Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 03:54 AM EDT

PDB ID	:	3E7J
Title	:	HeparinaseII H202A/Y257A double mutant complexed with a heparan sulfate tetrasaccharide substrate
Authors	:	Shaya, D.; Cygler, M.
Deposited on	:	2008-08-18
Resolution	:	2.10 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 (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:

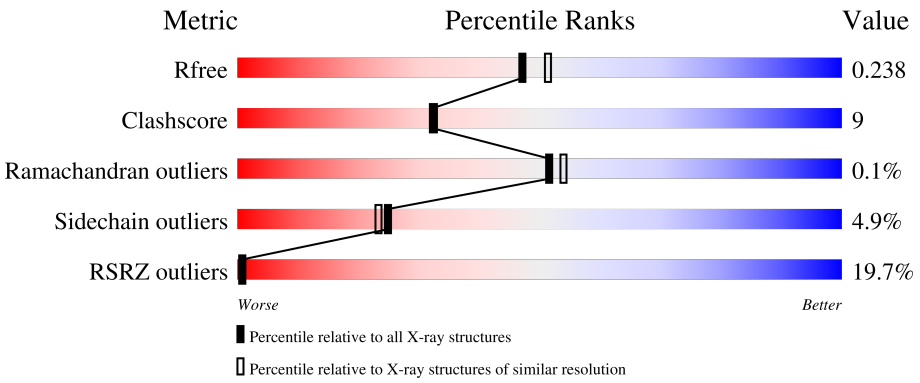
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	749	16% 82% 14% • •
1	B	749	23% 79% 16% • •
2	C	4	50% 50%
2	D	4	25% 75%

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	GCU	C	2	X	-	-	-
2	NAG	C	3	X	-	-	-
2	GCU	D	2	X	-	-	-
2	NAG	D	3	X	-	-	-
2	GCD	D	4	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12784 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 Heparinase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	743	5938	3823	1001	1091	23	0	0	0
1	B	743	5938	3823	1001	1091	23	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	HIS	engineered mutation	UNP Q46080
A	257	ALA	TYR	engineered mutation	UNP Q46080
A	758	ALA	PRO	SEE REMARK 999	UNP Q46080
B	202	ALA	HIS	engineered mutation	UNP Q46080
B	257	ALA	TYR	engineered mutation	UNP Q46080
B	758	ALA	PRO	SEE REMARK 999	UNP Q46080

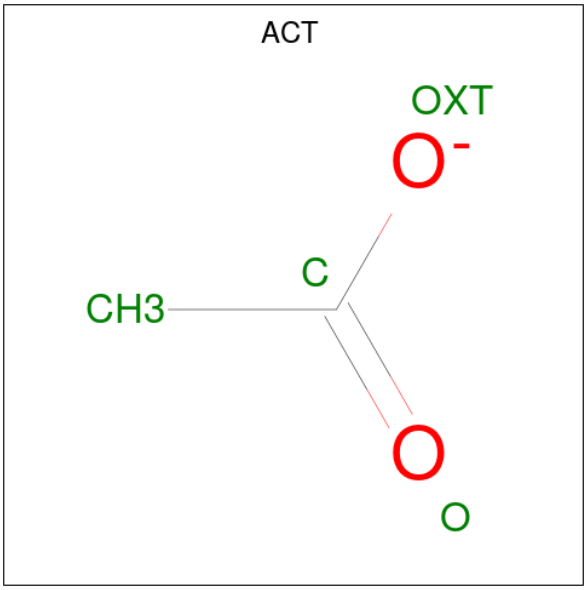
- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	4	52	28	2	22	0	0	0
2	D	4	52	28	2	22	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

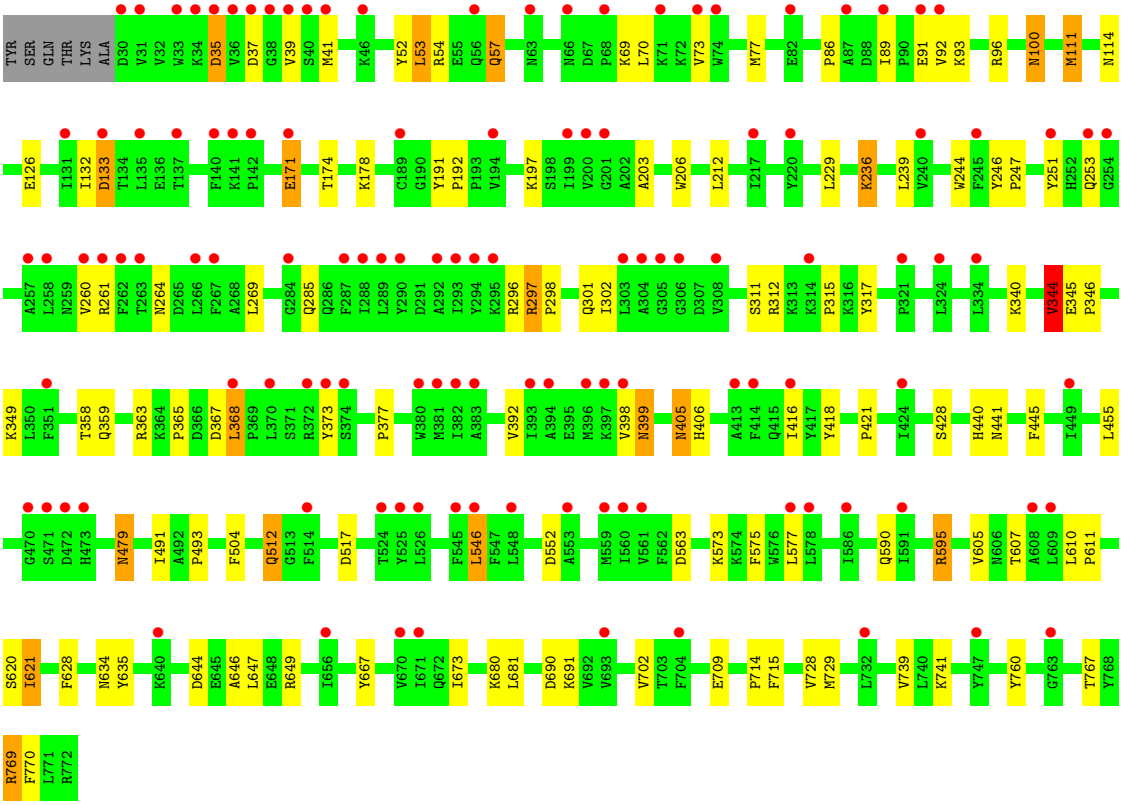
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	480	Total O 480 480	0	0
5	B	302	Total O 302 302	0	0

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 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.

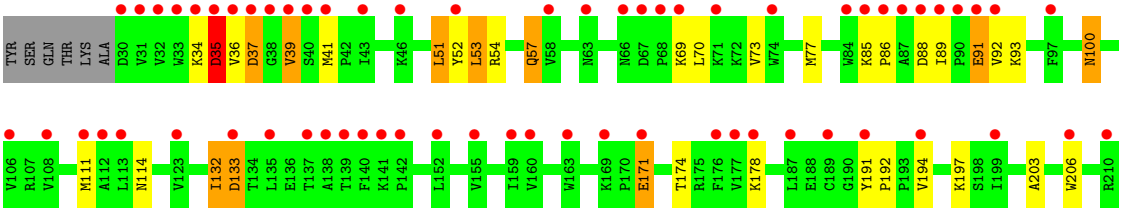
- Molecule 1: Heparinase II protein

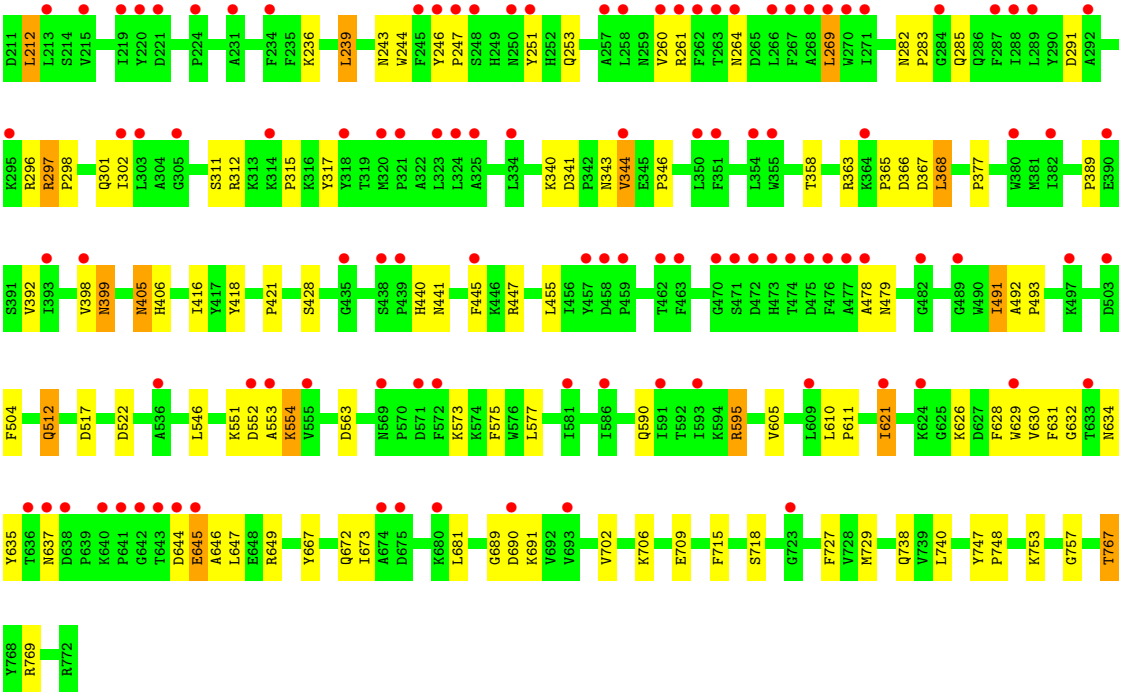
Chain A:



- Molecule 1: Heparinase II protein

Chain B:





• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranuronic acid-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 25% 75%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.95Å 162.21Å 93.84Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	42.52 – 2.10 42.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	82.9 (42.52-2.10) 82.9 (42.53-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.234 0.207 , 0.238	Depositor DCC
R_{free} test set	3630 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12784	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ACT, GCD, ZN, GCU

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	0.34	1/6098 (0.0%)	0.55	6/8253 (0.1%)
1	B	0.35	2/6098 (0.0%)	0.57	8/8253 (0.1%)
All	All	0.34	3/12196 (0.0%)	0.56	14/16506 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	344	VAL	CB-CG2	-7.57	1.36	1.52
1	A	344	VAL	CB-CG2	-7.40	1.37	1.52
1	B	344	VAL	CB-CG1	-7.18	1.37	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ASP	CB-CG-OD2	13.62	130.56	118.30
1	A	133	ASP	CB-CG-OD1	-12.07	107.43	118.30
1	A	133	ASP	CB-CG-OD2	11.43	128.59	118.30
1	A	35	ASP	CB-CG-OD2	10.50	127.75	118.30
1	B	133	ASP	CB-CG-OD1	-10.44	108.91	118.30
1	B	35	ASP	CB-CG-OD2	9.79	127.11	118.30
1	B	35	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	B	344	VAL	CG1-CB-CG2	-9.13	96.29	110.90
1	B	517	ASP	CB-CG-OD2	9.07	126.46	118.30
1	A	35	ASP	CB-CG-OD1	-8.56	110.60	118.30
1	A	517	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	552	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	552	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	91	GLU	CA-CB-CG	5.12	124.66	113.40

There are no chirality outliers.

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	5938	0	5853	103	0
1	B	5938	0	5853	106	0
2	C	52	0	37	1	0
2	D	52	0	37	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	0	12	1	0
4	B	4	0	3	0	0
5	A	480	0	0	5	0
5	B	302	0	0	2	0
All	All	12784	0	11795	210	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 (210) 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:628:PHE:H	1:A:634:ASN:HD21	1.05	1.02
1:A:769:ARG:HG2	1:A:769:ARG:HH21	1.23	1.01
1:A:769:ARG:HH21	1:A:769:ARG:CG	1.76	0.98
1:B:522:ASP:OD1	1:B:551:LYS:NZ	2.00	0.95
1:B:628:PHE:H	1:B:634:ASN:HD21	1.06	0.94
1:A:53:LEU:HB2	1:A:57:GLN:HG3	1.46	0.93
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.34	0.92
1:A:253:GLN:HE22	1:A:405:ASN:HB3	1.34	0.90
1:A:590:GLN:NE2	1:A:607:THR:OG1	2.06	0.88
1:B:261:ARG:HH11	1:B:261:ARG:HG3	1.42	0.83
1:B:398:VAL:O	1:B:399:ASN:HB2	1.79	0.81
1:A:269:LEU:HD23	1:A:285:GLN:HE22	1.46	0.80
1:A:171:GLU:H	1:A:171:GLU:CD	1.86	0.78
1:B:690:ASP:O	1:B:715:PHE:HB2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ARG:HB3	1:B:298:PRO:HD2	1.66	0.76
1:A:269:LEU:CD2	1:A:285:GLN:HE22	1.99	0.76
1:A:628:PHE:H	1:A:634:ASN:ND2	1.84	0.75
1:B:628:PHE:H	1:B:634:ASN:ND2	1.84	0.74
1:B:53:LEU:HB2	1:B:57:GLN:HG3	1.68	0.74
1:B:191:TYR:HA	1:B:192:PRO:C	2.08	0.74
1:A:261:ARG:HG3	1:A:261:ARG:HH11	1.52	0.73
1:B:546:LEU:HD22	1:B:702:VAL:HG21	1.70	0.73
1:B:92:VAL:HG13	1:B:92:VAL:O	1.89	0.72
1:A:455:LEU:HD11	1:A:577:LEU:HD11	1.72	0.72
1:B:171:GLU:CD	1:B:171:GLU:H	1.94	0.71
1:A:297:ARG:HB3	1:A:298:PRO:HD2	1.73	0.70
1:A:398:VAL:O	1:A:399:ASN:HB2	1.90	0.70
1:B:86:PRO:HA	1:B:89:ILE:HD12	1.75	0.69
1:A:416:ILE:HG21	1:A:673:ILE:HD12	1.77	0.67
1:A:111:MET:HE2	1:A:126:GLU:HG2	1.77	0.67
1:B:455:LEU:HD11	1:B:577:LEU:HD11	1.76	0.67
1:B:573:LYS:HD3	1:B:575:PHE:CZ	2.30	0.67
1:B:92:VAL:O	1:B:92:VAL:CG1	2.42	0.66
1:A:621:ILE:HD13	1:A:621:ILE:N	2.10	0.66
1:A:628:PHE:N	1:A:634:ASN:HD21	1.87	0.66
1:A:573:LYS:HD3	1:A:575:PHE:CZ	2.31	0.66
1:A:92:VAL:O	1:A:92:VAL:HG13	1.96	0.66
1:B:644:ASP:OD2	1:B:649:ARG:HD2	1.96	0.66
1:A:644:ASP:OD2	1:A:649:ARG:HD2	1.96	0.65
1:B:269:LEU:HG	1:B:285:GLN:HE22	1.61	0.65
1:B:301:GLN:NE2	1:B:311:SER:O	2.29	0.64
1:A:301:GLN:NE2	1:A:311:SER:O	2.30	0.64
1:A:769:ARG:HG2	1:A:769:ARG:NH2	2.05	0.63
1:B:51:LEU:HD13	1:B:52:TYR:CE1	2.33	0.63
1:A:345:GLU:OE1	5:A:1211:HOH:O	2.16	0.63
1:A:590:GLN:HE21	1:A:607:THR:HG23	1.65	0.62
1:A:610:LEU:HA	1:A:611:PRO:C	2.19	0.61
1:B:261:ARG:HG3	1:B:261:ARG:NH1	2.15	0.61
1:B:365:PRO:HA	1:B:368:LEU:HD12	1.83	0.60
1:A:86:PRO:HA	1:A:89:ILE:HD12	1.84	0.59
1:B:629:TRP:CH2	1:B:632:GLY:O	2.54	0.59
1:A:416:ILE:HG21	1:A:673:ILE:CD1	2.32	0.59
1:A:35:ASP:HB2	5:A:1234:HOH:O	2.03	0.59
1:A:769:ARG:CG	1:A:769:ARG:NH2	2.46	0.59
1:B:610:LEU:HA	1:B:611:PRO:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:PRO:HA	1:A:368:LEU:HD12	1.87	0.57
1:A:253:GLN:HE22	1:A:406:HIS:H	1.52	0.57
1:A:92:VAL:O	1:A:92:VAL:CG1	2.52	0.57
1:B:73:VAL:O	1:B:77:MET:HG3	2.05	0.57
1:B:53:LEU:CB	1:B:57:GLN:HG3	2.34	0.57
1:A:563:ASP:HB2	1:A:667:TYR:HB2	1.86	0.56
1:A:590:GLN:NE2	1:A:607:THR:HG23	2.21	0.56
1:B:253:GLN:HE21	1:B:261:ARG:HH12	1.54	0.55
1:A:546:LEU:HD22	1:A:702:VAL:HG21	1.88	0.55
1:A:741:LYS:HA	1:A:767:THR:O	2.07	0.55
1:A:73:VAL:O	1:A:77:MET:HG3	2.07	0.55
1:A:620:SER:C	1:A:621:ILE:HD13	2.27	0.55
1:B:628:PHE:N	1:B:634:ASN:HD21	1.89	0.55
1:B:296:ARG:HE	1:B:302:ILE:HD13	1.72	0.55
1:B:563:ASP:HB2	1:B:667:TYR:HB2	1.87	0.54
1:B:621:ILE:CD1	1:B:621:ILE:N	2.70	0.54
4:A:5:ACT:H3	2:C:2:GCU:H3	1.90	0.54
1:B:260:VAL:HG13	1:B:261:ARG:N	2.23	0.54
1:B:253:GLN:HE22	1:B:406:HIS:H	1.55	0.54
1:A:428:SER:H	1:A:440:HIS:HE1	1.55	0.53
1:A:253:GLN:NE2	1:A:405:ASN:HB3	2.15	0.53
1:A:191:TYR:HA	1:A:192:PRO:C	2.29	0.53
1:B:689:GLY:O	1:B:706:LYS:NZ	2.41	0.53
1:B:260:VAL:CG1	1:B:261:ARG:N	2.70	0.53
1:A:244:TRP:CZ3	1:A:377:PRO:HG3	2.44	0.53
1:B:398:VAL:O	1:B:399:ASN:CB	2.54	0.53
1:B:312:ARG:NH1	1:B:646:ALA:HB2	2.23	0.53
1:A:359:GLN:HG3	5:A:1237:HOH:O	2.09	0.52
1:B:312:ARG:HG3	1:B:312:ARG:HH11	1.74	0.52
1:B:672:GLN:OE1	1:B:681:LEU:HB3	2.09	0.52
1:A:261:ARG:HG3	1:A:261:ARG:NH1	2.21	0.52
1:B:769:ARG:HH11	1:B:769:ARG:HG2	1.73	0.52
1:B:34:LYS:NZ	5:B:1311:HOH:O	2.41	0.52
1:A:111:MET:HE2	1:A:126:GLU:CG	2.39	0.52
1:B:296:ARG:HE	1:B:302:ILE:CD1	2.23	0.52
1:A:111:MET:CE	1:A:126:GLU:CD	2.78	0.51
1:A:246:TYR:N	1:A:247:PRO:CD	2.73	0.51
1:B:70:LEU:HG	1:B:358:THR:HG21	1.92	0.51
1:B:428:SER:H	1:B:440:HIS:HE1	1.57	0.51
1:A:39:VAL:HG13	1:A:41:MET:HE3	1.93	0.51
1:B:244:TRP:CZ3	1:B:377:PRO:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TYR:N	1:B:247:PRO:CD	2.72	0.51
1:B:269:LEU:HG	1:B:285:GLN:NE2	2.26	0.51
1:A:35:ASP:HA	1:A:39:VAL:O	2.10	0.51
1:A:171:GLU:OE1	1:A:171:GLU:N	2.41	0.51
1:A:760:TYR:HE1	5:A:1212:HOH:O	1.95	0.50
1:B:416:ILE:HG21	1:B:673:ILE:HD12	1.94	0.50
1:A:728:VAL:HG22	1:A:760:TYR:HD1	1.76	0.50
1:B:341:ASP:OD1	1:B:343:ASN:ND2	2.43	0.50
1:B:491:ILE:HD12	1:B:492:ALA:H	1.76	0.50
1:A:590:GLN:NE2	1:A:607:THR:CB	2.75	0.49
1:A:373:TYR:CD2	1:A:512:GLN:NE2	2.80	0.49
1:B:37:ASP:HB3	1:B:236:LYS:NZ	2.28	0.49
1:A:253:GLN:NE2	1:A:406:HIS:H	2.10	0.49
1:A:70:LEU:HG	1:A:358:THR:HG21	1.94	0.49
1:A:171:GLU:CD	1:A:171:GLU:N	2.61	0.48
1:A:605:VAL:HG21	1:A:681:LEU:HD11	1.94	0.48
1:A:421:PRO:HD2	1:A:595:ARG:HD2	1.95	0.48
1:B:645:GLU:H	1:B:645:GLU:CD	2.17	0.48
1:B:191:TYR:CA	1:B:192:PRO:C	2.81	0.48
1:A:690:ASP:O	1:A:715:PHE:HB2	2.13	0.48
1:A:714:PRO:HA	1:A:770:PHE:O	2.13	0.48
1:B:718:SER:OG	1:B:767:THR:HG22	2.14	0.48
1:A:440:HIS:HD2	1:A:635:TYR:O	1.97	0.47
1:A:344:VAL:HG12	1:A:349:LYS:HD3	1.96	0.47
1:A:590:GLN:NE2	1:A:607:THR:CG2	2.78	0.47
1:B:315:PRO:HB2	1:B:317:TYR:CZ	2.49	0.47
1:B:174:THR:O	1:B:178:LYS:HG3	2.15	0.47
1:B:296:ARG:HH12	1:B:340:LYS:HE2	1.79	0.47
1:B:440:HIS:HD2	1:B:635:TYR:O	1.97	0.47
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.40	0.47
1:B:421:PRO:HD2	1:B:595:ARG:HD2	1.96	0.47
1:A:398:VAL:O	1:A:399:ASN:CB	2.60	0.46
1:A:253:GLN:HE21	1:A:261:ARG:HH12	1.61	0.46
1:A:455:LEU:CD1	1:A:577:LEU:HD11	2.45	0.46
1:A:260:VAL:HG13	1:A:261:ARG:N	2.30	0.46
1:B:171:GLU:CD	1:B:171:GLU:N	2.67	0.46
1:B:253:GLN:NE2	1:B:406:HIS:H	2.14	0.46
1:A:296:ARG:HE	1:A:302:ILE:CD1	2.29	0.46
1:A:260:VAL:CG1	1:A:261:ARG:N	2.79	0.45
1:B:192:PRO:HB2	1:B:194:VAL:HG13	1.97	0.45
1:A:39:VAL:HG11	1:A:236:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:TRP:HA	1:B:264:ASN:OD1	2.16	0.45
1:B:621:ILE:HG22	1:B:626:LYS:HB3	1.97	0.45
1:A:493:PRO:HD3	1:A:504:PHE:CE2	2.52	0.45
1:A:690:ASP:O	1:A:691:LYS:HB2	2.16	0.45
1:A:680:LYS:HD3	1:A:681:LEU:O	2.17	0.45
1:B:296:ARG:NH1	1:B:340:LYS:HE2	2.32	0.45
1:B:553:ALA:O	1:B:554:LYS:C	2.52	0.45
1:B:605:VAL:HG21	1:B:681:LEU:HD11	1.99	0.45
1:B:54:ARG:O	1:B:57:GLN:HG2	2.16	0.45
1:B:738:GLN:HE21	1:B:740:LEU:HD11	1.82	0.45
1:A:312:ARG:NH1	1:A:646:ALA:HB2	2.31	0.45
1:B:690:ASP:O	1:B:691:LYS:HB2	2.17	0.44
1:B:239:LEU:HD22	1:B:243:ASN:ND2	2.32	0.44
1:A:54:ARG:O	1:A:57:GLN:HG2	2.16	0.44
1:B:36:VAL:O	1:B:37:ASP:HB2	2.17	0.44
1:A:769:ARG:HD2	1:A:769:ARG:HA	1.81	0.44
1:A:96:ARG:HD2	5:A:1209:HOH:O	2.18	0.44
1:A:111:MET:CE	1:A:126:GLU:OE1	2.66	0.44
1:A:769:ARG:HH21	1:A:769:ARG:HG3	1.74	0.44
1:B:253:GLN:NE2	1:B:405:ASN:HB3	2.16	0.44
1:B:197:LYS:O	1:B:203:ALA:HB3	2.17	0.44
1:A:206:TRP:HA	1:A:264:ASN:OD1	2.17	0.43
1:A:296:ARG:HE	1:A:302:ILE:HD13	1.83	0.43
1:A:647:LEU:HD12	1:A:649:ARG:HD3	2.00	0.43
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.90	0.43
1:B:416:ILE:HG21	1:B:673:ILE:CD1	2.48	0.43
1:B:35:ASP:HA	1:B:39:VAL:O	2.18	0.43
1:B:455:LEU:HB2	1:B:575:PHE:HB2	2.00	0.43
1:A:111:MET:CE	1:A:126:GLU:CG	2.97	0.43
1:B:100:ASN:HD22	1:B:346:PRO:HG2	1.83	0.43
1:B:512:GLN:OE1	1:B:512:GLN:C	2.57	0.43
1:A:197:LYS:O	1:A:203:ALA:HB3	2.18	0.43
1:B:37:ASP:HB3	1:B:236:LYS:HZ1	1.84	0.43
1:A:296:ARG:NH1	1:A:340:LYS:HE2	2.33	0.43
1:A:479:ASN:C	1:A:479:ASN:HD22	2.21	0.43
1:B:621:ILE:N	1:B:621:ILE:HD12	2.33	0.43
1:B:647:LEU:HD12	1:B:649:ARG:HD3	1.99	0.42
1:A:52:TYR:O	1:A:53:LEU:HB3	2.19	0.42
1:A:192:PRO:HB3	1:A:229:LEU:HD13	2.01	0.42
1:A:363:ARG:NH1	1:A:367:ASP:OD2	2.52	0.42
1:B:769:ARG:HG2	1:B:769:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:VAL:HG22	1:B:418:TYR:CD1	2.54	0.42
1:B:447:ARG:NH2	1:B:478:ALA:O	2.45	0.42
1:B:493:PRO:HD3	1:B:504:PHE:CE2	2.55	0.42
1:A:100:ASN:HA	1:A:346:PRO:HG2	2.01	0.42
1:A:174:THR:O	1:A:178:LYS:HG3	2.19	0.42
1:B:132:ILE:HD13	1:B:132:ILE:O	2.19	0.42
1:A:769:ARG:NH2	1:A:769:ARG:HG3	2.32	0.42
1:A:392:VAL:HG22	1:A:418:TYR:CD1	2.55	0.42
1:B:298:PRO:CB	1:B:389:PRO:HA	2.50	0.42
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.46	0.42
1:B:85:LYS:O	1:B:88:ASP:N	2.45	0.42
1:A:455:LEU:HB2	1:A:575:PHE:HB2	2.02	0.41
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.86	0.41
1:A:739:VAL:HG22	1:A:770:PHE:CD2	2.55	0.41
1:B:440:HIS:CD2	1:B:637:ASN:HB2	2.55	0.41
1:A:315:PRO:HB2	1:A:317:TYR:CZ	2.55	0.41
1:A:41:MET:HE3	1:A:41:MET:HB3	1.52	0.41
1:A:605:VAL:HG21	1:A:681:LEU:CD1	2.51	0.41
1:B:291:ASP:HB3	5:B:1352:HOH:O	2.21	0.41
1:B:753:LYS:O	1:B:757:GLY:N	2.52	0.41
1:A:441:ASN:HA	1:A:445:PHE:HB3	2.03	0.41
1:B:57:GLN:HE21	1:B:57:GLN:HB3	1.65	0.41
1:B:630:VAL:O	1:B:631:PHE:C	2.60	0.41
1:B:747:TYR:HA	1:B:748:PRO:HD2	1.90	0.40
1:B:441:ASN:HA	1:B:445:PHE:HB3	2.03	0.40
1:B:455:LEU:CD1	1:B:577:LEU:HD11	2.48	0.40
1:B:709:GLU:HA	1:B:709:GLU:OE1	2.20	0.40
1:B:39:VAL:HG13	1:B:41:MET:HG2	2.03	0.40
1:B:282:ASN:HA	1:B:283:PRO:HD3	1.94	0.40
1:B:53:LEU:HB2	1:B:57:GLN:CG	2.45	0.40
1:B:363:ARG:NH1	1:B:367:ASP:OD2	2.53	0.40
1:B:727:PHE:HB3	1:B:729:MET:HE3	2.03	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	741/749 (99%)	710 (96%)	30 (4%)	1 (0%)	51	54
1	B	741/749 (99%)	707 (95%)	33 (4%)	1 (0%)	51	54
All	All	1482/1498 (99%)	1417 (96%)	63 (4%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	ASN
1	A	399	ASN

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	628/633 (99%)	599 (95%)	29 (5%)	27	26
1	B	628/633 (99%)	595 (95%)	33 (5%)	22	20
All	All	1256/1266 (99%)	1194 (95%)	62 (5%)	25	23

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	53	LEU
1	A	57	GLN
1	A	69	LYS
1	A	91	GLU
1	A	93	LYS
1	A	100	ASN
1	A	111	MET
1	A	114	ASN
1	A	132	ILE

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Mol	Chain	Res	Type
1	A	133	ASP
1	A	171	GLU
1	A	212	LEU
1	A	236	LYS
1	A	239	LEU
1	A	251	TYR
1	A	297	ARG
1	A	344	VAL
1	A	368	LEU
1	A	405	ASN
1	A	479	ASN
1	A	491	ILE
1	A	512	GLN
1	A	546	LEU
1	A	595	ARG
1	A	621	ILE
1	A	709	GLU
1	A	729	MET
1	A	769	ARG
1	B	35	ASP
1	B	37	ASP
1	B	39	VAL
1	B	51	LEU
1	B	53	LEU
1	B	57	GLN
1	B	69	LYS
1	B	91	GLU
1	B	93	LYS
1	B	100	ASN
1	B	111	MET
1	B	114	ASN
1	B	132	ILE
1	B	133	ASP
1	B	171	GLU
1	B	212	LEU
1	B	239	LEU
1	B	251	TYR
1	B	269	LEU
1	B	297	ARG
1	B	344	VAL
1	B	366	ASP
1	B	368	LEU

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Mol	Chain	Res	Type
1	B	405	ASN
1	B	479	ASN
1	B	491	ILE
1	B	512	GLN
1	B	554	LYS
1	B	590	GLN
1	B	595	ARG
1	B	621	ILE
1	B	645	GLU
1	B	767	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	66	ASN
1	A	100	ASN
1	A	114	ASN
1	A	253	GLN
1	A	285	GLN
1	A	335	ASN
1	A	440	HIS
1	A	479	ASN
1	A	590	GLN
1	A	634	ASN
1	B	63	ASN
1	B	66	ASN
1	B	100	ASN
1	B	114	ASN
1	B	253	GLN
1	B	285	GLN
1	B	335	ASN
1	B	440	HIS
1	B	590	GLN
1	B	634	ASN
1	B	738	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

8 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	NAG	C	1	2	15,15,15	0.51	0	21,21,21	0.93	0
2	GCU	C	2	2	12,12,13	0.81	0	14,17,19	0.79	0
2	NAG	C	3	2	14,14,15	0.48	0	17,19,21	0.98	0
2	GCD	C	4	2	10,11,12	1.54	1 (10%)	13,15,17	1.96	3 (23%)
2	NAG	D	1	2	15,15,15	0.53	0	21,21,21	1.09	1 (4%)
2	GCU	D	2	2	12,12,13	0.81	0	14,17,19	0.74	0
2	NAG	D	3	2	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
2	GCD	D	4	2	10,11,12	1.56	1 (10%)	13,15,17	1.91	3 (23%)

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	NAG	C	1	2	-	0/6/26/26	0/1/1/1
2	GCU	C	2	2	1/1/5/6	0/4/21/24	0/1/1/1
2	NAG	C	3	2	1/1/5/7	0/6/23/26	0/1/1/1
2	GCD	C	4	2	-	0/4/17/20	0/1/1/1
2	NAG	D	1	2	-	0/6/26/26	0/1/1/1
2	GCU	D	2	2	1/1/5/6	0/4/21/24	0/1/1/1
2	NAG	D	3	2	1/1/5/7	2/6/23/26	0/1/1/1
2	GCD	D	4	2	1/1/4/6	0/4/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	GCD	O5-C5	4.09	1.43	1.37
2	C	4	GCD	O5-C5	4.07	1.43	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4	GCD	C2-C3-C4	-4.23	106.54	112.32
2	C	4	GCD	C2-C3-C4	-4.20	106.58	112.32
2	C	4	GCD	O5-C5-C6	3.71	117.08	111.52
2	D	4	GCD	O5-C5-C6	3.42	116.66	111.52
2	C	4	GCD	C4-C5-C6	-2.92	117.35	123.65
2	D	4	GCD	C4-C5-C6	-2.91	117.37	123.65
2	D	1	NAG	C1-C2-N2	-2.61	107.70	110.73
2	D	3	NAG	C2-N2-C7	2.33	126.22	122.90

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	GCU	C1
2	C	3	NAG	C1
2	D	2	GCU	C1
2	D	3	NAG	C1
2	D	4	GCD	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2

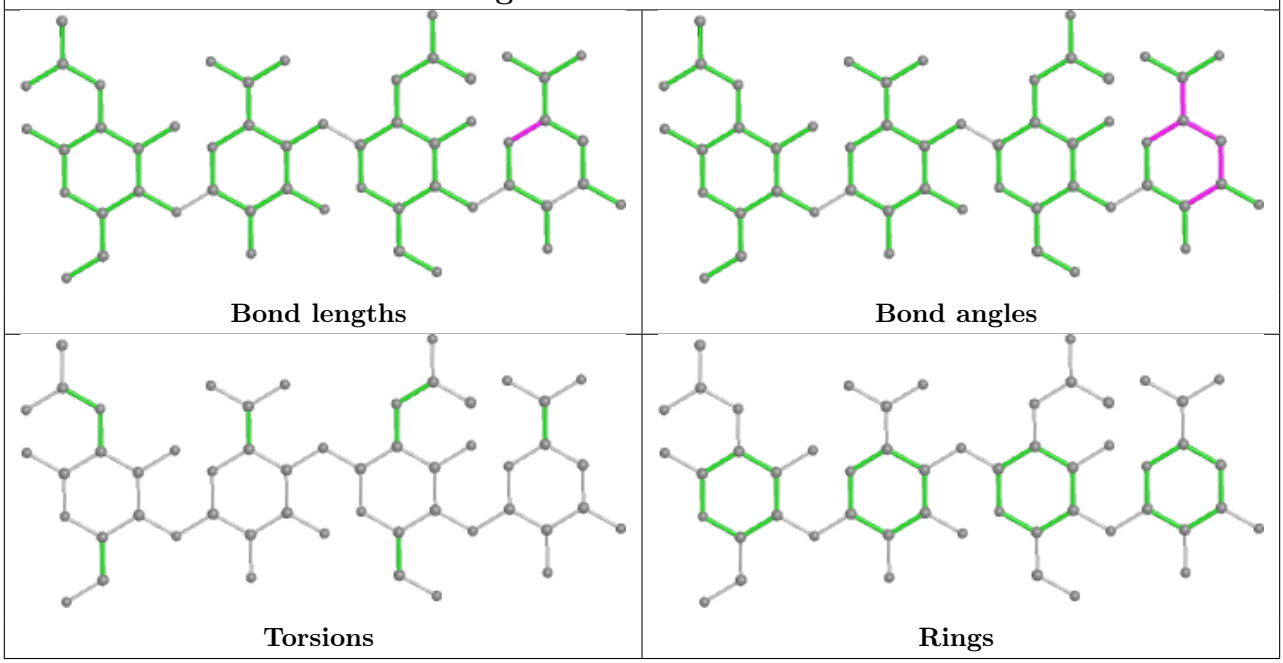
There are no ring outliers.

1 monomer is involved in 1 short contact:

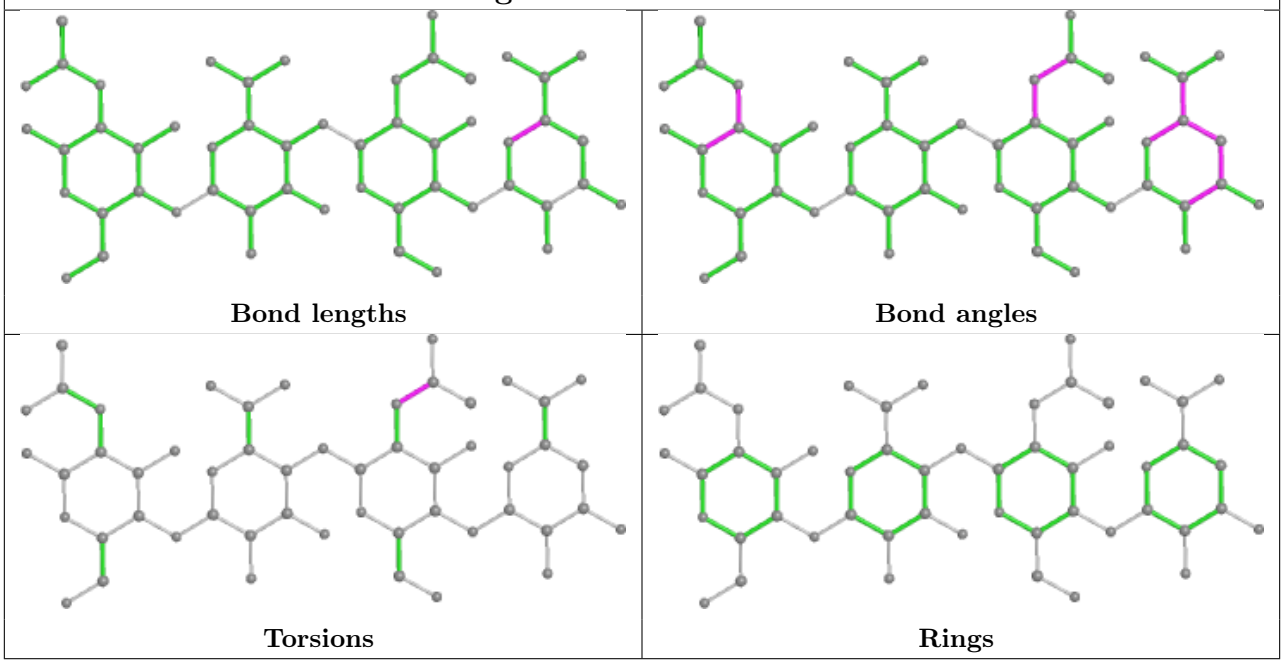
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GCU	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	ACT	A	4	-	3,3,3	0.79	0	3,3,3	1.35	0
4	ACT	A	3	-	3,3,3	0.80	0	3,3,3	1.36	0
4	ACT	A	773	-	3,3,3	0.76	0	3,3,3	1.29	0
4	ACT	B	773	-	3,3,3	0.78	0	3,3,3	1.29	0
4	ACT	A	5	-	3,3,3	0.73	0	3,3,3	1.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5	ACT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	743/749 (99%)	1.08	120 (16%)	1	2	47, 50, 50, 53	0
1	B	743/749 (99%)	1.46	172 (23%)	0	0	47, 50, 50, 53	0
All	All	1486/1498 (99%)	1.27	292 (19%)	1	1	47, 50, 50, 53	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ALA	10.4
1	B	36	VAL	9.7
1	B	37	ASP	8.1
1	B	39	VAL	7.6
1	B	470	GLY	7.4
1	B	471	SER	7.1
1	A	36	VAL	7.0
1	B	35	ASP	6.9
1	A	37	ASP	6.9
1	B	472	ASP	6.8
1	B	473	HIS	6.6
1	B	34	LYS	6.5
1	B	133	ASP	6.3
1	B	92	VAL	6.2
1	B	640	LYS	5.5
1	B	139	THR	5.5
1	B	267	PHE	5.4
1	A	133	ASP	5.4
1	B	258	LEU	5.4
1	B	324	LEU	5.4
1	A	472	ASP	5.3
1	B	641	PRO	5.3
1	B	91	GLU	5.3
1	B	32	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	38	GLY	5.2
1	B	643	THR	5.1
1	A	33	TRP	5.1
1	B	141	LYS	5.0
1	B	90	PRO	5.0
1	B	88	ASP	5.0
1	B	474	THR	4.9
1	A	30	ASP	4.8
1	B	68	PRO	4.8
1	B	262	PHE	4.7
1	B	266	LEU	4.6
1	A	91	GLU	4.6
1	B	553	ALA	4.6
1	B	288	ILE	4.5
1	B	351	PHE	4.4
1	B	633	THR	4.4
1	B	66	ASN	4.4
1	B	33	TRP	4.3
1	A	258	LEU	4.3
1	B	89	ILE	4.3
1	B	38	GLY	4.2
1	A	471	SER	4.2
1	A	40	SER	4.2
1	B	40	SER	4.1
1	A	288	ILE	4.0
1	B	41	MET	4.0
1	B	459	PRO	4.0
1	A	34	LYS	3.9
1	B	85	LYS	3.9
1	A	31	VAL	3.8
1	A	35	ASP	3.8
1	B	477	ALA	3.8
1	B	220	TYR	3.8
1	B	260	VAL	3.8
1	B	263	THR	3.7
1	A	305	GLY	3.7
1	B	140	PHE	3.7
1	B	269	LEU	3.7
1	A	292	ALA	3.7
1	B	289	LEU	3.7
1	A	545	PHE	3.7
1	B	251	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	31	VAL	3.7
1	B	489	GLY	3.6
1	B	63	ASN	3.6
1	A	63	ASN	3.6
1	A	251	TYR	3.6
1	B	245	PHE	3.5
1	B	142	PRO	3.5
1	B	364	LYS	3.5
1	A	470	GLY	3.5
1	B	478	ALA	3.4
1	B	723	GLY	3.4
1	A	74	TRP	3.4
1	A	526	LEU	3.4
1	A	39	VAL	3.4
1	B	435	GLY	3.4
1	B	292	ALA	3.3
1	B	438	SER	3.3
1	B	321	PRO	3.3
1	B	135	LEU	3.3
1	B	199	ILE	3.3
1	B	106	VAL	3.2
1	A	266	LEU	3.2
1	A	591	ILE	3.2
1	B	178	LYS	3.2
1	A	303	LEU	3.2
1	B	536	ALA	3.2
1	A	324	LEU	3.2
1	B	642	GLY	3.2
1	A	586	ILE	3.2
1	B	71	LYS	3.2
1	A	66	ASN	3.1
1	A	609	LEU	3.1
1	B	572	PHE	3.1
1	A	293	ILE	3.1
1	B	552	ASP	3.1
1	A	87	ALA	3.1
1	B	302	ILE	3.1
1	B	97	PHE	3.1
1	B	123	VAL	3.1
1	A	306	GLY	3.0
1	B	690	ASP	3.0
1	A	290	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	383	ALA	3.0
1	B	137	THR	3.0
1	B	571	ASP	3.0
1	A	68	PRO	3.0
1	A	304	ALA	3.0
1	B	187	LEU	3.0
1	A	382	ILE	2.9
1	B	159	ILE	2.9
1	B	270	TRP	2.9
1	B	318	TYR	2.9
1	B	320	MET	2.9
1	B	680	LYS	2.9
1	B	350	LEU	2.9
1	B	74	TRP	2.9
1	B	284	GLY	2.9
1	A	220	TYR	2.9
1	A	308	VAL	2.9
1	A	46	LYS	2.9
1	B	629	TRP	2.9
1	A	396	MET	2.9
1	A	71	LYS	2.9
1	B	189	CYS	2.9
1	B	177	VAL	2.8
1	A	262	PHE	2.8
1	B	246	TYR	2.8
1	B	462	THR	2.8
1	B	250	ASN	2.8
1	A	245	PHE	2.8
1	A	142	PRO	2.8
1	B	482	GLY	2.8
1	B	138	ALA	2.8
1	A	41	MET	2.8
1	A	525	TYR	2.8
1	B	171	GLU	2.8
1	A	370	LEU	2.8
1	B	354	LEU	2.8
1	A	398	VAL	2.8
1	B	163	TRP	2.8
1	A	763	GLY	2.8
1	B	86	PRO	2.7
1	B	636	THR	2.7
1	B	624	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	323	LEU	2.7
1	B	46	LYS	2.7
1	B	231	ALA	2.7
1	B	268	ALA	2.7
1	B	439	PRO	2.7
1	B	693	VAL	2.7
1	A	89	ILE	2.7
1	A	560	ILE	2.7
1	A	524	THR	2.7
1	B	215	VAL	2.7
1	B	398	VAL	2.7
1	A	82	GLU	2.7
1	B	113	LEU	2.7
1	A	559	MET	2.7
1	A	92	VAL	2.7
1	A	693	VAL	2.7
1	B	476	PHE	2.6
1	B	111	MET	2.6
1	B	176	PHE	2.6
1	A	189	CYS	2.6
1	B	271	ILE	2.6
1	B	30	ASP	2.6
1	B	169	LYS	2.6
1	B	43	ILE	2.6
1	A	416	ILE	2.6
1	A	671	ILE	2.6
1	B	591	ILE	2.6
1	B	210	ARG	2.5
1	B	638	ASP	2.5
1	A	56	GLN	2.5
1	A	373	TYR	2.5
1	A	131	ILE	2.5
1	B	355	TRP	2.5
1	A	380	TRP	2.5
1	A	294	TYR	2.5
1	B	457	TYR	2.5
1	A	393	ILE	2.5
1	B	248	SER	2.5
1	B	593	ILE	2.5
1	A	284	GLY	2.5
1	B	221	ASP	2.5
1	A	381	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	497	LYS	2.5
1	B	108	VAL	2.5
1	A	413	ALA	2.5
1	B	257	ALA	2.5
1	A	253	GLN	2.4
1	A	473	HIS	2.4
1	A	267	PHE	2.4
1	B	569	ASN	2.4
1	B	609	LEU	2.4
1	B	155	VAL	2.4
1	B	206	TRP	2.4
1	A	608	ALA	2.4
1	B	325	ALA	2.4
1	B	224	PRO	2.4
1	A	287	PHE	2.4
1	B	303	LEU	2.4
1	B	219	ILE	2.4
1	A	254	GLY	2.4
1	A	546	LEU	2.4
1	B	305	GLY	2.4
1	A	670	VAL	2.4
1	B	67	ASP	2.4
1	B	458	ASP	2.4
1	B	675	ASP	2.4
1	B	84	TRP	2.4
1	B	393	ILE	2.4
1	A	135	LEU	2.4
1	A	200	VAL	2.4
1	B	160	VAL	2.4
1	B	344	VAL	2.4
1	B	555	VAL	2.4
1	A	257	ALA	2.4
1	B	637	ASN	2.3
1	A	260	VAL	2.3
1	B	69	LYS	2.3
1	A	424	ILE	2.3
1	A	414	PHE	2.3
1	A	578	LEU	2.3
1	B	334	LEU	2.3
1	A	201	GLY	2.3
1	A	141	LYS	2.3
1	A	372	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	314	LYS	2.3
1	A	334	LEU	2.3
1	B	213	LEU	2.3
1	B	445	PHE	2.3
1	B	380	TRP	2.3
1	A	732	LEU	2.3
1	A	397	LYS	2.3
1	B	264	ASN	2.3
1	B	586	ILE	2.3
1	B	295	LYS	2.2
1	A	240	VAL	2.2
1	A	295	LYS	2.2
1	A	394	ALA	2.2
1	A	137	THR	2.2
1	A	449	ILE	2.2
1	A	656	ILE	2.2
1	B	382	ILE	2.2
1	A	263	THR	2.2
1	B	261	ARG	2.2
1	A	140	PHE	2.2
1	A	704	PHE	2.2
1	B	52	TYR	2.2
1	B	58	VAL	2.2
1	A	553	ALA	2.2
1	A	368	LEU	2.2
1	A	548	LEU	2.2
1	A	171	GLU	2.2
1	A	514	PHE	2.2
1	B	463	PHE	2.2
1	B	503	ASP	2.2
1	B	112	ALA	2.2
1	A	217	ILE	2.1
1	B	581	ILE	2.1
1	A	747	TYR	2.1
1	A	640	LYS	2.1
1	B	390	GLU	2.1
1	B	621	ILE	2.1
1	B	152	LEU	2.1
1	B	475	ASP	2.1
1	B	644	ASP	2.1
1	A	374	SER	2.1
1	A	577	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	194	VAL	2.1
1	B	314	LYS	2.1
1	A	321	PRO	2.1
1	A	289	LEU	2.1
1	A	73	VAL	2.1
1	A	194	VAL	2.1
1	B	247	PRO	2.1
1	B	234	PHE	2.1
1	B	287	PHE	2.1
1	B	191	TYR	2.1
1	B	645	GLU	2.0
1	A	351	PHE	2.0
1	A	199	ILE	2.0
1	B	674	ALA	2.0
1	A	261	ARG	2.0
1	A	561	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

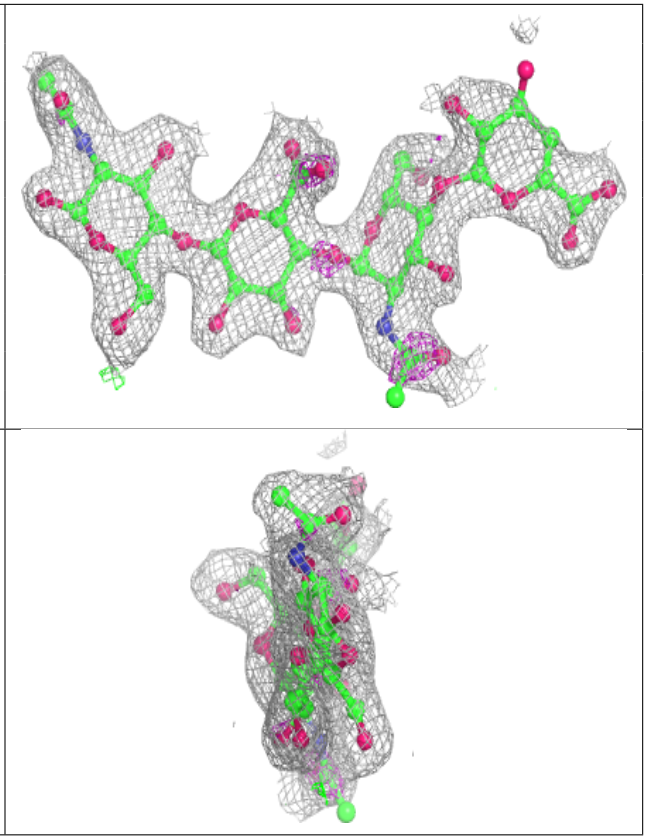
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	3	14/15	0.75	0.27	76,77,79,80	0
2	NAG	C	3	14/15	0.79	0.19	62,64,67,67	0
2	GCD	D	4	11/12	0.81	0.31	97,97,97,97	0
2	GCD	C	4	11/12	0.83	0.21	88,89,89,89	0
2	NAG	D	1	15/15	0.83	0.23	58,60,61,62	0
2	GCU	D	2	12/13	0.88	0.29	64,64,65,65	0
2	GCU	C	2	12/13	0.90	0.20	53,54,55,55	0
2	NAG	C	1	15/15	0.91	0.15	49,49,50,51	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

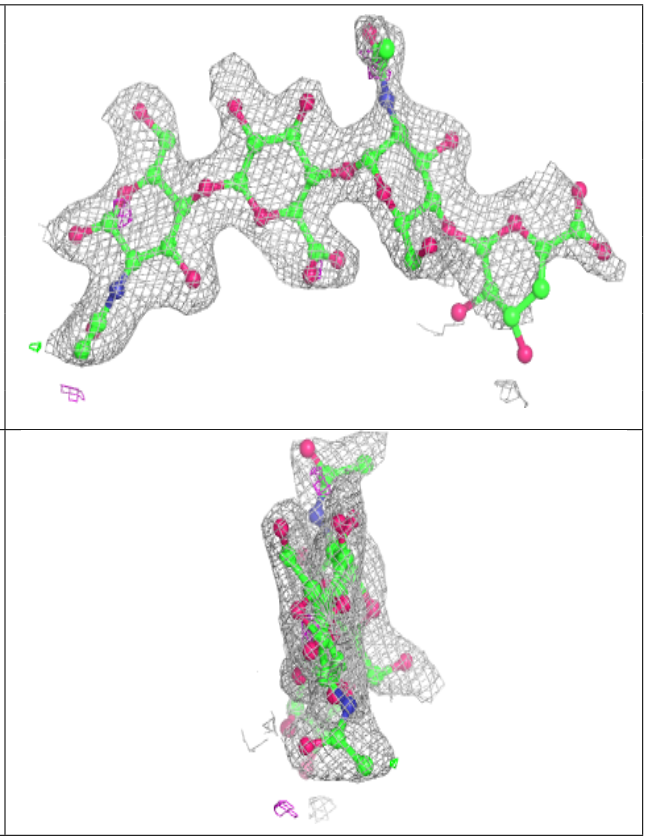
Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	ACT	A	4	4/4	0.62	0.26	70,70,70,70	0
4	ACT	B	773	4/4	0.84	0.19	67,67,67,67	0
4	ACT	A	5	4/4	0.88	0.14	58,58,58,58	0
4	ACT	A	3	4/4	0.92	0.18	61,61,61,61	0
4	ACT	A	773	4/4	0.93	0.15	64,64,64,64	0
3	ZN	B	2	1/1	0.99	0.05	55,55,55,55	0
3	ZN	A	1	1/1	1.00	0.03	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.