



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:53 PM UTC

PDB ID : 1MS0 / pdb_00001ms0
Title : Monoclinic form of Trypanosoma cruzi trans-sialidase, in complex with 3-deoxy-2,3-dehydro-N-acetylneuraminic acid (DANA) and lactose
Authors : Buschiazzi, A.; Amaya, M.F.; Cremona, M.L.; Frasch, A.C.; Alzari, P.M.
Deposited on : 2002-09-19
Resolution : 2.50 Å (reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

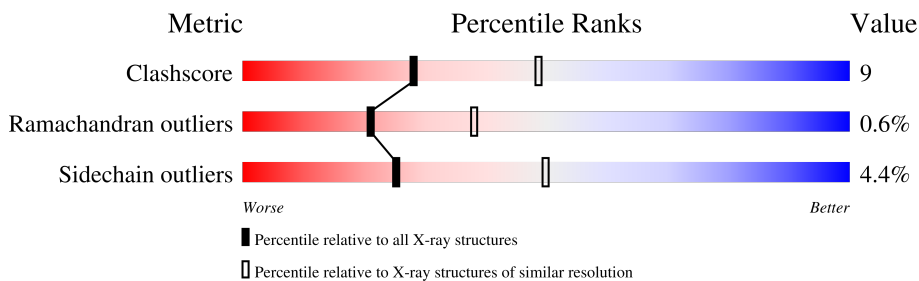
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	648	
1	B	648	
2	C	2	
2	D	2	

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
2	BGC	C	1	X	-	-	-
2	BGC	D	1	X	-	-	-
3	DAN	A	700	-	-	X	-
3	DAN	B	701	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10372 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 trans-sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			4835	3061	844	916	14			
1	B	623	Total	C	N	O	S	0	0	0
			4835	3061	844	916	14			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q26964
A	-12	GLY	-	expression tag	UNP Q26964
A	-11	GLY	-	expression tag	UNP Q26964
A	-10	SER	-	expression tag	UNP Q26964
A	-9	HIS	-	expression tag	UNP Q26964
A	-8	HIS	-	expression tag	UNP Q26964
A	-7	HIS	-	expression tag	UNP Q26964
A	-6	HIS	-	expression tag	UNP Q26964
A	-5	HIS	-	expression tag	UNP Q26964
A	-4	HIS	-	expression tag	UNP Q26964
A	-3	GLY	-	expression tag	UNP Q26964
A	-2	MET	-	expression tag	UNP Q26964
A	-1	ALA	-	expression tag	UNP Q26964
A	0	SER	-	expression tag	UNP Q26964
A	58	PHE	ASN	engineered mutation	UNP Q26964
A	262	THR	SER	SEE REMARK 999	UNP Q26964
A	476	HIS	ARG	SEE REMARK 999	UNP Q26964
A	484	LEU	VAL	SEE REMARK 999	UNP Q26964
A	495	LYS	SER	engineered mutation	UNP Q26964
A	496	GLY	VAL	engineered mutation	UNP Q26964
A	520	LYS	GLU	engineered mutation	UNP Q26964
A	558	VAL	GLU	SEE REMARK 999	UNP Q26964
A	593	GLY	ASP	engineered mutation	UNP Q26964
A	597	ASP	ILE	engineered mutation	UNP Q26964
A	599	ARG	HIS	engineered mutation	UNP Q26964

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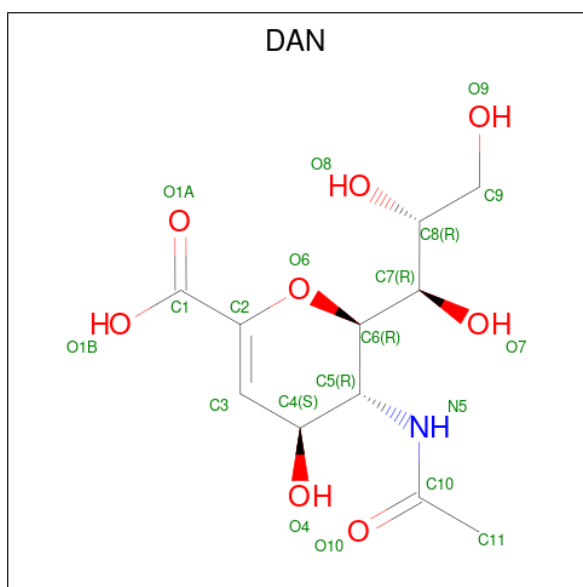
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP Q26964
B	-12	GLY	-	expression tag	UNP Q26964
B	-11	GLY	-	expression tag	UNP Q26964
B	-10	SER	-	expression tag	UNP Q26964
B	-9	HIS	-	expression tag	UNP Q26964
B	-8	HIS	-	expression tag	UNP Q26964
B	-7	HIS	-	expression tag	UNP Q26964
B	-6	HIS	-	expression tag	UNP Q26964
B	-5	HIS	-	expression tag	UNP Q26964
B	-4	HIS	-	expression tag	UNP Q26964
B	-3	GLY	-	expression tag	UNP Q26964
B	-2	MET	-	expression tag	UNP Q26964
B	-1	ALA	-	expression tag	UNP Q26964
B	0	SER	-	expression tag	UNP Q26964
B	58	PHE	ASN	engineered mutation	UNP Q26964
B	262	THR	SER	SEE REMARK 999	UNP Q26964
B	476	HIS	ARG	SEE REMARK 999	UNP Q26964
B	484	LEU	VAL	SEE REMARK 999	UNP Q26964
B	495	LYS	SER	engineered mutation	UNP Q26964
B	496	GLY	VAL	engineered mutation	UNP Q26964
B	520	LYS	GLU	engineered mutation	UNP Q26964
B	558	VAL	GLU	SEE REMARK 999	UNP Q26964
B	593	GLY	ASP	engineered mutation	UNP Q26964
B	597	ASP	ILE	engineered mutation	UNP Q26964
B	599	ARG	HIS	engineered mutation	UNP Q26964

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (CCD ID: DAN) (formula: C₁₁H₁₇NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	11	1	8		
3	B	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is water.

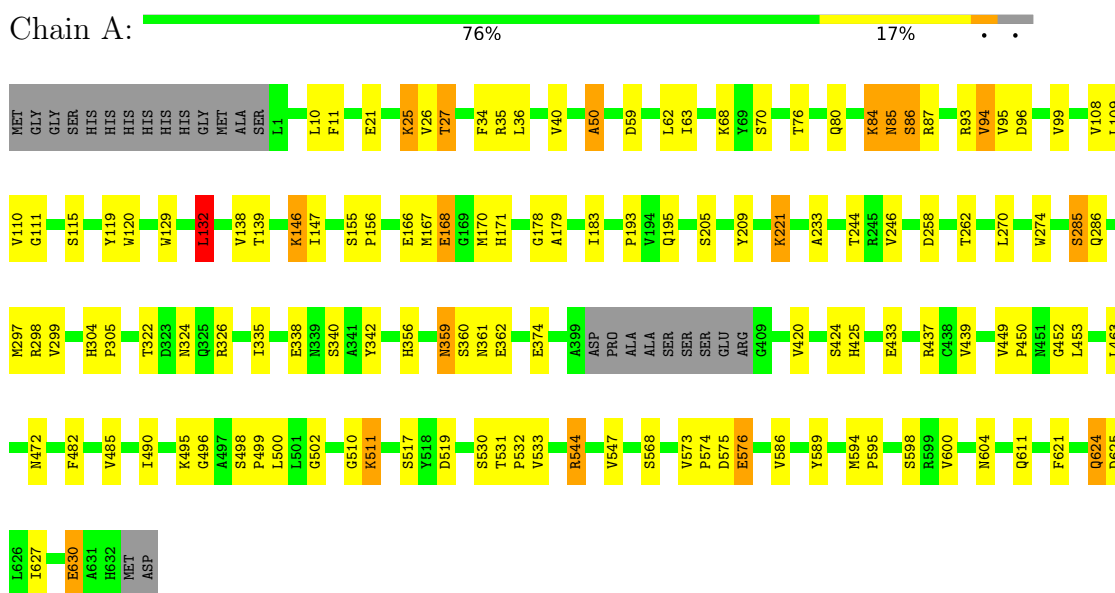
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	339	Total	O	0	0
			339	339		
4	B	277	Total	O	0	0
			277	277		

3 Residue-property plots

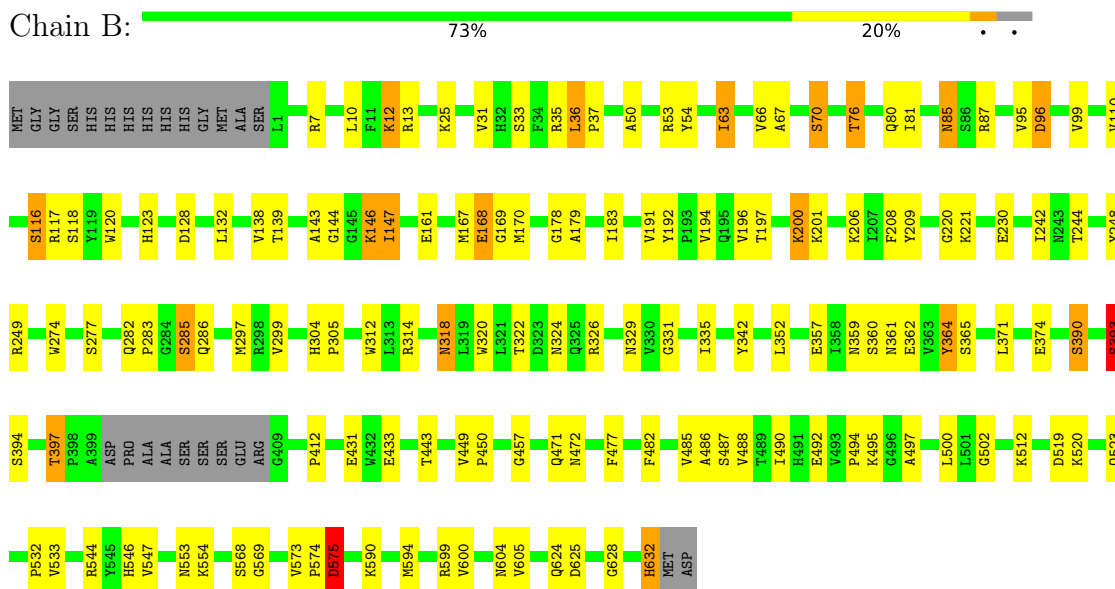
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: trans-sialidase



- Molecule 1: trans-sialidase



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:  50% 50%

BGC1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain D:  100%

BGC1
GAL2

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.22Å 133.37Å 90.61Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.1 (15.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.191 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10372	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, BGC, DAN

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	0.88	1/4948 (0.0%)	1.24	47/6718 (0.7%)
1	B	0.84	2/4948 (0.0%)	1.22	42/6718 (0.6%)
All	All	0.86	3/9896 (0.0%)	1.23	89/13436 (0.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	MET	SD-CE	8.27	2.00	1.79
1	B	297	MET	SD-CE	7.35	1.98	1.79
1	B	208	PHE	CA-C	5.35	1.58	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ILE	N-CA-C	8.45	120.90	108.65
1	B	533	VAL	N-CA-C	8.20	120.39	108.58
1	A	129	TRP	N-CA-C	7.88	122.86	110.17
1	B	54	TYR	N-CA-C	7.55	119.15	111.07
1	B	393	SER	N-CA-C	-7.49	101.20	110.41
1	A	244	THR	N-CA-C	7.44	121.67	110.14
1	A	183	ILE	N-CA-C	7.42	119.94	108.44
1	A	356	HIS	N-CA-C	7.34	120.08	109.14
1	A	420	VAL	N-CA-C	7.12	117.67	111.90
1	A	630	GLU	N-CA-C	7.10	119.63	111.11
1	A	627	ILE	N-CA-C	7.04	119.80	112.83
1	A	40	VAL	N-CA-C	6.94	117.00	108.53
1	A	10	LEU	N-CA-C	6.94	119.86	111.40
1	B	628	GLY	N-CA-C	6.91	119.87	111.93
1	B	95	VAL	N-CA-C	6.88	118.85	108.80
1	A	95	VAL	N-CA-C	6.81	118.63	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	VAL	N-CA-C	6.75	118.19	108.48
1	B	209	TYR	N-CA-C	6.75	119.43	109.24
1	A	519	ASP	N-CA-C	6.62	118.20	108.86
1	B	502	GLY	N-CA-C	6.44	120.15	110.75
1	A	586	VAL	N-CA-C	6.41	117.25	107.77
1	B	99	VAL	N-CA-C	6.40	117.81	108.53
1	B	433	GLU	N-CA-C	6.31	119.79	109.76
1	A	285	SER	N-CA-C	6.28	117.77	108.60
1	A	258	ASP	N-CA-C	6.25	118.11	109.54
1	A	547	VAL	N-CA-C	6.25	116.86	108.11
1	B	604	ASN	N-CA-C	6.25	118.83	111.02
1	B	443	THR	N-CA-C	6.23	118.88	109.41
1	A	115	SER	N-CA-C	6.15	123.65	113.50
1	B	96	ASP	CB-CA-C	-5.95	106.97	111.20
1	B	10	LEU	N-CA-C	5.94	117.75	111.28
1	B	244	THR	N-CA-C	5.94	119.62	110.42
1	A	193	PRO	CA-C-O	-5.92	114.28	121.03
1	B	31	VAL	N-CA-C	5.90	116.44	108.17
1	A	573	VAL	CB-CA-C	-5.89	103.98	110.52
1	B	331	GLY	N-CA-C	5.88	119.03	110.63
1	B	12	LYS	N-CA-C	5.85	117.83	108.41
1	A	63	ILE	N-CA-C	5.84	116.70	108.17
1	A	86	SER	N-CA-C	5.83	120.01	113.01
1	A	205	SER	N-CA-C	5.82	118.95	109.59
1	A	221	LYS	N-CA-C	5.80	118.55	111.82
1	A	108	VAL	N-CA-C	5.78	116.18	107.80
1	B	63	ILE	N-CA-C	5.78	117.07	108.46
1	B	37	PRO	CB-CA-C	-5.76	104.03	111.46
1	B	132	LEU	N-CA-C	5.68	118.82	109.85
1	B	33	SER	N-CA-C	5.65	118.67	109.24
1	A	359	ASN	N-CA-C	5.63	117.55	107.80
1	B	76	THR	N-CA-C	5.63	118.39	109.50
1	B	285	SER	N-CA-C	5.59	116.77	108.60
1	B	547	VAL	N-CA-C	5.59	115.94	108.11
1	A	433	GLU	N-CA-C	5.56	118.98	110.20
1	A	50	ALA	N-CA-C	5.55	115.16	107.73
1	B	220	GLY	N-CA-C	-5.50	105.50	112.54
1	B	50	ALA	N-CA-C	5.44	116.41	108.14
1	B	110	VAL	CB-CA-C	-5.42	101.00	110.71
1	B	299	VAL	N-CA-C	5.41	116.49	108.65
1	A	485	VAL	N-CA-C	5.41	116.51	108.46
1	A	502	GLY	N-CA-C	5.40	118.47	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LEU	N-CA-C	5.39	120.87	113.97
1	A	138	VAL	N-CA-C	5.39	115.86	107.99
1	A	209	TYR	N-CA-C	5.39	117.88	109.52
1	A	533	VAL	N-CA-C	5.38	116.46	108.23
1	B	364	TYR	N-CA-C	5.35	118.12	109.40
1	A	437	ARG	N-CA-C	5.35	119.38	112.86
1	B	512	LYS	N-CA-C	5.33	118.76	110.17
1	B	488	VAL	N-CA-C	5.31	117.42	108.81
1	A	246	VAL	CB-CA-C	-5.31	104.36	110.41
1	A	624	GLN	N-CA-C	5.28	117.72	111.33
1	A	132	LEU	N-CA-C	5.28	117.70	109.52
1	A	624	GLN	CB-CA-C	-5.28	101.71	110.68
1	A	322	THR	N-CA-C	5.27	117.27	108.99
1	B	138	VAL	N-CA-C	5.26	115.43	107.80
1	A	340	SER	N-CA-C	5.24	115.96	107.32
1	A	233	ALA	N-CA-C	5.22	117.61	109.52
1	B	431	GLU	N-CA-C	5.19	117.62	108.75
1	B	486	ALA	N-CA-C	5.16	116.69	108.79
1	B	147	ILE	N-CA-C	5.15	116.23	109.58
1	A	485	VAL	CB-CA-C	-5.14	102.59	110.50
1	B	192	TYR	CB-CA-C	-5.11	104.28	110.15
1	A	93	ARG	N-CA-C	5.10	116.27	108.52
1	A	110	VAL	N-CA-C	5.07	117.03	108.81
1	A	27	THR	N-CA-C	5.06	117.67	109.06
1	B	191	VAL	N-CA-C	5.05	115.13	107.80
1	A	62	LEU	N-CA-C	5.05	117.02	109.59
1	B	393	SER	CA-C-N	-5.05	117.52	126.45
1	B	393	SER	C-N-CA	-5.05	117.52	126.45
1	B	194	VAL	N-CA-C	5.04	116.86	108.99
1	B	457	GLY	N-CA-C	5.03	120.25	112.81
1	A	439	VAL	CB-CA-C	-5.00	104.71	110.41

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	4835	0	4761	72	0
1	B	4835	0	4761	94	0
2	C	23	0	21	3	0
2	D	23	0	21	4	0
3	A	20	0	16	8	0
3	B	20	0	16	9	0
4	A	339	0	0	4	0
4	B	277	0	0	8	0
All	All	10372	0	9596	173	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 9.

All (173) 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)
3:B:701:DAN:H3	2:D:2:GAL:O3	1.55	1.05
1:B:352:LEU:HD23	1:B:371:LEU:HD12	1.42	1.01
1:A:544:ARG:NH2	1:A:625:ASP:OD1	2.01	0.93
1:B:146:LYS:HD3	1:B:146:LYS:H	1.35	0.91
1:B:352:LEU:CD2	1:B:371:LEU:HD12	2.03	0.87
1:B:393:SER:O	1:B:394:SER:HB2	1.72	0.87
1:B:178:GLY:O	1:B:179:ALA:HB3	1.77	0.84
1:B:35:ARG:HD2	1:B:357:GLU:OE1	1.78	0.82
1:B:374:GLU:N	1:B:374:GLU:OE1	2.12	0.81
3:B:701:DAN:H3	2:D:2:GAL:HO3	1.42	0.81
1:A:342:TYR:OH	3:A:700:DAN:O1B	1.99	0.79
1:A:574:PRO:O	1:A:576:GLU:N	2.18	0.76
1:B:85:ASN:HD22	1:B:87:ARG:H	1.34	0.76
1:A:498:SER:O	1:A:517:SER:HB3	1.87	0.75
1:B:146:LYS:HD3	1:B:146:LYS:N	2.02	0.74
1:A:85:ASN:ND2	1:A:87:ARG:H	1.86	0.74
1:A:85:ASN:HD22	1:A:87:ARG:H	1.36	0.73
1:B:70:SER:HB2	1:B:76:THR:O	1.89	0.72
1:A:359:ASN:HD21	1:A:362:GLU:H	1.35	0.72
1:B:359:ASN:HD22	1:B:360:SER:N	1.89	0.70
1:B:248:TYR:O	1:B:249:ARG:HG2	1.91	0.70
1:B:304:HIS:CD2	1:B:305:PRO:HD2	2.27	0.70
1:B:85:ASN:ND2	1:B:87:ARG:H	1.90	0.69
3:B:701:DAN:C3	2:D:2:GAL:O3	2.39	0.69
1:A:359:ASN:C	1:A:359:ASN:ND2	2.52	0.67
1:A:85:ASN:HD22	1:A:85:ASN:C	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:O	1:A:179:ALA:HB3	1.96	0.66
1:B:144:GLY:HA3	1:B:146:LYS:HE2	1.78	0.66
3:B:701:DAN:H113	3:B:701:DAN:H7	1.78	0.66
1:B:66:VAL:HG22	1:B:67:ALA:N	2.11	0.65
1:A:359:ASN:HD22	1:A:360:SER:N	1.94	0.65
1:A:544:ARG:HH22	1:A:625:ASP:CG	2.05	0.65
1:B:532:PRO:O	4:B:801:HOH:O	2.13	0.65
1:B:85:ASN:ND2	1:B:87:ARG:HH11	1.94	0.64
1:B:118:SER:O	1:B:123:HIS:HE1	1.80	0.64
1:A:359:ASN:C	1:A:359:ASN:HD22	2.05	0.64
1:B:487:SER:OG	1:B:624:GLN:NE2	2.30	0.64
1:B:318:ASN:ND2	1:B:329:ASN:OD1	2.30	0.64
1:B:116:SER:OG	1:B:128:ASP:OD2	2.16	0.62
1:A:139:THR:HG23	4:A:818:HOH:O	1.99	0.62
1:B:304:HIS:CG	1:B:305:PRO:HD2	2.34	0.62
1:A:304:HIS:CD2	1:A:305:PRO:HD2	2.34	0.62
1:A:195:GLN:OE1	3:A:700:DAN:H91	2.00	0.61
1:B:546:HIS:CD2	4:B:875:HOH:O	2.53	0.61
1:A:304:HIS:HD2	1:A:305:PRO:O	1.83	0.61
1:B:304:HIS:HD2	1:B:305:PRO:O	1.85	0.60
1:A:511:LYS:CE	1:A:511:LYS:HA	2.32	0.60
1:B:248:TYR:C	1:B:249:ARG:HG2	2.27	0.60
1:A:574:PRO:C	1:A:576:GLU:H	2.10	0.59
1:B:85:ASN:HD22	1:B:85:ASN:C	2.10	0.59
1:B:546:HIS:HD2	4:B:875:HOH:O	1.85	0.59
1:B:625:ASP:HB2	4:B:856:HOH:O	2.01	0.59
1:A:120:TRP:HE1	3:A:700:DAN:H92	1.67	0.59
1:B:490:ILE:HA	1:B:600:VAL:HG12	1.84	0.58
1:B:342:TYR:OH	3:B:701:DAN:C2	2.51	0.58
1:A:463:LEU:C	1:A:463:LEU:HD23	2.29	0.58
1:B:144:GLY:HA3	1:B:146:LYS:CE	2.34	0.58
1:B:397:THR:HG23	4:B:820:HOH:O	2.04	0.57
1:A:342:TYR:N	1:A:342:TYR:CD1	2.72	0.57
1:A:70:SER:HB2	1:A:76:THR:O	2.05	0.57
1:A:85:ASN:ND2	1:A:85:ASN:C	2.62	0.56
1:A:511:LYS:HA	1:A:511:LYS:HE2	1.86	0.56
1:A:621:PHE:O	1:A:624:GLN:HG3	2.04	0.56
1:A:510:GLY:O	1:A:511:LYS:HE3	2.05	0.56
1:B:178:GLY:O	1:B:179:ALA:CB	2.44	0.56
1:A:342:TYR:N	1:A:342:TYR:HD1	2.02	0.56
1:B:66:VAL:CG2	1:B:67:ALA:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:ASN:ND2	1:B:360:SER:N	2.54	0.56
1:A:490:ILE:HA	1:A:600:VAL:HG12	1.87	0.55
1:A:611:GLN:NE2	4:A:805:HOH:O	2.39	0.55
1:A:544:ARG:NH2	1:A:625:ASP:CG	2.64	0.54
1:B:85:ASN:HD21	1:B:87:ARG:HH11	1.55	0.54
1:B:161:GLU:HG2	4:B:807:HOH:O	2.06	0.54
1:B:167:MET:O	1:B:168:GLU:C	2.51	0.54
1:A:449:VAL:HB	1:A:450:PRO:HD2	1.89	0.53
1:B:282:GLN:HB3	1:B:283:PRO:CD	2.38	0.53
1:A:574:PRO:C	1:A:576:GLU:N	2.66	0.52
1:A:425:HIS:CE1	1:A:630:GLU:HG3	2.45	0.52
1:B:599:ARG:O	1:B:600:VAL:HG13	2.10	0.52
1:B:35:ARG:HD3	1:B:364:TYR:CD2	2.44	0.51
1:B:13:ARG:HG2	1:B:365:SER:OG	2.10	0.51
1:A:499:PRO:HG3	1:A:589:TYR:CZ	2.46	0.51
1:B:120:TRP:HE1	3:B:701:DAN:H92	1.76	0.51
1:B:573:VAL:O	1:B:575:ASP:N	2.43	0.51
1:A:36:LEU:N	1:A:36:LEU:HD12	2.26	0.50
1:B:359:ASN:HD22	1:B:360:SER:H	1.59	0.50
1:A:335:ILE:O	1:A:338:GLU:HG2	2.10	0.50
1:B:397:THR:HG21	1:B:412:PRO:O	2.11	0.50
1:A:25:LYS:HE3	1:A:26:VAL:N	2.27	0.50
1:A:85:ASN:HD22	1:A:86:SER:N	2.08	0.50
1:B:169:GLY:O	4:B:802:HOH:O	2.19	0.50
1:A:59:ASP:OD1	2:C:2:GAL:O3	2.22	0.50
1:A:449:VAL:HB	1:A:450:PRO:CD	2.42	0.50
1:A:499:PRO:HG3	1:A:589:TYR:CE1	2.46	0.50
1:B:230:GLU:OE2	3:B:701:DAN:H8	2.12	0.49
1:B:167:MET:HB2	1:B:170:MET:CE	2.42	0.49
1:A:361:ASN:O	1:A:362:GLU:HB2	2.12	0.49
1:B:274:TRP:HA	1:B:472:ASN:HD22	1.77	0.49
1:A:374:GLU:OE1	1:A:374:GLU:N	2.44	0.49
1:B:449:VAL:HB	1:B:450:PRO:CD	2.42	0.49
1:B:352:LEU:HD23	1:B:371:LEU:CD1	2.28	0.49
1:B:485:VAL:O	1:B:605:VAL:HA	2.12	0.49
3:A:700:DAN:H111	4:A:872:HOH:O	2.12	0.49
1:B:36:LEU:HD12	1:B:96:ASP:HA	1.94	0.49
1:B:53:ARG:HG2	1:B:63:ILE:HG12	1.95	0.48
1:A:25:LYS:HE3	1:A:25:LYS:CA	2.43	0.48
1:B:494:PRO:O	1:B:520:LYS:HB3	2.14	0.48
1:B:482:PHE:C	1:B:482:PHE:CD1	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:MET:O	1:A:168:GLU:C	2.57	0.48
1:B:200:LYS:O	1:B:201:LYS:HB2	2.12	0.48
1:B:519:ASP:OD1	1:B:519:ASP:C	2.57	0.48
1:B:118:SER:O	1:B:123:HIS:CE1	2.65	0.47
1:B:360:SER:O	1:B:361:ASN:C	2.56	0.47
1:A:21:GLU:OE1	1:A:84:LYS:HE3	2.15	0.47
1:B:342:TYR:OH	3:B:701:DAN:O6	2.33	0.47
1:B:312:TRP:CZ2	2:D:1:BGC:H6C1	2.49	0.47
1:A:36:LEU:N	1:A:36:LEU:CD1	2.78	0.47
1:B:477:PHE:C	1:B:477:PHE:CD2	2.93	0.46
1:A:496:GLY:HA3	4:A:812:HOH:O	2.15	0.46
1:A:166:GLU:OE2	1:A:171:HIS:CE1	2.69	0.46
1:B:277:SER:O	1:B:471:GLN:HG3	2.16	0.46
1:A:274:TRP:HA	1:A:472:ASN:HD22	1.80	0.46
1:A:36:LEU:HD23	1:A:96:ASP:HA	1.99	0.45
1:B:7:ARG:CZ	1:B:335:ILE:HD12	2.47	0.45
1:A:25:LYS:HE3	1:A:26:VAL:H	1.81	0.45
1:B:314:ARG:NH1	3:B:701:DAN:O1B	2.41	0.45
1:B:320:TRP:CZ3	1:B:329:ASN:HB2	2.51	0.45
3:A:700:DAN:C10	3:A:700:DAN:H7	2.47	0.45
1:B:304:HIS:CD2	1:B:305:PRO:O	2.68	0.45
1:B:449:VAL:HB	1:B:450:PRO:HD2	1.99	0.44
1:A:94:VAL:HA	1:A:111:GLY:O	2.18	0.44
1:B:282:GLN:HB3	1:B:283:PRO:HD2	1.99	0.44
1:A:11:PHE:CZ	1:A:68:LYS:HD2	2.53	0.44
1:A:452:GLY:O	1:A:453:LEU:HD23	2.18	0.44
1:B:632:HIS:ND1	1:B:632:HIS:N	2.66	0.44
1:B:146:LYS:H	1:B:146:LYS:CD	2.18	0.43
1:B:599:ARG:O	1:B:600:VAL:CG1	2.66	0.43
1:A:298:ARG:C	1:A:299:VAL:HG13	2.42	0.43
1:B:12:LYS:O	1:B:13:ARG:C	2.62	0.43
1:B:599:ARG:C	1:B:600:VAL:HG13	2.43	0.43
1:A:109:LEU:HD12	1:A:132:LEU:O	2.18	0.43
1:A:531:THR:HG23	1:A:532:PRO:HD2	2.00	0.43
1:B:285:SER:OG	1:B:286:GLN:N	2.52	0.43
1:A:155:SER:HA	1:A:156:PRO:HD3	1.85	0.43
3:A:700:DAN:C3	2:C:2:GAL:O3	2.67	0.43
1:B:196:VAL:HG12	1:B:197:THR:N	2.33	0.43
1:B:359:ASN:ND2	1:B:359:ASN:C	2.76	0.43
1:B:35:ARG:CD	1:B:357:GLU:OE1	2.59	0.43
1:A:146:LYS:HE3	1:A:146:LYS:HB2	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LYS:HE3	1:B:495:LYS:HB2	1.77	0.42
1:B:523:GLN:NE2	4:B:810:HOH:O	2.47	0.42
1:A:495:LYS:HB2	1:A:495:LYS:HE3	1.81	0.42
1:B:492:GLU:HB3	1:B:599:ARG:HG3	2.01	0.42
1:B:359:ASN:HD21	1:B:362:GLU:HA	1.85	0.42
1:B:390:SER:O	1:B:393:SER:O	2.36	0.42
1:B:553:ASN:O	1:B:554:LYS:HB2	2.19	0.42
1:A:285:SER:OG	1:A:286:GLN:N	2.51	0.42
1:B:568:SER:OG	1:B:569:GLY:N	2.53	0.42
1:A:424:SER:OG	1:A:604:ASN:ND2	2.53	0.42
1:A:594:MET:HA	1:A:595:PRO:HD3	1.93	0.42
1:B:393:SER:O	1:B:394:SER:CB	2.48	0.42
1:B:85:ASN:ND2	1:B:87:ARG:NH1	2.66	0.41
1:B:167:MET:HB2	1:B:170:MET:HE3	2.02	0.41
1:A:35:ARG:O	1:A:50:ALA:HB1	2.21	0.41
1:A:482:PHE:CD1	1:A:482:PHE:C	2.99	0.41
1:A:11:PHE:HB3	1:A:34:PHE:CD1	2.56	0.41
1:A:120:TRP:NE1	3:A:700:DAN:H92	2.35	0.41
1:A:195:GLN:CD	3:A:700:DAN:H91	2.44	0.41
1:B:85:ASN:ND2	1:B:85:ASN:C	2.77	0.41
1:A:166:GLU:HG2	1:A:170:MET:O	2.22	0.40
1:A:119:TYR:CE1	2:C:1:BGC:H5	2.57	0.40
1:B:85:ASN:HD22	1:B:87:ARG:N	2.10	0.40
1:B:206:LYS:HE3	1:B:206:LYS:HB3	1.96	0.40

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	619/648 (96%)	581 (94%)	35 (6%)	3 (0%)	24 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	619/648 (96%)	584 (94%)	30 (5%)	5 (1%)	16	31
All	All	1238/1296 (96%)	1165 (94%)	65 (5%)	8 (1%)	21	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	GLU
1	A	575	ASP
1	A	576	GLU
1	B	143	ALA
1	B	575	ASP
1	B	168	GLU
1	B	497	ALA
1	B	574	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	526/547 (96%)	507 (96%)	19 (4%)	31	58
1	B	526/547 (96%)	499 (95%)	27 (5%)	21	43
All	All	1052/1094 (96%)	1006 (96%)	46 (4%)	25	50

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	27	THR
1	A	80	GLN
1	A	84	LYS
1	A	85	ASN
1	A	94	VAL
1	A	132	LEU
1	A	146	LYS

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Mol	Chain	Res	Type
1	A	147	ILE
1	A	221	LYS
1	A	262	THR
1	A	324	ASN
1	A	326	ARG
1	A	500	LEU
1	A	511	LYS
1	A	530	SER
1	A	544	ARG
1	A	568	SER
1	A	598	SER
1	B	25	LYS
1	B	36	LEU
1	B	70	SER
1	B	80	GLN
1	B	81	ILE
1	B	85	ASN
1	B	116	SER
1	B	117	ARG
1	B	139	THR
1	B	146	LYS
1	B	147	ILE
1	B	200	LYS
1	B	221	LYS
1	B	242	ILE
1	B	318	ASN
1	B	322	THR
1	B	324	ASN
1	B	326	ARG
1	B	390	SER
1	B	393	SER
1	B	397	THR
1	B	500	LEU
1	B	544	ARG
1	B	575	ASP
1	B	590	LYS
1	B	594	MET
1	B	632	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	123	HIS
1	A	171	HIS
1	A	174	GLN
1	A	304	HIS
1	A	324	ASN
1	A	359	ASN
1	A	472	ASN
1	A	476	HIS
1	A	480	HIS
1	A	546	HIS
1	A	604	ASN
1	A	611	GLN
1	A	624	GLN
1	B	85	ASN
1	B	123	HIS
1	B	171	HIS
1	B	173	ASN
1	B	174	GLN
1	B	304	HIS
1	B	324	ASN
1	B	359	ASN
1	B	472	ASN
1	B	480	HIS
1	B	546	HIS
1	B	603	ASN
1	B	624	GLN

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 ⓘ

4 monosaccharides 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	BGC	C	1	2	12,12,12	0.54	0	17,17,17	0.75	0
2	GAL	C	2	2	11,11,12	0.64	0	15,15,17	0.90	1 (6%)
2	BGC	D	1	2	12,12,12	0.69	0	17,17,17	1.44	2 (11%)
2	GAL	D	2	2	11,11,12	0.53	0	15,15,17	1.27	2 (13%)

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	BGC	C	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	BGC	D	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	BGC	C1-C2-C3	3.41	117.32	110.36
2	D	1	BGC	C4-C3-C2	2.90	115.93	110.83
2	D	2	GAL	C2-C3-C4	-2.48	106.49	110.86
2	D	2	GAL	C3-C4-C5	-2.46	105.77	110.23
2	C	2	GAL	C1-C2-C3	2.42	113.17	109.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	BGC	C1
2	D	1	BGC	C1

All (6) torsion outliers are listed below:

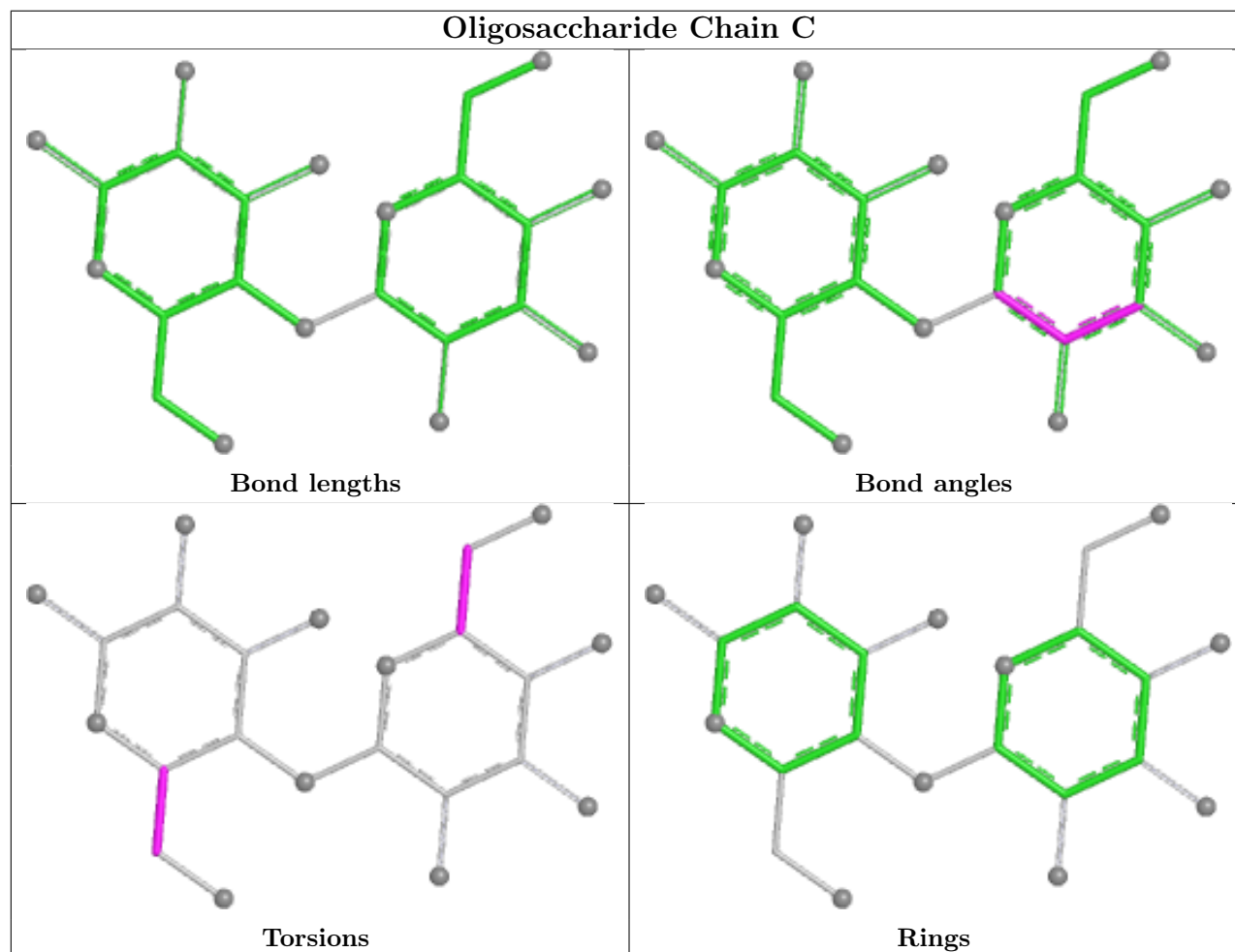
Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6
2	C	2	GAL	O5-C5-C6-O6

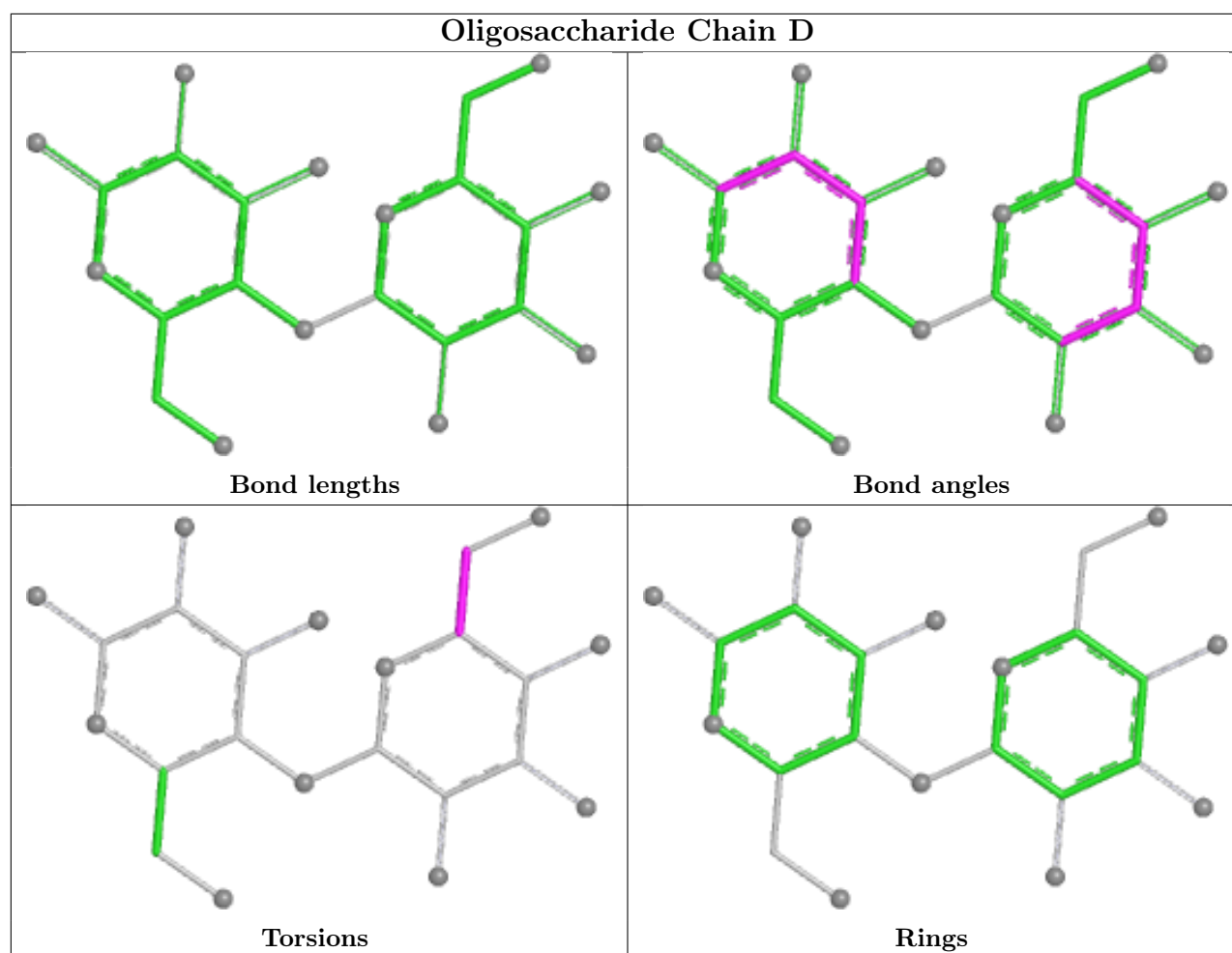
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GAL	2	0
2	C	1	BGC	1	0
2	D	2	GAL	3	0
2	D	1	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 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	DAN	B	701	-	20,20,20	3.70	5 (25%)	24,28,28	1.97	6 (25%)
3	DAN	A	700	-	20,20,20	3.74	6 (30%)	24,28,28	2.18	8 (33%)

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	DAN	B	701	-	-	11/18/34/34	0/1/1/1
3	DAN	A	700	-	-	8/18/34/34	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	DAN	C3-C2	10.61	1.51	1.33
3	B	701	DAN	C3-C2	10.40	1.51	1.33
3	B	701	DAN	O10-C10	8.28	1.41	1.23
3	A	700	DAN	O10-C10	8.26	1.41	1.23
3	A	700	DAN	O1A-C1	8.18	1.42	1.22
3	B	701	DAN	O1A-C1	8.11	1.42	1.22
3	B	701	DAN	C2-C1	-3.38	1.41	1.48
3	B	701	DAN	O6-C2	-2.95	1.26	1.37
3	A	700	DAN	C2-C1	-2.91	1.42	1.48
3	A	700	DAN	O6-C2	-2.75	1.27	1.37
3	A	700	DAN	C4-C3	2.00	1.53	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	DAN	C4-C3-C2	-6.07	111.17	121.45
3	A	700	DAN	C4-C3-C2	-5.41	112.30	121.45
3	A	700	DAN	O6-C6-C7	4.54	113.97	105.98
3	A	700	DAN	O1B-C1-C2	3.27	121.47	114.06
3	B	701	DAN	O6-C2-C1	3.24	118.47	112.02
3	A	700	DAN	O1B-C1-O1A	-3.19	116.30	123.90
3	A	700	DAN	O6-C2-C1	3.18	118.36	112.02
3	B	701	DAN	O6-C2-C3	-3.06	121.19	124.62
3	A	700	DAN	O4-C4-C5	-2.64	107.92	112.66
3	B	701	DAN	O6-C6-C7	2.59	110.54	105.98
3	A	700	DAN	O6-C2-C3	-2.46	121.87	124.62
3	B	701	DAN	O1B-C1-O1A	-2.42	118.14	123.90
3	B	701	DAN	O1B-C1-C2	2.29	119.24	114.06
3	A	700	DAN	O7-C7-C6	2.04	113.86	109.44

There are no chirality outliers.

All (19) torsion outliers are listed below:

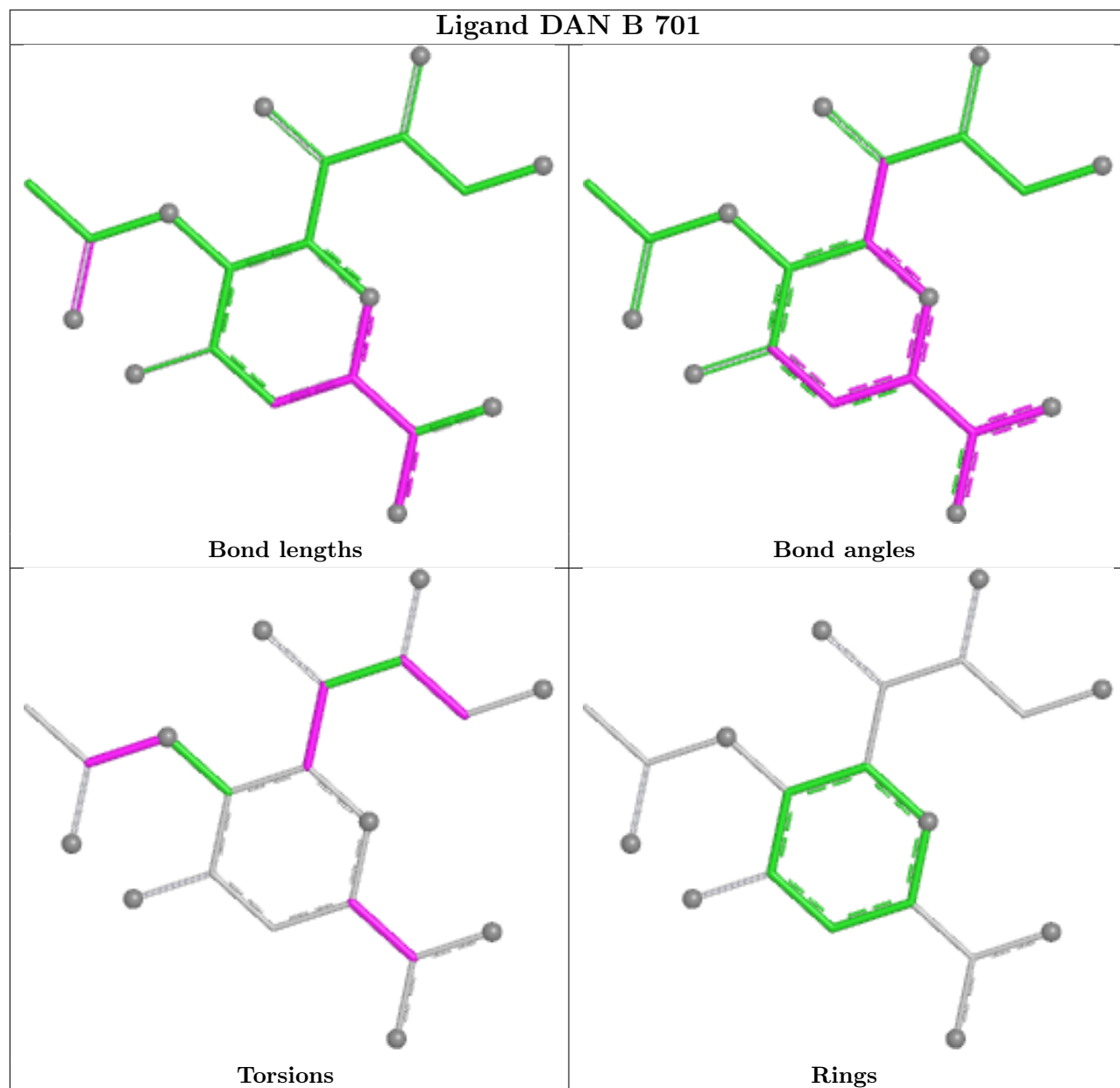
Mol	Chain	Res	Type	Atoms
3	A	700	DAN	O1A-C1-C2-C3
3	A	700	DAN	O1A-C1-C2-O6
3	A	700	DAN	O1B-C1-C2-C3
3	A	700	DAN	O1B-C1-C2-O6
3	A	700	DAN	C11-C10-N5-C5
3	B	701	DAN	O1A-C1-C2-C3
3	B	701	DAN	O1A-C1-C2-O6
3	B	701	DAN	O1B-C1-C2-C3
3	B	701	DAN	O1B-C1-C2-O6
3	B	701	DAN	C5-C6-C7-C8
3	B	701	DAN	C5-C6-C7-O7
3	B	701	DAN	O6-C6-C7-C8
3	B	701	DAN	O6-C6-C7-O7
3	A	700	DAN	O10-C10-N5-C5
3	B	701	DAN	C11-C10-N5-C5
3	B	701	DAN	O10-C10-N5-C5
3	B	701	DAN	C7-C8-C9-O9
3	A	700	DAN	O8-C8-C9-O9
3	A	700	DAN	C7-C8-C9-O9

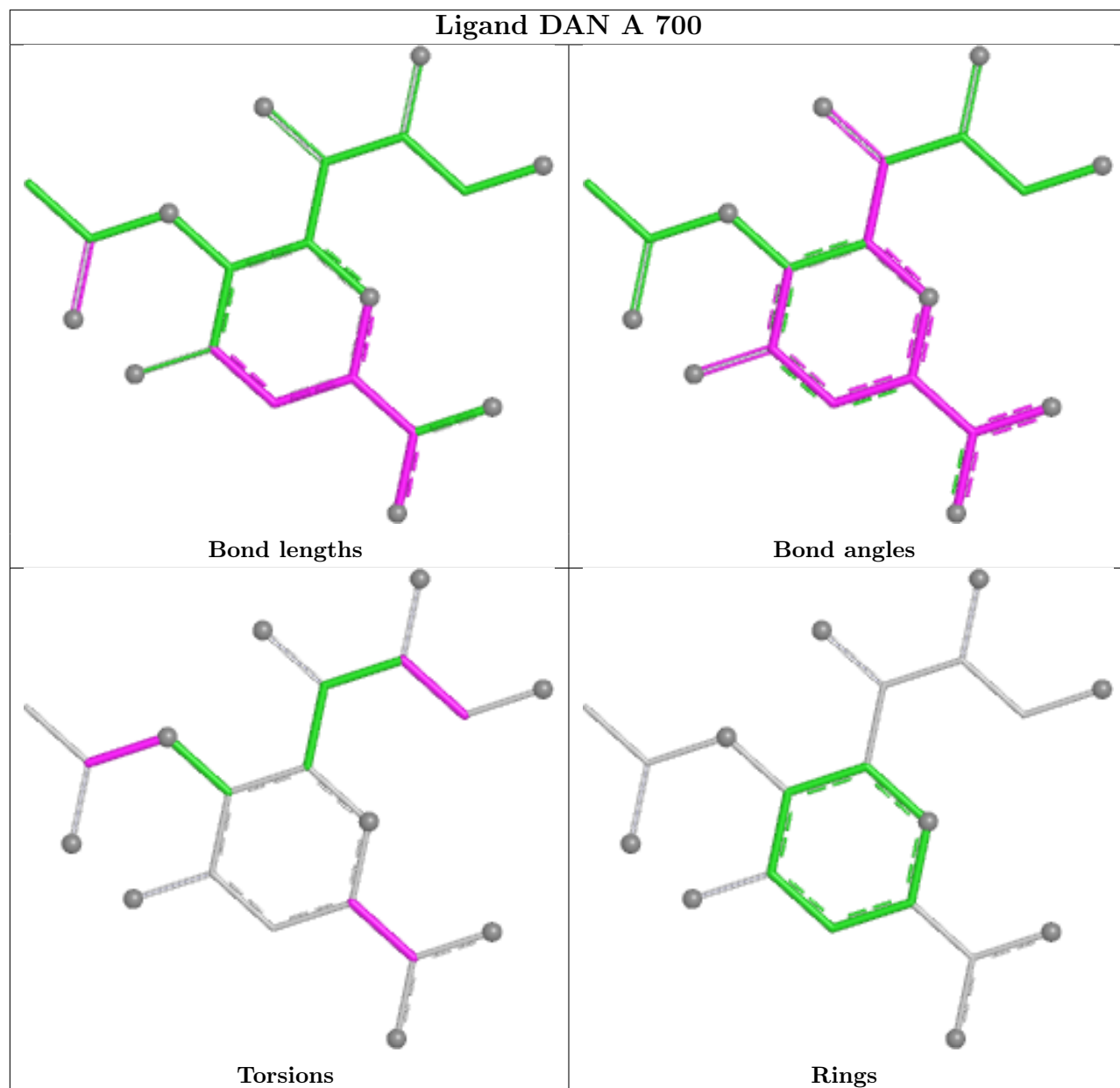
There are no ring outliers.

2 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	DAN	9	0
3	A	700	DAN	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.