:HH22	3:A:705:GLC:H1	1.70	0.56
1:B:399:GLU:HG3	1:B:437:MET:SD	2.47	0.54

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	500/523 (96%)	497 (99%)	3 (1%)	0	100	100
1	B	500/523 (96%)	491 (98%)	9 (2%)	0	100	100
2	C	8/13 (62%)	7 (88%)	1 (12%)	0	100	100
All	All	1008/1059 (95%)	995 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	410/431 (95%)	405 (99%)	5 (1%)	67	72
1	B	405/431 (94%)	400 (99%)	5 (1%)	67	72
2	C	8/8 (100%)	8 (100%)	0	100	100
All	All	823/870 (95%)	813 (99%)	10 (1%)	67	72

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	229	LEU
1	B	430	ASN
1	B	515	ARG
1	A	430	ASN
1	A	515	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	B5I	C	6	2	7,9,10	0.64	0	5,11,13	0.68	0
1	CSO	B	466	1	3,6,7	0.71	0	0,6,8	-	-
1	CSO	A	466	1	3,6,7	0.69	0	0,6,8	-	-
2	MH8	C	2	2	6,9,10	0.59	0	5,11,13	1.76	1 (20%)
2	MH8	C	9	2	6,9,10	0.61	0	5,11,13	0.43	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
2	B5I	C	6	2	-	1/6/11/14	-
1	CSO	B	466	1	-	0/1/5/7	-
1	CSO	A	466	1	-	0/1/5/7	-
2	MH8	C	2	2	-	2/7/9/12	-
2	MH8	C	9	2	-	0/7/9/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2	MH8	CB2-CG-CD	3.82	115.49	111.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	B5I	CE-CD-CK-CA
2	C	2	MH8	CA-CB2-CG-CD
2	C	2	MH8	CE-CD-CG-CB2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	466	CSO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	9	MH8	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	TRS	B	702	-	7,7,7	0.14	0	9,9,9	0.30	0
3	GLC	B	705	-	12,12,12	0.47	0	17,17,17	0.55	0
3	GLC	A	701	-	12,12,12	0.55	0	17,17,17	0.96	1 (5%)
3	GLC	A	705	-	12,12,12	0.60	0	17,17,17	0.56	0
3	GLC	B	704	-	12,12,12	0.58	0	17,17,17	0.89	1 (5%)
4	TRS	A	703	-	7,7,7	0.14	0	9,9,9	0.22	0
4	TRS	B	701	-	7,7,7	0.17	0	9,9,9	0.36	0
3	GLC	B	706	-	12,12,12	0.53	0	17,17,17	0.66	0
3	GLC	A	704	-	12,12,12	0.47	0	17,17,17	0.45	0
3	GLC	B	703	-	12,12,12	0.59	0	17,17,17	0.93	0
4	TRS	A	702	-	7,7,7	0.17	0	9,9,9	0.37	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	TRS	B	702	-	-	0/9/9/9	-
3	GLC	B	705	-	-	1/2/22/22	0/1/1/1
3	GLC	A	701	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	A	705	-	-	0/2/22/22	0/1/1/1
3	GLC	B	704	-	-	2/2/22/22	0/1/1/1
4	TRS	A	703	-	-	0/9/9/9	-
4	TRS	B	701	-	-	3/9/9/9	-
3	GLC	B	706	-	-	2/2/22/22	0/1/1/1
3	GLC	A	704	-	-	0/2/22/22	0/1/1/1
3	GLC	B	703	-	-	0/2/22/22	0/1/1/1
4	TRS	A	702	-	-	0/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	GLC	O5-C5-C6	2.44	112.51	106.44
3	B	704	GLC	O5-C5-C6	2.01	111.44	106.44

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	TRS	C3-C-C2-O2
4	B	701	TRS	N-C-C2-O2
3	B	706	GLC	O5-C5-C6-O6
3	B	704	GLC	O5-C5-C6-O6
3	B	704	GLC	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	GLC	2	0
3	A	705	GLC	1	0
4	B	701	TRS	1	0
3	A	704	GLC	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 ⓘ

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(Å²)	Q<0.9
1	A	503/523 (96%)	0.64	74 (14%)	7	9	13, 41, 89, 139	1 (0%)
1	B	502/523 (95%)	0.68	85 (16%)	5	7	13, 36, 124, 186	2 (0%)
2	C	8/13 (61%)	1.59	3 (37%)	1	1	55, 65, 79, 81	0
All	All	1013/1059 (95%)	0.67	162 (15%)	6	8	13, 38, 110, 186	3 (0%)

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	ILE	7.8
1	B	156	LEU	6.9
1	A	153	ILE	6.8
1	B	211	ALA	6.7
1	B	189	MET	6.6

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, 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(Å²)	Q<0.9
2	MH8	C	2	10/11	0.84	0.16	58,69,78,79	0
2	B5I	C	6	10/11	0.88	0.12	57,72,86,88	0
2	MH8	C	9	10/11	0.91	0.12	59,64,65,68	0
1	CSO	A	466	7/8	0.95	0.07	21,23,40,42	0
1	CSO	B	466	7/8	0.96	0.07	21,22,37,43	0

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	GLC	B	706	12/12	0.74	0.18	58,81,99,109	0
4	TRS	B	702	8/8	0.76	0.18	74,93,105,127	0
3	GLC	A	705	12/12	0.77	0.16	60,88,108,109	0
6	NA	A	707	1/1	0.77	0.13	54,54,54,54	0
3	GLC	A	701	12/12	0.80	0.16	65,69,91,105	0
4	TRS	A	703	8/8	0.80	0.20	69,97,104,109	0
3	GLC	B	704	12/12	0.81	0.17	63,86,106,125	0
3	GLC	B	705	12/12	0.81	0.12	66,83,100,110	0
3	GLC	B	703	12/12	0.82	0.14	59,70,77,90	0
3	GLC	A	704	12/12	0.83	0.19	71,95,117,152	0
6	NA	B	707	1/1	0.84	0.14	52,52,52,52	0
4	TRS	B	701	8/8	0.86	0.17	51,58,64,90	0
4	TRS	A	702	8/8	0.87	0.15	37,59,66,73	0
5	CL	A	706	1/1	0.99	0.03	30,30,30,30	0

6.5   Other polymers ⓘ

There are no such residues in this entry.