Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 04:55 PM EDT

PDB ID	:	1WHT
Title	:	STRUCTURE OF THE COMPLEX OF L-BENZYLSUCCINATE WITH WHEAT SERINE CARBOXYPEPTIDASE II AT 2.0 ANGSTROMS RESOLUTION
Authors	:	Bullock, T.L.; Remington, S.J.
Deposited on	:	1994-03-07
Resolution	:	2.00 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:

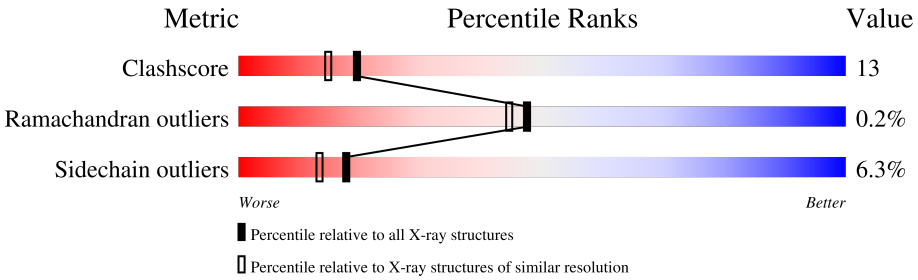
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	68% 27% .
2	B	153	71% 20% 8% .
3	C	3	100%
4	D	2	50% 50%

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
3	NDG	C	3	X	-	-	-
4	NAG	D	2	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3741 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.

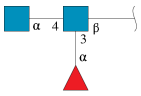
- Molecule 1 is a protein called SERINE CARBOXYPEPTIDASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2003	1282	335	379	7	0	0	0

- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II.

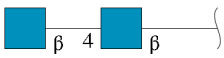
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	153	1213	778	208	221	6	0	0	0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



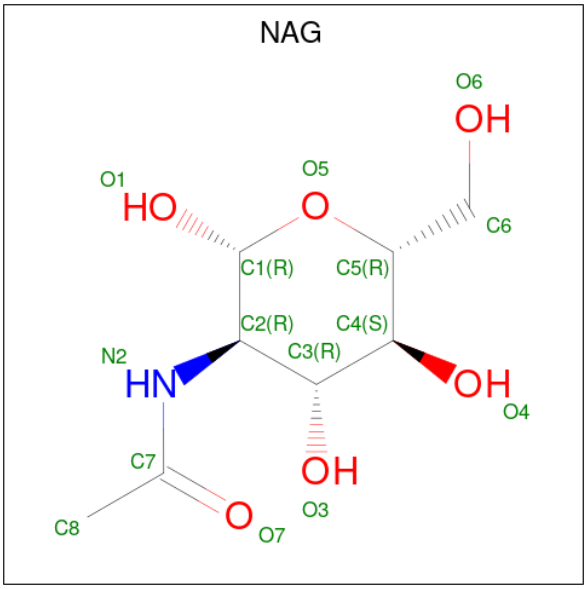
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0

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



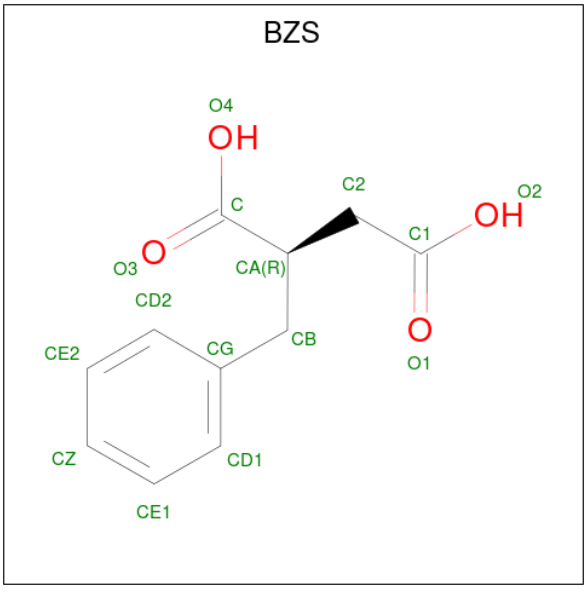
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is L-BENZYLSUCCINIC ACID (three-letter code: BZS) (formula: $C_{11}H_{12}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	259	Total O 259 259	0	0
7	B	171	Total O 171 171	0	0

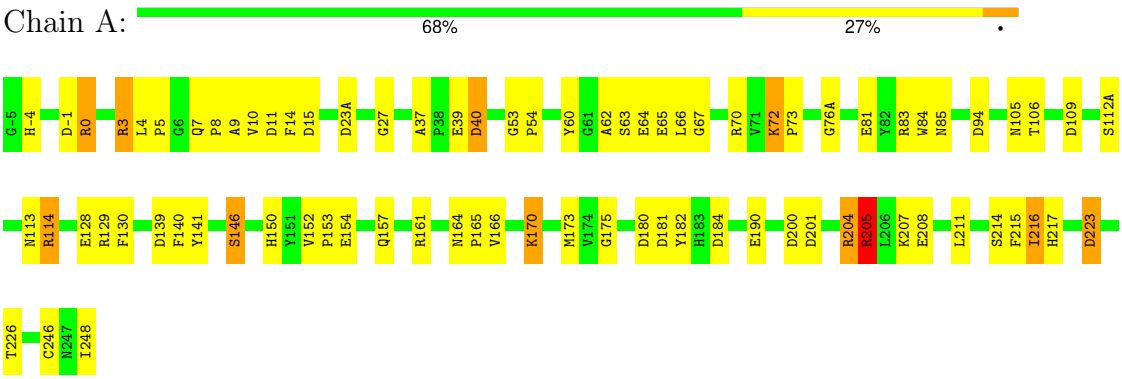
3 Residue-property plots (i)

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.

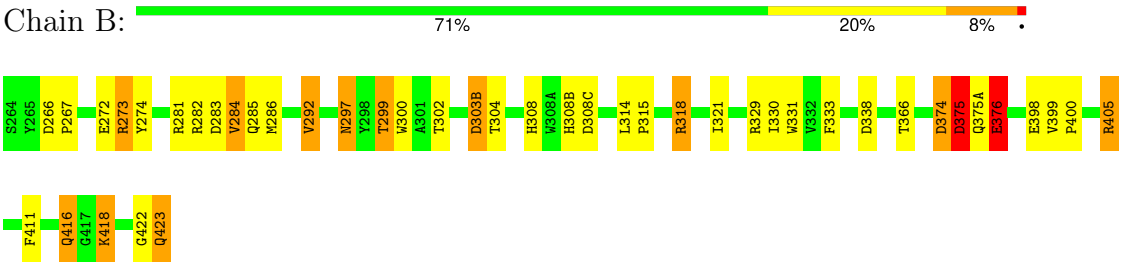
• Molecule 1: SERINE CARBOXYPEPTIDASE II

Chain A:



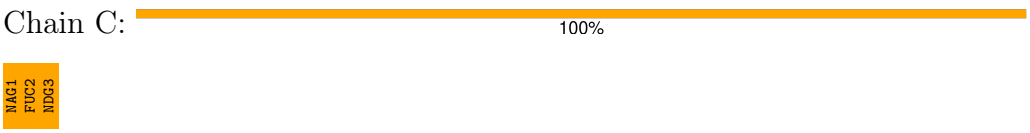
• Molecule 2: SERINE CARBOXYPEPTIDASE II

Chain B:



• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.50Å 95.50Å 208.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3741	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: BZS, NAG, FUC, NDG

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	1.15	9/2066 (0.4%)	1.60	38/2819 (1.3%)
2	B	1.17	5/1253 (0.4%)	1.58	21/1718 (1.2%)
All	All	1.16	14/3319 (0.4%)	1.59	59/4537 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
2	B	2	0
All	All	3	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	376	GLU	CD-OE2	12.47	1.39	1.25
1	A	81	GLU	CD-OE1	10.51	1.37	1.25
1	A	128	GLU	CD-OE2	8.23	1.34	1.25
1	A	39	GLU	CD-OE1	8.09	1.34	1.25
1	A	154	GLU	CD-OE2	8.07	1.34	1.25
1	A	190	GLU	CD-OE1	6.90	1.33	1.25
1	A	208	GLU	CD-OE1	6.59	1.32	1.25
2	B	398	GLU	CD-OE2	-6.41	1.18	1.25
1	A	65	GLU	CD-OE1	5.82	1.32	1.25
2	B	272	GLU	CD-OE1	5.61	1.31	1.25
2	B	375	ASP	CG-OD2	5.37	1.37	1.25
1	A	64	GLU	CD-OE1	5.22	1.31	1.25
1	A	208	GLU	CD-OE2	-5.17	1.20	1.25
2	B	422	GLY	CA-C	5.01	1.59	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	ARG	NE-CZ-NH1	22.07	131.34	120.30
1	A	114	ARG	NE-CZ-NH1	18.39	129.50	120.30
2	B	405	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	A	114	ARG	NE-CZ-NH2	-13.29	113.66	120.30
2	B	303(B)	ASP	CB-CG-OD1	-11.30	108.12	118.30
1	A	205	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	129	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	200	ASP	CB-CG-OD1	8.91	126.32	118.30
1	A	205	ARG	CD-NE-CZ	8.59	135.62	123.60
2	B	318	ARG	NE-CZ-NH2	-8.46	116.07	120.30
2	B	318	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	15	ASP	CB-CG-OD2	-8.21	110.91	118.30
2	B	405	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	114	ARG	CD-NE-CZ	8.00	134.81	123.60
1	A	201	ASP	CB-CG-OD1	-7.91	111.19	118.30
2	B	308(C)	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	A	0	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	204	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	204	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	200	ASP	CB-CG-OD2	-7.46	111.58	118.30
2	B	375	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	40	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	184	ASP	CB-CG-OD2	7.04	124.64	118.30
2	B	303(B)	ASP	CA-CB-CG	-7.02	97.96	113.40
2	B	329	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	B	308(C)	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	94	ASP	CB-CG-OD1	6.93	124.54	118.30
2	B	374	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	181	ASP	CB-CG-OD2	-6.67	112.30	118.30
2	B	266	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	B	266	ASP	CB-CG-OD1	6.57	124.21	118.30
2	B	318	ARG	CD-NE-CZ	6.38	132.54	123.60
1	A	223	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	204	ARG	CD-NE-CZ	6.30	132.43	123.60
2	B	338	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	23(A)	ASP	CB-CG-OD1	-6.20	112.72	118.30
2	B	338	ASP	CB-CG-OD1	6.15	123.84	118.30
1	A	181	ASP	CB-CG-OD1	6.14	123.83	118.30
2	B	273	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	182	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	94	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	B	375	ASP	CB-CG-OD1	5.98	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	LYS	CB-CA-C	-5.96	98.47	110.40
1	A	0	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	11	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	B	375	ASP	CA-CB-CG	5.83	126.23	113.40
1	A	83	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	-1	ASP	CB-CG-OD2	5.74	123.46	118.30
1	A	223	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	15	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	146	SER	N-CA-CB	-5.38	102.43	110.50
2	B	303(B)	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	70	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	416	GLN	CB-CA-C	5.21	120.83	110.40
1	A	180	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	139	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	140	PHE	N-CA-CB	-5.16	101.31	110.60
1	A	83	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	40	ASP	CB-CG-OD1	5.12	122.91	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	226	THR	CB
2	B	302	THR	CB
2	B	366	THR	CB

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2003	0	1855	46	0
2	B	1213	0	1150	34	0
3	C	38	0	33	5	0
4	D	28	0	25	5	0
5	A	14	0	13	4	0
6	A	15	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	259	0	0	6	1
7	B	171	0	0	5	0
All	All	3741	0	3086	82	1

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 13.

All (82) 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)
2:B:297:ASN:H	2:B:297:ASN:ND2	1.65	0.94
2:B:297:ASN:HD22	2:B:297:ASN:N	1.56	0.88
2:B:285:GLN:HE22	4:D:1:NAG:H83	1.43	0.83
3:C:2:FUC:H3	3:C:3:NDG:H6C1	1.59	0.82
2:B:297:ASN:H	2:B:297:ASN:HD22	0.86	0.80
3:C:2:FUC:H3	3:C:3:NDG:C6	2.12	0.79
2:B:281:ARG:HB2	2:B:284:VAL:HG13	1.66	0.77
1:A:223:ASP:HA	1:A:226:THR:HG22	1.68	0.74
1:A:4:LEU:H	1:A:7:GLN:NE2	1.87	0.72
3:C:2:FUC:H5	3:C:3:NDG:C1	2.22	0.70
4:D:1:NAG:H61	4:D:2:NAG:H82	1.75	0.68
2:B:282:ARG:O	2:B:286:MET:HG3	1.93	0.67
2:B:375:ASP:CG	2:B:375(A):GLN:H	1.99	0.64
1:A:3:ARG:NH1	1:A:9:ALA:N	2.49	0.61
2:B:304:THR:O	2:B:308:HIS:HD2	1.85	0.60
2:B:300:TRP:HB2	4:D:1:NAG:H81	1.82	0.60
1:A:3:ARG:HH12	1:A:9:ALA:N	1.99	0.60
1:A:226:THR:HG23	7:A:1309:HOH:O	2.02	0.59
1:A:113:ASN:HD22	5:A:1131:NAG:H83	1.68	0.58
1:A:207:LYS:HE2	7:A:1203:HOH:O	2.05	0.57
2:B:416:GLN:NE2	7:B:2979:HOH:O	2.36	0.56
1:A:226:THR:HG21	7:A:1248:HOH:O	2.05	0.55
2:B:318:ARG:HD3	7:B:3011:HOH:O	2.06	0.55
1:A:-4:HIS:NE2	7:A:1262:HOH:O	2.32	0.55
1:A:5:PRO:HG2	2:B:284:VAL:HG12	1.89	0.54
2:B:281:ARG:HB3	2:B:283:ASP:OD1	2.07	0.54
1:A:113:ASN:ND2	5:A:1131:NAG:H83	2.22	0.54
1:A:4:LEU:H	1:A:7:GLN:HE21	1.52	0.54
1:A:204:ARG:HH21	1:A:205:ARG:HB2	1.72	0.53
1:A:27:GLY:HA3	1:A:105:ASN:HB2	1.89	0.53
2:B:321:ILE:HG13	2:B:330:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:HG2	1:A:8:PRO:O	2.09	0.53
1:A:164:ASN:OD1	1:A:165:PRO:HD2	2.10	0.52
1:A:106:THR:O	1:A:109:ASP:HB2	2.10	0.52
1:A:72:LYS:HB3	1:A:73:PRO:HD2	1.92	0.52
1:A:60:TYR:OH	2:B:302:THR:HG21	2.10	0.51
2:B:374:ASP:OD2	2:B:405:ARG:NH1	2.37	0.51
1:A:152:VAL:HB	1:A:153:PRO:HD3	1.93	0.51
5:A:1131:NAG:H83	7:A:1316:HOH:O	2.10	0.50
2:B:281:ARG:O	2:B:285:GLN:HG3	2.11	0.50
2:B:304:THR:O	2:B:308:HIS:CD2	2.65	0.50
1:A:214:SER:OG	1:A:217:HIS:N	2.42	0.50
1:A:3:ARG:NH1	1:A:9:ALA:CA	2.75	0.49
3:C:1:NAG:H61	3:C:3:NDG:H2	1.94	0.49
1:A:62:ALA:O	1:A:67:GLY:HA3	2.12	0.49
1:A:223:ASP:HA	1:A:226:THR:CG2	2.39	0.49
2:B:274:TYR:N	2:B:274:TYR:CD1	2.78	0.48
3:C:2:FUC:C3	3:C:3:NDG:H6C1	2.37	0.48
1:A:72:LYS:HG2	1:A:76(A):GLY:C	2.34	0.47
1:A:84:TRP:HB3	2:B:411:PHE:CE2	2.49	0.47
1:A:114:ARG:HD2	7:A:1166:HOH:O	2.14	0.46
2:B:314:LEU:N	2:B:315:PRO:CD	2.78	0.46
2:B:374:ASP:O	2:B:376:GLU:HG3	2.16	0.46
1:A:246:CYS:HA	2:B:267:PRO:HG2	1.98	0.45
1:A:146:SER:OG	6:A:430:BZS:O2	2.30	0.45
2:B:375:ASP:OD1	2:B:375(A):GLN:N	2.32	0.44
1:A:-4:HIS:HB2	1:A:130:PHE:CE2	2.53	0.44
2:B:299:THR:HA	4:D:2:NAG:O6	2.18	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.69	0.43
1:A:223:ASP:CA	1:A:226:THR:HG22	2.43	0.43
1:A:175:GLY:HA3	2:B:333:PHE:CZ	2.54	0.43
2:B:423:GLN:N	7:B:3081:HOH:O	2.34	0.43
2:B:416:GLN:HG3	2:B:418:LYS:HB2	2.01	0.43
1:A:53:GLY:HA3	1:A:54:PRO:C	2.38	0.43
1:A:216:ILE:HG23	1:A:216:ILE:HD13	1.62	0.42
2:B:292:VAL:HG23	7:B:3073:HOH:O	2.18	0.42
2:B:423:GLN:HB3	7:B:3080:HOH:O	2.20	0.42
4:D:1:NAG:HO3	4:D:2:NAG:HO6	1.58	0.42
1:A:112(A):SER:O	2:B:308(B):HIS:HD2	2.03	0.42
1:A:141:TYR:CE2	1:A:170:LYS:HB2	2.55	0.42
5:A:1131:NAG:H82	5:A:1131:NAG:H2	1.75	0.42
1:A:157:GLN:HG2	1:A:161:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HB	1:A:14:PHE:CE2	2.55	0.41
1:A:150:HIS:O	1:A:153:PRO:HD2	2.20	0.41
1:A:173:MET:HA	2:B:331:TRP:O	2.21	0.41
1:A:37:ALA:HA	1:A:85:ASN:O	2.20	0.41
1:A:216:ILE:HD12	1:A:216:ILE:HG21	1.61	0.41
1:A:72:LYS:HB3	1:A:73:PRO:CD	2.51	0.40
1:A:72:LYS:HD2	1:A:72:LYS:HA	1.38	0.40
1:A:164:ASN:OD1	1:A:166:VAL:HG22	2.21	0.40
2:B:399:VAL:HB	2:B:400:PRO:HD3	2.02	0.40
2:B:418:LYS:HA	2:B:418:LYS:HD3	1.73	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1308:HOH:O	7:A:1308:HOH:O[8_665]	1.81	0.39

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	254/256 (99%)	242 (95%)	12 (5%)	0	100	100
2	B	151/153 (99%)	144 (95%)	6 (4%)	1 (1%)	22	16
All	All	405/409 (99%)	386 (95%)	18 (4%)	1 (0%)	47	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	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	205/208 (99%)	195 (95%)	10 (5%)	25 21
2	B	126/128 (98%)	115 (91%)	11 (9%)	10 6
All	All	331/336 (98%)	310 (94%)	21 (6%)	18 13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	ARG
1	A	3	ARG
1	A	40	ASP
1	A	63	SER
1	A	66	LEU
1	A	170	LYS
1	A	205	ARG
1	A	215	PHE
1	A	216	ILE
1	A	248	ILE
2	B	273	ARG
2	B	284	VAL
2	B	292	VAL
2	B	297	ASN
2	B	299	THR
2	B	303(B)	ASP
2	B	366	THR
2	B	375	ASP
2	B	376	GLU
2	B	418	LYS
2	B	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN

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Mol	Chain	Res	Type
1	A	117	HIS
1	A	217	HIS
1	A	233	GLN
2	B	285	GLN
2	B	297	ASN
2	B	308	HIS

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

5 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.69	0	17,19,21	2.26	6 (35%)
3	FUC	C	2	3	10,10,11	3.15	4 (40%)	14,14,16	3.22	4 (28%)
3	NDG	C	3	3	14,14,15	0.75	0	17,19,21	2.97	5 (29%)
4	NAG	D	1	2,4	14,14,15	0.79	0	17,19,21	1.72	3 (17%)
4	NAG	D	2	4	14,14,15	1.78	5 (35%)	17,19,21	2.70	7 (41%)

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	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
3	NDG	C	3	3	1/1/5/7	5/6/23/26	1/1/1/1
4	NAG	D	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	2/2/5/7	4/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FUC	O5-C1	7.53	1.56	1.43
3	C	2	FUC	O5-C5	5.08	1.53	1.43
4	D	2	NAG	C2-N2	3.05	1.51	1.46
4	D	2	NAG	C3-C2	2.56	1.57	1.52
3	C	2	FUC	C4-C3	2.54	1.58	1.52
4	D	2	NAG	O4-C4	2.53	1.49	1.43
4	D	2	NAG	C4-C3	2.39	1.58	1.52
4	D	2	NAG	O3-C3	2.08	1.48	1.43
3	C	2	FUC	C1-C2	-2.00	1.47	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	NDG	O6-C6-C5	9.04	142.10	111.33
3	C	2	FUC	O3-C3-C2	8.43	127.26	110.05
3	C	2	FUC	C2-C3-C4	-6.87	98.78	110.86
3	C	1	NAG	C1-O5-C5	5.98	120.20	112.19
4	D	2	NAG	O7-C7-C8	-4.92	113.29	122.05
3	C	3	NDG	O5-C1-C2	-4.58	104.21	111.29
4	D	2	NAG	C3-C4-C5	4.34	118.10	110.23
4	D	2	NAG	O6-C6-C5	-4.08	97.44	111.33
3	C	1	NAG	O3-C3-C2	-4.07	100.94	109.40
4	D	2	NAG	C1-C2-N2	3.88	116.54	110.43
4	D	2	NAG	C4-C3-C2	3.85	116.66	111.02
3	C	3	NDG	C1-C2-N2	3.82	116.45	110.43
4	D	2	NAG	O7-C7-N2	3.74	128.59	121.98
4	D	1	NAG	C4-C3-C2	-3.67	105.64	111.02
3	C	3	NDG	C4-C3-C2	-3.42	106.01	111.02
4	D	2	NAG	C2-N2-C7	3.40	127.46	122.90
3	C	1	NAG	O6-C6-C5	-2.90	101.46	111.33
3	C	2	FUC	O2-C2-C3	2.74	115.82	110.15
4	D	1	NAG	C2-N2-C7	2.70	126.51	122.90
3	C	2	FUC	O3-C3-C4	-2.63	104.17	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	C3-C4-C5	2.60	114.95	110.23
3	C	3	NDG	C6-C5-C4	2.46	119.06	113.02
3	C	1	NAG	O5-C5-C6	-2.21	103.35	107.66
3	C	1	NAG	O3-C3-C4	-2.17	105.26	110.38
4	D	1	NAG	O4-C4-C3	2.01	115.11	110.38

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	NDG	C2
4	D	2	NAG	C2
4	D	2	NAG	C5

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NDG	C1-C2-N2-C7
3	C	3	NDG	C8-C7-N2-C2
3	C	3	NDG	O7-C7-N2-C2
4	D	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
3	C	3	NDG	O5-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
3	C	3	NDG	C4-C5-C6-O6
4	D	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NDG	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	FUC	4	0
3	C	1	NAG	1	0
4	D	2	NAG	3	0

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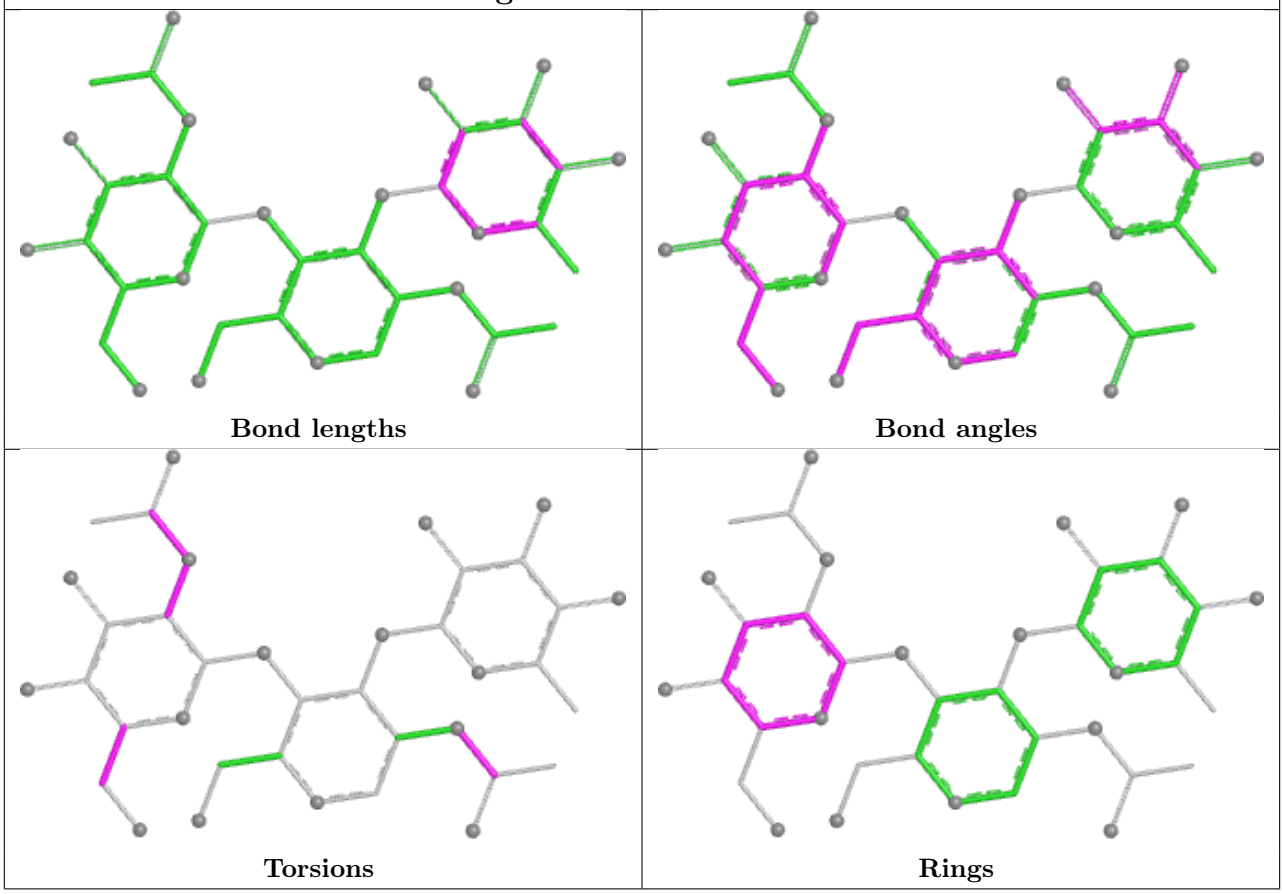
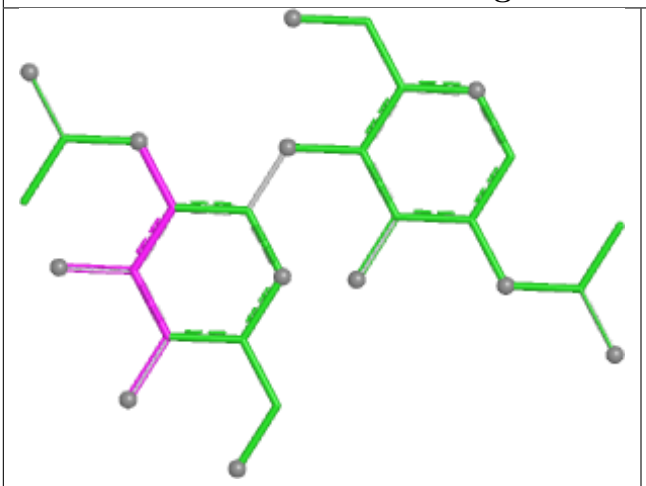
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	4	0
3	C	3	NDG	5	0

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

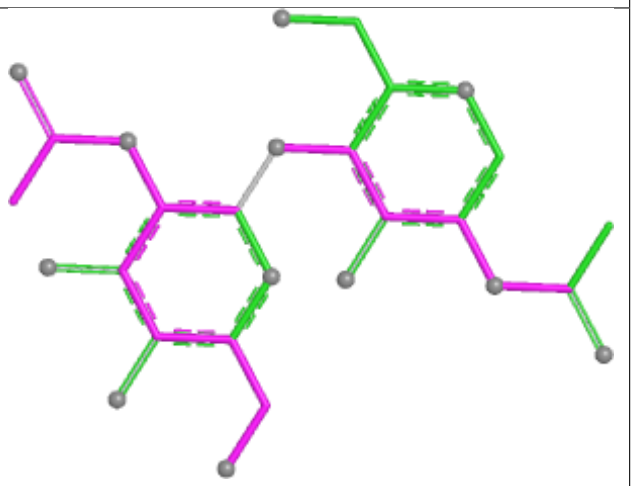
Oligosaccharide Chain C



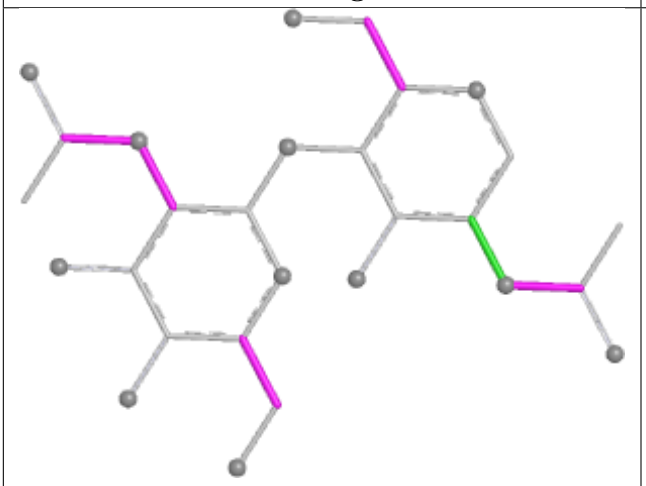
Oligosaccharide Chain D



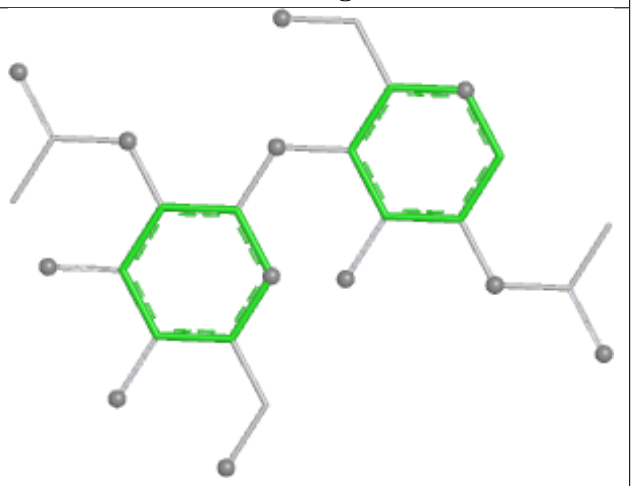
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
5	NAG	A	1131	1	14,14,15	0.84	0	17,19,21	2.05	3 (17%)
6	BZS	A	430	-	15,15,15	1.26	2 (13%)	19,19,19	1.38	2 (10%)

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
5	NAG	A	1131	1	-	2/6/23/26	0/1/1/1
6	BZS	A	430	-	-	2/12/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	430	BZS	O1-C1	2.30	1.29	1.22
6	A	430	BZS	O2-C1	-2.17	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1131	NAG	C4-C3-C2	-5.39	103.12	111.02
5	A	1131	NAG	C2-N2-C7	-5.24	115.87	122.90
6	A	430	BZS	CZ-CE2-CD2	-2.88	116.69	120.24
6	A	430	BZS	O3-C-CA	-2.76	115.52	122.86
5	A	1131	NAG	O5-C1-C2	-2.06	108.10	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1131	NAG	C8-C7-N2-C2
5	A	1131	NAG	O7-C7-N2-C2
6	A	430	BZS	O3-C-CA-C2
6	A	430	BZS	O4-C-CA-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1131	NAG	4	0
6	A	430	BZS	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

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.