



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:55 PM UTC

PDB ID : 4YH7 / pdb_00004yh7
Title : Crystal structure of PTPdelta ectodomain in complex with IL1RAPL1
Authors : Yamagata, A.; Fukai, S.
Deposited on : 2015-02-27
Resolution : 4.40 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

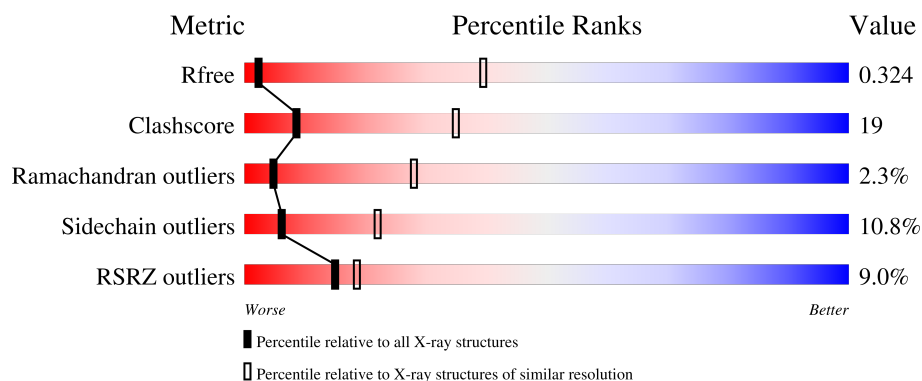
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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 $\leq 5\%$. 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	841	7% 36% 28% 5% 30%
2	B	348	6% 55% 30% 8% 7%
3	C	2	100%
4	D	5	60% 40%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7240 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 Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	4515	2820	784	894	17	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	862	LYS	-	expression tag	UNP Q64487
A	863	HIS	-	expression tag	UNP Q64487
A	864	HIS	-	expression tag	UNP Q64487
A	865	HIS	-	expression tag	UNP Q64487
A	866	HIS	-	expression tag	UNP Q64487
A	867	HIS	-	expression tag	UNP Q64487
A	868	HIS	-	expression tag	UNP Q64487

- Molecule 2 is a protein called Interleukin-1 receptor accessory protein-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	324	2608	1658	436	498	16	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	-	expression tag	UNP P59823
B	13	GLN	-	expression tag	UNP P59823
B	14	PRO	-	expression tag	UNP P59823
B	15	ALA	-	expression tag	UNP P59823
B	16	ALA	-	expression tag	UNP P59823
B	17	ARG	-	expression tag	UNP P59823
B	18	ASP	-	expression tag	UNP P59823
B	353	LYS	-	expression tag	UNP P59823
B	354	HIS	-	expression tag	UNP P59823

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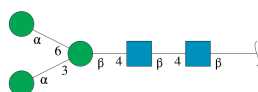
Chain	Residue	Modelled	Actual	Comment	Reference
B	355	HIS	-	expression tag	UNP P59823
B	356	HIS	-	expression tag	UNP P59823
B	357	HIS	-	expression tag	UNP P59823
B	358	HIS	-	expression tag	UNP P59823
B	359	HIS	-	expression tag	UNP P59823

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



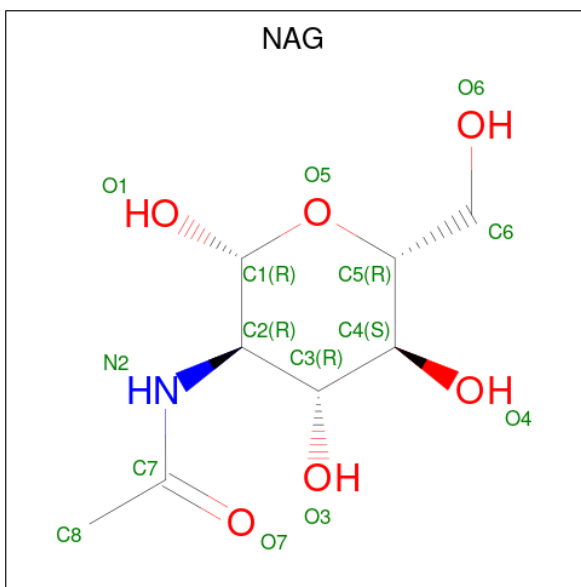
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

NAG1	NAG2	BMA3	MAN4	MAN5
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4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	286.30Å 286.30Å 70.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 4.40 39.09 – 4.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (39.09-4.40) 95.3 (39.09-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.290 , 0.325 0.293 , 0.324	Depositor DCC
R_{free} test set	896 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	175.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 103.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.149 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

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	0.53	0/4615	1.33	59/6296 (0.9%)
2	B	0.37	0/2666	0.84	7/3600 (0.2%)
All	All	0.48	0/7281	1.17	66/9896 (0.7%)

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
2	B	0	1

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	THR	N-CA-C	11.41	127.53	109.39
1	A	413	GLU	CA-C-N	-11.30	109.24	120.31
1	A	413	GLU	C-N-CA	-11.30	109.24	120.31
1	A	473	TRP	N-CA-C	11.29	123.33	111.14
1	A	452	ASN	N-CA-C	11.20	126.52	112.86
1	A	447	GLU	CA-C-N	9.33	129.39	119.78
1	A	447	GLU	C-N-CA	9.33	129.39	119.78
1	A	300	ASP	N-CA-C	8.77	120.91	108.54
1	A	354	ASN	CA-C-N	8.58	128.20	118.85
1	A	354	ASN	C-N-CA	8.58	128.20	118.85
1	A	507	ASP	N-CA-C	8.30	123.31	110.20
1	A	422	GLN	N-CA-C	8.28	122.81	112.87
1	A	514	ILE	N-CA-C	8.04	119.37	108.11
1	A	459	ARG	N-CA-C	8.00	121.45	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	SER	N-CA-C	7.91	122.50	113.01
1	A	171	LEU	CA-C-N	7.84	127.60	119.76
1	A	171	LEU	C-N-CA	7.84	127.60	119.76
1	A	367	PRO	N-CA-C	7.60	123.00	111.14
1	A	522	VAL	CA-C-N	7.47	127.42	120.03
1	A	522	VAL	C-N-CA	7.47	127.42	120.03
1	A	302	ARG	N-CA-C	-7.01	95.86	110.80
1	A	431	VAL	N-CA-C	-7.01	99.59	108.84
1	A	245	PHE	N-CA-C	6.93	119.42	108.67
1	A	489	LEU	N-CA-C	-6.92	100.28	110.52
1	A	470	VAL	N-CA-C	6.91	119.69	111.05
1	A	356	GLU	CA-C-N	6.80	128.34	119.84
1	A	356	GLU	C-N-CA	6.80	128.34	119.84
1	A	372	GLU	CA-C-N	-6.76	112.82	119.78
1	A	372	GLU	C-N-CA	-6.76	112.82	119.78
1	A	377	ILE	N-CA-C	6.68	117.25	107.37
1	A	291	ILE	N-CA-C	6.64	117.20	107.37
1	A	358	VAL	CG1-CB-CG2	-6.52	96.45	110.80
1	A	452	ASN	N-CA-CB	-6.51	102.33	112.41
1	A	454	GLN	N-CA-C	-6.40	100.36	109.96
1	A	284	THR	CA-C-N	6.21	126.42	119.90
1	A	284	THR	C-N-CA	6.21	126.42	119.90
1	A	504	SER	N-CA-C	6.13	118.76	111.71
1	A	326	VAL	N-CA-C	6.12	116.74	108.17
1	A	601	GLY	N-CA-C	6.06	120.25	112.13
1	A	299	ASN	N-CA-C	5.99	123.55	110.80
1	A	474	MET	N-CA-CB	5.90	120.46	110.49
2	B	290	ILE	N-CA-C	5.87	116.00	110.30
1	A	435	MET	N-CA-C	5.86	118.95	110.28
1	A	363	ILE	N-CA-C	5.85	116.72	108.36
1	A	356	GLU	N-CA-C	5.80	117.27	110.31
1	A	65	ASN	N-CA-C	5.78	118.89	109.59
1	A	518	THR	CB-CA-C	-5.65	102.90	112.00
2	B	326	GLU	N-CA-C	5.61	121.02	113.72
1	A	306	ASN	N-CA-C	5.59	117.52	108.41
1	A	338	VAL	N-CA-C	5.55	116.76	108.54
2	B	32	THR	N-CA-C	5.52	117.47	108.63
1	A	500	LEU	N-CA-C	5.52	118.07	109.52
1	A	106	VAL	N-CA-C	5.42	115.66	107.75
1	A	186	ARG	N-CA-C	5.42	117.92	108.76
1	A	472	ASN	N-CA-C	5.41	119.99	113.17
1	A	329	LEU	CA-C-N	5.34	125.28	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	LEU	C-N-CA	5.34	125.28	119.78
1	A	78	VAL	N-CA-C	5.26	115.67	107.99
1	A	606	GLU	N-CA-C	5.24	117.02	108.63
1	A	232	VAL	N-CA-C	5.21	115.98	107.24
1	A	520	THR	N-CA-C	5.20	118.42	110.36
2	B	121	ARG	N-CA-C	5.20	116.84	108.32
2	B	194	ILE	N-CA-C	5.11	113.73	106.53
1	A	307	TYR	N-CA-C	5.08	116.81	108.52
2	B	176	GLU	CA-C-N	-5.03	115.60	120.98
2	B	176	GLU	C-N-CA	-5.03	115.60	120.98

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	88	PRO	Peptide

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	4515	0	4454	203	0
2	B	2608	0	2540	75	0
3	C	28	0	25	0	0
4	D	61	0	52	2	0
5	B	28	0	26	1	0
All	All	7240	0	7097	271	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 19.

All (271) 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:462:TYR:HE1	1:A:476:HIS:HB2	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:PRO:HB2	1:A:421:GLU:OE2	1.74	0.88
1:A:98:ARG:NH2	2:B:291:GLU:OE2	2.09	0.85
1:A:124:ARG:O	1:A:127:GLN:NE2	2.13	0.82
1:A:424:PRO:HA	1:A:452:ASN:HD22	1.44	0.80
2:B:144:TYR:HB3	2:B:228:THR:HG21	1.63	0.80
1:A:241:VAL:HB	1:A:269:SER:H	1.47	0.78
1:A:462:TYR:CE1	1:A:476:HIS:HB2	2.19	0.78
2:B:122:ASN:HB2	2:B:125:TYR:HB3	1.67	0.77
1:A:196:ARG:NH2	2:B:37:ASP:OD1	2.19	0.76
1:A:265:VAL:HG22	1:A:293:ARG:HG3	1.70	0.74
1:A:521:GLY:O	1:A:598:GLN:NE2	2.20	0.74
2:B:326:GLU:N	2:B:327:GLY:HA3	2.03	0.73
1:A:143:VAL:HG22	1:A:231:TYR:HB2	1.69	0.73
1:A:533:PRO:HA	1:A:539:ILE:HG12	1.69	0.73
1:A:66:LYS:HB3	1:A:71:VAL:HG11	1.69	0.72
1:A:368:LYS:HG2	1:A:395:ASP:HB3	1.70	0.72
1:A:473:TRP:O	1:A:474:MET:HG3	1.89	0.71
1:A:145:GLU:OE1	1:A:236:ARG:N	2.23	0.71
1:A:464:MET:HG2	1:A:495:TYR:HE1	1.56	0.70
1:A:450:GLU:HB3	1:A:452:ASN:HD21	1.56	0.69
1:A:277:MET:HE2	1:A:310:VAL:HG21	1.74	0.69
1:A:314:THR:HA	2:B:121:ARG:HH22	1.59	0.68
2:B:55:LEU:HD21	2:B:129:VAL:HB	1.75	0.68
2:B:167:ILE:O	2:B:169:ASP:N	2.27	0.68
1:A:390:LEU:HD21	1:A:419:THR:HG21	1.76	0.68
1:A:429:ARG:HD2	1:A:430:ASP:H	1.60	0.67
1:A:435:MET:HE1	1:A:437:SER:O	1.94	0.67
1:A:425:SER:H	1:A:452:ASN:ND2	1.92	0.67
2:B:95:ARG:NH1	2:B:112:ASP:OD2	2.28	0.66
1:A:329:LEU:HA	1:A:406:ILE:HD13	1.76	0.65
1:A:196:ARG:HH22	2:B:38:ILE:HG22	1.60	0.65
1:A:422:GLN:HG3	1:A:505:ILE:HG21	1.78	0.65
2:B:306:LEU:HD11	2:B:316:SER:HB2	1.79	0.65
1:A:459:ARG:HH22	1:A:475:LYS:HG2	1.62	0.63
1:A:252:HIS:HB2	1:A:324:ILE:HD12	1.80	0.63
1:A:366:LYS:HD3	1:A:367:PRO:HD2	1.81	0.63
1:A:90:ARG:NH1	1:A:213:GLU:OE1	2.31	0.63
1:A:540:LEU:HG	1:A:578:ARG:HD2	1.80	0.63
1:A:184:GLN:NE2	1:A:198:ALA:O	2.31	0.63
2:B:220:TYR:O	2:B:223:PHE:N	2.31	0.63
1:A:126:ASP:OD1	1:A:126:ASP:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:MET:HB3	1:A:317:VAL:HG22	1.80	0.62
2:B:355:HIS:O	2:B:357:HIS:N	2.33	0.61
1:A:181:ARG:HG2	1:A:182:ILE:HG13	1.82	0.61
1:A:463:THR:HB	1:A:473:TRP:HB3	1.81	0.61
2:B:254:VAL:HG13	2:B:348:LEU:HB3	1.83	0.61
1:A:399:ARG:HB2	1:A:411:ALA:HB1	1.82	0.61
1:A:476:HIS:CE1	1:A:484:THR:HG1	2.18	0.61
1:A:108:SER:HB3	1:A:113:GLU:HG3	1.82	0.61
1:A:168:LYS:HE3	1:A:209:GLN:O	2.00	0.60
1:A:435:MET:HB2	1:A:521:GLY:HA2	1.83	0.60
1:A:62:ILE:HD11	1:A:105:CYS:SG	2.41	0.60
1:A:435:MET:CB	1:A:521:GLY:HA2	2.32	0.59
1:A:242:PRO:HG3	1:A:315:LEU:HG	1.85	0.59
1:A:177:ASN:O	1:A:179:ASN:N	2.35	0.59
1:A:236:ARG:CZ	1:A:236:ARG:HA	2.32	0.59
1:A:352:SER:HB3	1:A:361:TYR:OH	2.03	0.58
1:A:426:SER:C	1:A:509:PRO:HG2	2.29	0.57
1:A:125:GLU:HA	1:A:128:ILE:HG13	1.85	0.57
1:A:142:LYS:HE2	1:A:151:THR:H	1.69	0.57
1:A:257:GLY:HA2	1:A:300:ASP:HA	1.86	0.57
1:A:397:GLU:OE2	1:A:414:PRO:HB3	2.03	0.57
2:B:182:TYR:OH	2:B:217:GLU:OE1	2.21	0.57
1:A:343:ALA:O	1:A:392:PRO:HA	2.04	0.57
1:A:133:PRO:HA	1:A:157:SER:O	2.05	0.56
1:A:557:VAL:HG13	1:A:566:GLU:HG3	1.85	0.56
1:A:196:ARG:NH2	2:B:38:ILE:HG22	2.19	0.56
1:A:424:PRO:HA	1:A:452:ASN:ND2	2.16	0.55
2:B:110:LEU:HD23	2:B:135:VAL:HG12	1.87	0.55
1:A:104:GLU:HG2	1:A:117:SER:HA	1.87	0.55
1:A:75:ARG:NH2	1:A:95:ARG:HB2	2.22	0.55
1:A:536:GLU:HG2	1:A:537:THR:HG23	1.88	0.55
2:B:182:TYR:HB2	2:B:215:THR:HG23	1.89	0.55
1:A:329:LEU:HD13	1:A:410:PRO:HD2	1.88	0.55
1:A:557:VAL:O	1:A:590:PHE:HA	2.06	0.55
1:A:242:PRO:HA	1:A:315:LEU:HB3	1.89	0.55
1:A:429:ARG:HH11	1:A:430:ASP:H	1.55	0.55
2:B:43:VAL:HG21	2:B:49:VAL:HG13	1.88	0.55
1:A:236:ARG:HA	1:A:236:ARG:NH1	2.23	0.54
2:B:46:GLY:H	2:B:108:THR:HG22	1.73	0.54
2:B:92:ASP:OD1	2:B:94:SER:N	2.40	0.54
1:A:364:GLN:HA	1:A:375:LYS:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:N	1:A:127:GLN:HE22	2.06	0.53
1:A:459:ARG:NH2	1:A:475:LYS:HG2	2.22	0.53
1:A:406:ILE:HD12	1:A:407:GLY:H	1.73	0.53
1:A:556:LEU:HB2	1:A:571:ILE:HD11	1.91	0.53
1:A:435:MET:SD	1:A:441:ILE:HG22	2.48	0.53
1:A:458:TYR:HB2	1:A:478:VAL:HB	1.90	0.52
1:A:241:VAL:HB	1:A:269:SER:N	2.20	0.52
1:A:490:VAL:N	1:A:495:TYR:OH	2.42	0.52
2:B:267:CYS:HB2	2:B:283:TRP:CZ2	2.45	0.52
1:A:450:GLU:O	1:A:452:ASN:ND2	2.42	0.52
1:A:350:TRP:O	1:A:383:THR:HB	2.09	0.51
1:A:476:HIS:CG	1:A:477:ASN:H	2.29	0.51
1:A:136:ASP:OD2	1:A:157:SER:OG	2.28	0.51
1:A:177:ASN:C	1:A:179:ASN:H	2.17	0.51
2:B:294:ASP:OD1	2:B:298:VAL:N	2.31	0.51
1:A:83:ASP:C	1:A:85:SER:H	2.18	0.51
1:A:146:ARG:N	1:A:233:ARG:O	2.41	0.51
2:B:263:ALA:HB3	2:B:321:VAL:HB	1.93	0.51
1:A:500:LEU:HD23	1:A:510:LEU:HD13	1.92	0.50
1:A:175:THR:HG21	1:A:182:ILE:HG22	1.92	0.50
1:A:358:VAL:HG11	1:A:402:ALA:HB1	1.92	0.50
1:A:366:LYS:HD3	1:A:367:PRO:CD	2.41	0.50
1:A:335:THR:O	1:A:337:VAL:N	2.45	0.50
1:A:276:TRP:HD1	1:A:294:ASN:ND2	2.09	0.50
1:A:66:LYS:H	1:A:71:VAL:HG13	1.77	0.50
1:A:169:ASP:O	1:A:170:PHE:HB2	2.11	0.49
1:A:395:ASP:OD1	1:A:418:GLN:HG3	2.12	0.49
2:B:100:GLU:HG2	2:B:101:ASP:H	1.77	0.49
1:A:333:PRO:HD2	1:A:400:VAL:O	2.12	0.49
1:A:476:HIS:CG	1:A:477:ASN:N	2.80	0.49
2:B:247:PRO:HG3	2:B:347:VAL:HG22	1.94	0.49
1:A:148:ARG:HD3	1:A:239:ARG:NH2	2.26	0.49
1:A:394:SER:N	1:A:419:THR:OG1	2.44	0.49
1:A:429:ARG:HH11	1:A:430:ASP:N	2.11	0.49
1:A:304:SER:HB3	1:A:325:THR:HG22	1.95	0.49
2:B:326:GLU:H	2:B:327:GLY:HA3	1.75	0.49
1:A:393:TYR:HA	1:A:419:THR:O	2.13	0.48
1:A:144:VAL:HG11	1:A:150:ALA:HB2	1.93	0.48
1:A:253:GLU:C	1:A:254:ILE:HG13	2.38	0.48
1:A:447:GLU:HG3	1:A:458:TYR:OH	2.13	0.48
1:A:500:LEU:HD13	1:A:507:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG13	1:A:174:ASP:H	1.78	0.48
1:A:83:ASP:O	1:A:85:SER:N	2.46	0.48
1:A:271:MET:HE3	1:A:292:GLY:HA3	1.96	0.48
1:A:273:TYR:HE1	2:B:88:PRO:HB2	1.78	0.48
1:A:421:GLU:OE1	1:A:452:ASN:HB3	2.14	0.48
1:A:35:ARG:HD2	1:A:51:ILE:HG21	1.96	0.48
1:A:393:TYR:HB2	1:A:421:GLU:HG3	1.95	0.48
1:A:168:LYS:HE2	1:A:169:ASP:OD2	2.13	0.48
2:B:298:VAL:HG22	2:B:321:VAL:HG22	1.96	0.47
2:B:142:LEU:HD13	2:B:144:TYR:CZ	2.50	0.47
2:B:297:ARG:NH1	2:B:325:GLU:OE2	2.47	0.47
1:A:330:PRO:HB2	1:A:402:ALA:HB3	1.96	0.47
2:B:292:ASP:OD2	2:B:292:ASP:N	2.47	0.47
1:A:566:GLU:HG2	1:A:568:ARG:HH12	1.80	0.47
2:B:40:LYS:HG3	2:B:132:SER:HB3	1.96	0.47
2:B:82:PRO:HA	2:B:83:GLY:HA2	1.42	0.47
2:B:84:ASP:OD1	2:B:84:ASP:N	2.47	0.47
1:A:276:TRP:HB3	1:A:283:LEU:HD12	1.97	0.47
1:A:53:GLN:HA	1:A:86:GLY:HA3	1.97	0.47
1:A:184:GLN:NE2	1:A:185:LEU:O	2.45	0.47
1:A:75:ARG:NH2	1:A:99:ASP:OD1	2.47	0.47
1:A:317:VAL:HG23	2:B:121:ARG:HD3	1.97	0.47
1:A:426:SER:OG	1:A:450:GLU:HB2	2.14	0.47
1:A:413:GLU:H	1:A:413:GLU:HG3	1.39	0.47
1:A:464:MET:HG2	1:A:495:TYR:CE1	2.44	0.46
1:A:148:ARG:HD2	1:A:149:THR:H	1.79	0.46
1:A:424:PRO:HB2	1:A:508:GLY:HA3	1.97	0.46
1:A:468:GLN:O	1:A:473:TRP:NE1	2.27	0.46
2:B:181:TRP:CZ3	2:B:216:CYS:HB3	2.50	0.46
2:B:297:ARG:NH2	2:B:328:ASP:OD2	2.43	0.46
1:A:561:GLY:H	1:A:588:TYR:HA	1.81	0.46
1:A:592:LEU:HD23	1:A:593:SER:N	2.30	0.46
2:B:122:ASN:HB2	2:B:125:TYR:CB	2.41	0.46
1:A:52:CYS:HB2	1:A:64:TRP:CH2	2.51	0.46
1:A:424:PRO:CA	1:A:452:ASN:HD22	2.21	0.46
1:A:457:GLY:HA2	1:A:479:ALA:HA	1.97	0.46
1:A:459:ARG:NH1	1:A:476:HIS:H	2.13	0.46
1:A:422:GLN:HA	1:A:505:ILE:HG13	1.98	0.46
1:A:66:LYS:HD3	1:A:103:TYR:CE2	2.51	0.46
1:A:161:ASP:HB3	1:A:195:ILE:HD11	1.97	0.46
1:A:193:THR:OG1	1:A:194:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HH21	1:A:236:ARG:NH1	2.14	0.46
1:A:366:LYS:HE3	1:A:375:LYS:HE2	1.97	0.46
1:A:243:PRO:HG2	1:A:318:ILE:HG23	1.98	0.46
1:A:430:ASP:OD1	1:A:432:GLN:NE2	2.49	0.46
1:A:490:VAL:O	1:A:495:TYR:OH	2.26	0.45
1:A:557:VAL:HG21	1:A:591:ARG:HH21	1.81	0.45
1:A:276:TRP:CZ3	1:A:309:CYS:HB2	2.52	0.45
1:A:436:LEU:HD22	1:A:442:LEU:HD12	1.97	0.45
2:B:247:PRO:HG2	2:B:345:ALA:HB3	1.98	0.45
1:A:390:LEU:CD2	1:A:419:THR:HG21	2.45	0.45
2:B:75:MET:HB3	2:B:75:MET:HE3	1.69	0.45
1:A:331:LYS:N	1:A:354:ASN:OD1	2.44	0.45
1:A:308:THR:HG23	1:A:321:ILE:HG12	1.98	0.45
1:A:529:PHE:CE1	1:A:541:LEU:HD11	2.52	0.45
1:A:450:GLU:HB3	1:A:452:ASN:ND2	2.29	0.45
2:B:247:PRO:HG2	2:B:345:ALA:CB	2.47	0.45
4:D:3:BMA:H61	4:D:5:MAN:H2	1.42	0.45
1:A:233:ARG:NH2	1:A:236:ARG:HH12	2.16	0.44
1:A:123:LEU:HB3	1:A:127:GLN:NE2	2.32	0.44
1:A:327:LYS:H	1:A:327:LYS:HG2	1.69	0.44
1:A:403:VAL:HG22	1:A:408:ARG:HA	1.99	0.44
2:B:266:THR:HG23	2:B:318:SER:HB3	2.00	0.44
1:A:251:ASN:OD1	1:A:323:GLN:N	2.27	0.44
1:A:251:ASN:O	1:A:252:HIS:ND1	2.51	0.44
1:A:447:GLU:HA	1:A:448:PRO:HD2	1.66	0.44
2:B:125:TYR:CD1	5:B:401:NAG:H2	2.53	0.44
1:A:29:THR:H	1:A:57:ASP:HB3	1.82	0.44
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.85	0.44
1:A:359:SER:OG	1:A:404:ASN:HA	2.18	0.44
2:B:280:LEU:HD23	2:B:280:LEU:HA	1.75	0.44
2:B:350:HIS:CG	2:B:351:LYS:N	2.84	0.44
2:B:110:LEU:HD23	2:B:110:LEU:HA	1.87	0.44
1:A:35:ARG:HE	1:A:35:ARG:HB2	1.66	0.43
1:A:96:THR:HG21	1:A:124:ARG:HG2	2.00	0.43
1:A:281:GLU:OE2	1:A:283:LEU:HD23	2.18	0.43
1:A:404:ASN:OD1	1:A:406:ILE:HD11	2.17	0.43
1:A:367:PRO:HA	1:A:396:TYR:HA	2.00	0.43
1:A:431:VAL:HG21	1:A:511:SER:OG	2.18	0.43
1:A:75:ARG:HH22	1:A:99:ASP:CG	2.26	0.43
1:A:458:TYR:HE1	1:A:480:ASP:HA	1.82	0.43
1:A:589:TYR:CE1	1:A:606:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:MET:HG2	1:A:282:ASP:HA	1.99	0.43
1:A:462:TYR:O	1:A:474:MET:HB2	2.18	0.43
1:A:209:GLN:OE1	1:A:232:VAL:N	2.51	0.43
2:B:49:VAL:HG23	2:B:105:PHE:HB2	2.01	0.43
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.84	0.43
1:A:343:ALA:HB1	1:A:421:GLU:HG2	2.00	0.43
2:B:142:LEU:HD13	2:B:144:TYR:CE1	2.53	0.43
1:A:582:LEU:HD23	1:A:583:LYS:H	1.84	0.43
2:B:106:ARG:HA	2:B:107:PRO:HA	1.71	0.43
2:B:179:ILE:HD13	2:B:198:ARG:O	2.19	0.43
1:A:253:GLU:CD	1:A:327:LYS:HD3	2.43	0.43
1:A:555:GLU:CD	1:A:568:ARG:HE	2.25	0.43
1:A:366:LYS:HG3	1:A:373:PRO:O	2.19	0.42
2:B:184:GLU:CD	2:B:213:ASN:HD22	2.26	0.42
1:A:330:PRO:HG3	1:A:404:ASN:OD1	2.18	0.42
2:B:181:TRP:CD2	2:B:201:LEU:HD23	2.54	0.42
1:A:181:ARG:HG3	1:A:202:GLU:O	2.19	0.42
2:B:181:TRP:CE3	2:B:216:CYS:HB3	2.54	0.42
1:A:535:SER:C	1:A:612:MET:HG3	2.44	0.42
2:B:177:PRO:HG2	2:B:218:LEU:HD11	2.00	0.42
2:B:304:ARG:NH2	4:D:1:NAG:H3	2.35	0.42
1:A:209:GLN:CD	1:A:232:VAL:HB	2.45	0.42
1:A:276:TRP:CD1	1:A:296:LEU:HD13	2.54	0.42
2:B:37:ASP:OD1	2:B:59:TYR:OH	2.21	0.42
2:B:77:TYR:HB3	2:B:86:GLU:HB3	2.01	0.42
2:B:145:ASN:HB3	2:B:148:MET:HE2	2.02	0.42
1:A:486:ILE:O	1:A:486:ILE:HG13	2.20	0.42
2:B:76:TRP:CZ3	2:B:118:CYS:HB2	2.55	0.42
2:B:109:LEU:O	2:B:112:ASP:HB2	2.20	0.42
2:B:54:ALA:H	2:B:131:ILE:HD11	1.85	0.41
1:A:270:PRO:HD3	2:B:85:PHE:HZ	1.84	0.41
1:A:273:TYR:O	1:A:311:ALA:HA	2.21	0.41
1:A:364:GLN:HB3	1:A:374:TYR:HB3	2.01	0.41
2:B:298:VAL:HA	2:B:320:ILE:O	2.20	0.41
1:A:75:ARG:NH2	1:A:99:ASP:OD2	2.53	0.41
1:A:109:ASN:C	1:A:111:VAL:H	2.28	0.41
1:A:237:GLU:H	1:A:237:GLU:HG2	1.47	0.41
1:A:422:GLN:O	1:A:423:ALA:HB2	2.21	0.41
2:B:218:LEU:HD12	2:B:219:LYS:H	1.84	0.41
1:A:166:TRP:CZ3	1:A:214:CYS:HB3	2.55	0.41
1:A:463:THR:O	1:A:495:TYR:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:HD21	1:A:406:ILE:HG13	1.85	0.41
1:A:377:ILE:HG22	1:A:380:ILE:HD11	2.03	0.41
2:B:68:GLN:HE21	2:B:68:GLN:HB3	1.62	0.41
1:A:145:GLU:OE1	1:A:236:ARG:HG2	2.21	0.41
1:A:284:THR:HG22	1:A:285:PRO:HD2	2.02	0.41
1:A:520:THR:HB	1:A:598:GLN:HG3	2.02	0.41
2:B:31:CYS:HA	2:B:126:CYS:HB3	2.03	0.41
2:B:214:TYR:CE1	2:B:231:LEU:HD12	2.56	0.41
2:B:289:PHE:HE2	2:B:291:GLU:HB2	1.84	0.41
1:A:144:VAL:HG22	1:A:148:ARG:HB3	2.03	0.41
1:A:267:VAL:HG22	1:A:268:GLY:H	1.85	0.40
1:A:404:ASN:ND2	1:A:406:ILE:HG13	2.36	0.40
1:A:529:PHE:CZ	1:A:590:PHE:HE2	2.40	0.40
2:B:63:ASN:OD1	2:B:66:LEU:HG	2.21	0.40
2:B:94:SER:OG	2:B:95:ARG:N	2.54	0.40
1:A:147:THR:HA	1:A:203:GLN:HA	2.03	0.40
1:A:339:THR:O	1:A:340:GLU:HG2	2.20	0.40
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.68	0.40
2:B:106:ARG:HB2	2:B:223:PHE:CE2	2.57	0.40
2:B:149:LYS:HE3	2:B:230:GLU:OE2	2.21	0.40
1:A:276:TRP:CG	1:A:296:LEU:HD22	2.57	0.40
1:A:276:TRP:CD2	1:A:296:LEU:HD22	2.57	0.40
2:B:44:LEU:HD21	2:B:145:ASN:HB2	2.04	0.40
2:B:325:GLU:HB3	2:B:326:GLU:H	1.71	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	583/841 (69%)	523 (90%)	48 (8%)	12 (2%)	5 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	320/348 (92%)	274 (86%)	37 (12%)	9 (3%)	4	24
All	All	903/1189 (76%)	797 (88%)	85 (9%)	21 (2%)	5	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	85	SER
1	A	178	ASN
1	A	474	MET
1	A	482	GLN
1	A	513	ASP
2	B	89	ILE
2	B	168	GLU
2	B	294	ASP
2	B	356	HIS
1	A	84	GLY
1	A	174	ASP
1	A	516	VAL
1	A	68	GLY
1	A	100	GLU
2	B	45	VAL
2	B	122	ASN
2	B	140	THR
2	B	198	ARG
1	A	126	ASP
2	B	353	LYS

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	508/736 (69%)	467 (92%)	41 (8%)	11	31
2	B	289/309 (94%)	244 (84%)	45 (16%)	2	13
All	All	797/1045 (76%)	711 (89%)	86 (11%)	6	22

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	71	VAL
1	A	95	ARG
1	A	126	ASP
1	A	141	LEU
1	A	157	SER
1	A	163	GLU
1	A	168	LYS
1	A	173	VAL
1	A	176	SER
1	A	178	ASN
1	A	181	ARG
1	A	236	ARG
1	A	237	GLU
1	A	239	ARG
1	A	254	ILE
1	A	274	VAL
1	A	284	THR
1	A	297	GLU
1	A	308	THR
1	A	309	CYS
1	A	312	MET
1	A	317	VAL
1	A	326	VAL
1	A	331	LYS
1	A	346	ILE
1	A	352	SER
1	A	399	ARG
1	A	401	VAL
1	A	406	ILE
1	A	413	GLU
1	A	436	LEU
1	A	449	GLU
1	A	465	ASP
1	A	490	VAL
1	A	520	THR
1	A	532	GLU
1	A	535	SER
1	A	566	GLU
1	A	582	LEU
1	A	586	SER
2	B	40	LYS

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Mol	Chain	Res	Type
2	B	42	GLN
2	B	43	VAL
2	B	49	VAL
2	B	50	ARG
2	B	61	ARG
2	B	68	GLN
2	B	72	LEU
2	B	80	SER
2	B	84	ASP
2	B	100	GLU
2	B	102	SER
2	B	106	ARG
2	B	108	THR
2	B	120	ILE
2	B	122	ASN
2	B	130	SER
2	B	131	ILE
2	B	138	ASN
2	B	164	CYS
2	B	176	GLU
2	B	178	GLU
2	B	187	THR
2	B	201	LEU
2	B	205	GLU
2	B	215	THR
2	B	224	VAL
2	B	228	THR
2	B	229	THR
2	B	231	LEU
2	B	244	LEU
2	B	257	THR
2	B	280	LEU
2	B	291	GLU
2	B	292	ASP
2	B	295	GLU
2	B	310	LEU
2	B	319	LEU
2	B	333	SER
2	B	336	VAL
2	B	347	VAL
2	B	348	LEU
2	B	350	HIS

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Mol	Chain	Res	Type
2	B	351	LYS
2	B	355	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	178	ASN
1	A	323	GLN
1	A	365	HIS
1	A	432	GLN
1	A	452	ASN
1	A	456	GLN
1	A	482	GLN
2	B	68	GLN
2	B	355	HIS
2	B	356	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 ⓘ

7 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	3,2	14,14,15	0.36	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	D	1	2,4	14,14,15	0.28	0	17,19,21	0.62	0
4	NAG	D	2	4	14,14,15	0.59	1 (7%)	17,19,21	0.59	0
4	BMA	D	3	4	11,11,12	1.57	3 (27%)	15,15,17	1.53	2 (13%)
4	MAN	D	4	4	11,11,12	1.21	2 (18%)	15,15,17	0.90	1 (6%)
4	MAN	D	5	4	11,11,12	0.96	1 (9%)	15,15,17	1.27	1 (6%)

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	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	1/1/1/1
4	MAN	D	5	4	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	O3-C3	2.99	1.50	1.43
4	D	5	MAN	C1-C2	2.59	1.58	1.52
4	D	4	MAN	O5-C5	2.56	1.48	1.43
4	D	3	BMA	C4-C5	2.41	1.58	1.53
4	D	4	MAN	C1-C2	2.41	1.58	1.52
4	D	3	BMA	C4-C3	2.26	1.58	1.52
4	D	2	NAG	O5-C1	-2.04	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-C2-C3	-3.57	104.44	109.64
4	D	5	MAN	C1-O5-C5	3.40	116.74	112.19
4	D	3	BMA	O3-C3-C2	3.19	116.56	110.05
4	D	4	MAN	O2-C2-C3	-2.42	105.14	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	5	MAN	C4-C5-C6-O6
4	D	5	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

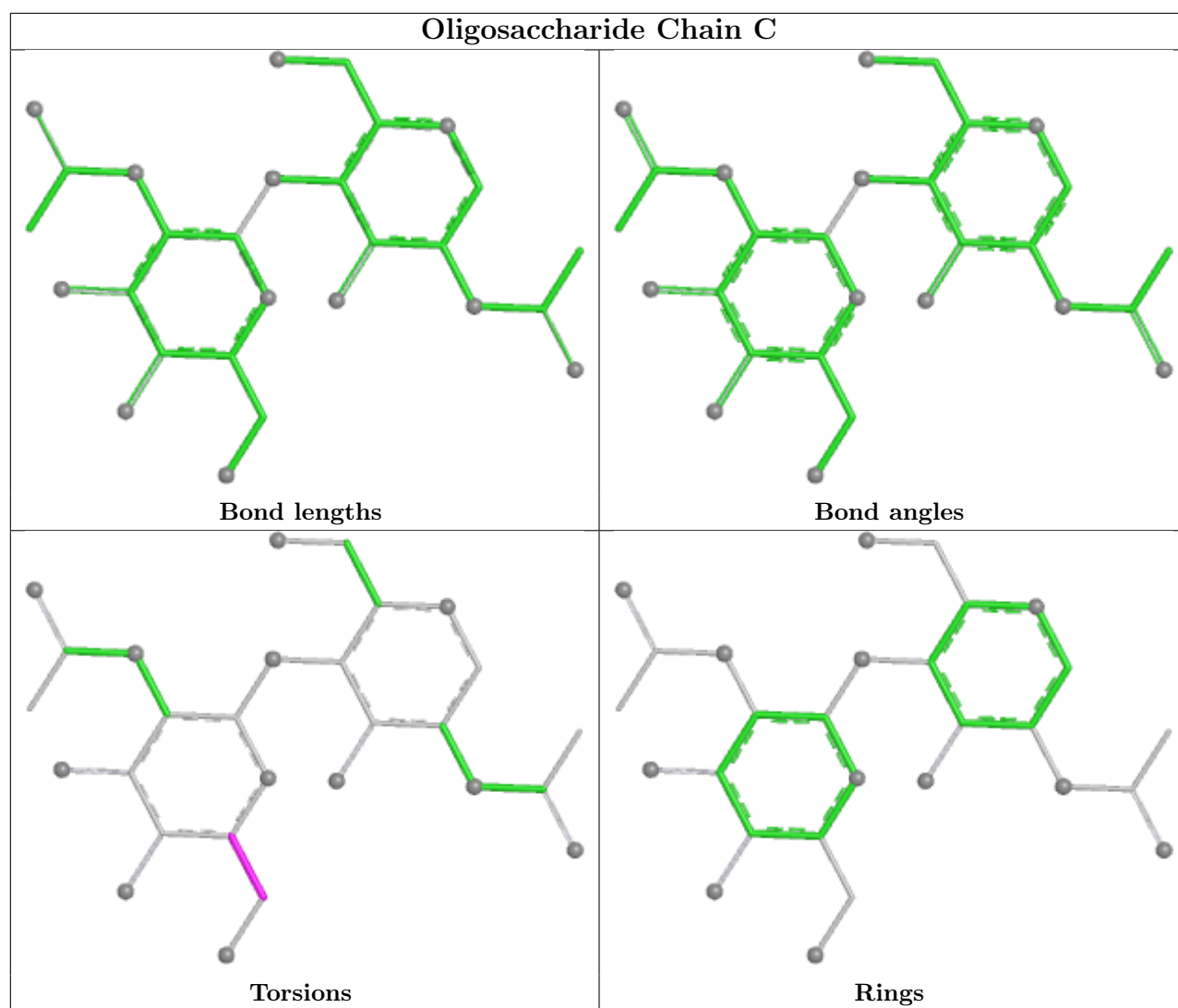
All (1) ring outliers are listed below:

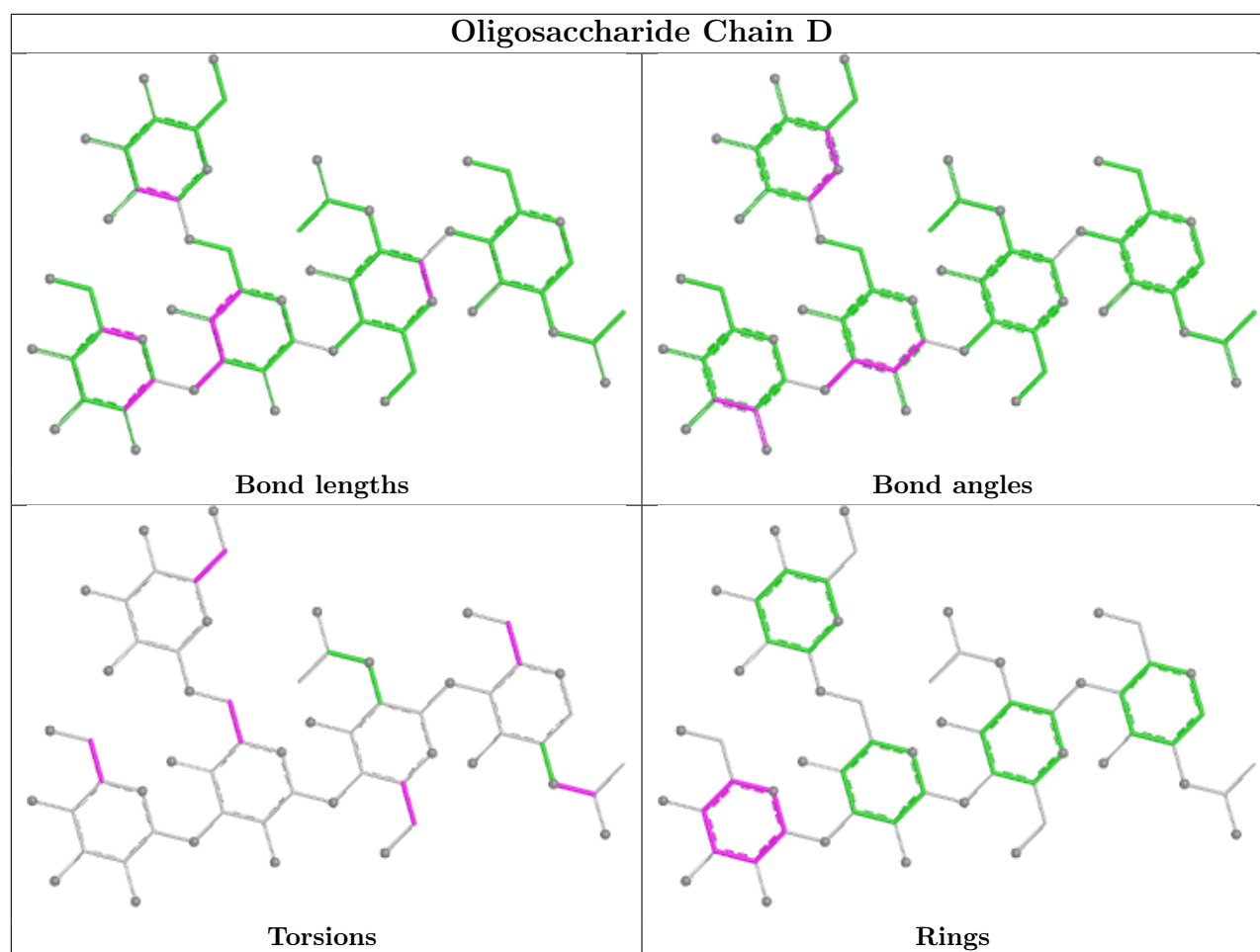
Mol	Chain	Res	Type	Atoms
4	D	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0
4	D	5	MAN	1	0
4	D	1	NAG	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	$\# Z > 2$
5	NAG	B	402	2	14,14,15	0.47	0	17,19,21	0.41	0
5	NAG	B	401	2	14,14,15	0.73	1 (7%)	17,19,21	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	402	2	-	0/6/23/26	0/1/1/1
5	NAG	B	401	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	NAG	C1-C2	2.06	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	NAG	O5-C5-C6-O6
5	B	401	NAG	C4-C5-C6-O6
5	B	401	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	585/841 (69%)	0.64	60 (10%)	12 15	70, 180, 242, 273	0
2	B	324/348 (93%)	0.39	22 (6%)	23 24	52, 98, 137, 206	0
All	All	909/1189 (76%)	0.55	82 (9%)	15 18	52, 137, 234, 273	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	VAL	7.6
1	A	433	ALA	7.2
2	B	170	PHE	5.6
1	A	398	PHE	4.6
1	A	501	ALA	4.3
1	A	68	GLY	4.0
1	A	470	VAL	3.9
1	A	432	GLN	3.8
2	B	282	TYR	3.6
1	A	399	ARG	3.5
1	A	328	ALA	3.5
2	B	83	GLY	3.4
1	A	363	ILE	3.4
1	A	516	VAL	3.3
2	B	116	TYR	3.3
1	A	576	SER	3.2
2	B	225	VAL	3.2
1	A	520	THR	3.1
1	A	107	ALA	3.1
1	A	67	LYS	3.1
1	A	408	ARG	3.1
1	A	48	ALA	3.0
2	B	283	TRP	3.0
1	A	298	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	417	THR	2.8
2	B	332	TYR	2.8
1	A	517	ILE	2.7
1	A	260	VAL	2.7
1	A	498	LYS	2.6
1	A	416	LEU	2.6
2	B	31	CYS	2.6
1	A	523	PRO	2.6
1	A	250	THR	2.5
2	B	119	VAL	2.5
1	A	527	LEU	2.5
2	B	218	LEU	2.5
1	A	515	GLN	2.5
1	A	460	VAL	2.5
1	A	427	ALA	2.5
1	A	492	GLN	2.4
1	A	314	THR	2.4
2	B	326	GLU	2.4
1	A	105	CYS	2.4
1	A	487	GLY	2.4
1	A	396	TYR	2.4
1	A	497	VAL	2.3
1	A	543	TRP	2.3
2	B	167	ILE	2.3
1	A	29	THR	2.3
1	A	575	THR	2.3
1	A	558	TYR	2.3
1	A	30	PRO	2.3
1	A	64	TRP	2.3
1	A	166	TRP	2.3
1	A	586	SER	2.3
1	A	329	LEU	2.3
1	A	364	GLN	2.3
1	A	574	GLY	2.3
1	A	289	MET	2.3
1	A	435	MET	2.3
2	B	220	TYR	2.2
1	A	316	GLY	2.2
2	B	240	LYS	2.2
1	A	152	MET	2.2
1	A	488	ASN	2.2
2	B	41	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	573	PRO	2.2
1	A	172	PRO	2.1
1	A	285	PRO	2.1
2	B	51	ILE	2.1
1	A	434	ARG	2.1
2	B	177	PRO	2.1
2	B	233	VAL	2.1
1	A	585	ASN	2.1
1	A	51	ILE	2.1
1	A	449	GLU	2.1
2	B	60	ILE	2.1
1	A	293	ARG	2.0
1	A	584	PRO	2.0
1	A	443	VAL	2.0
2	B	182	TYR	2.0
2	B	124	THR	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](#)

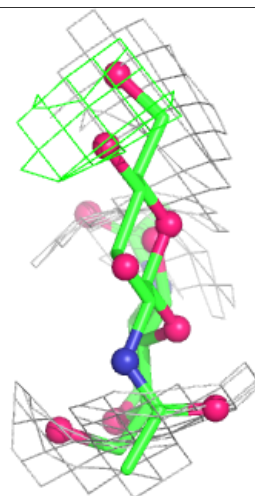
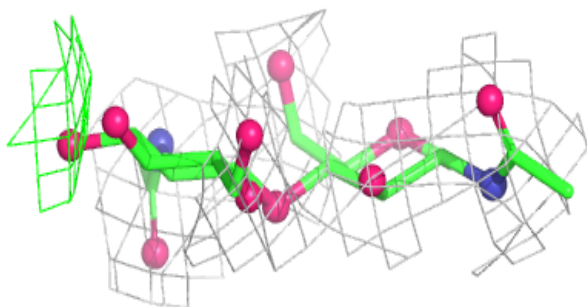
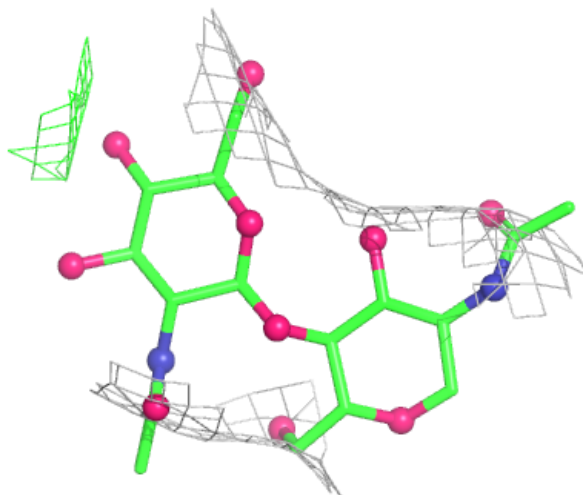
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

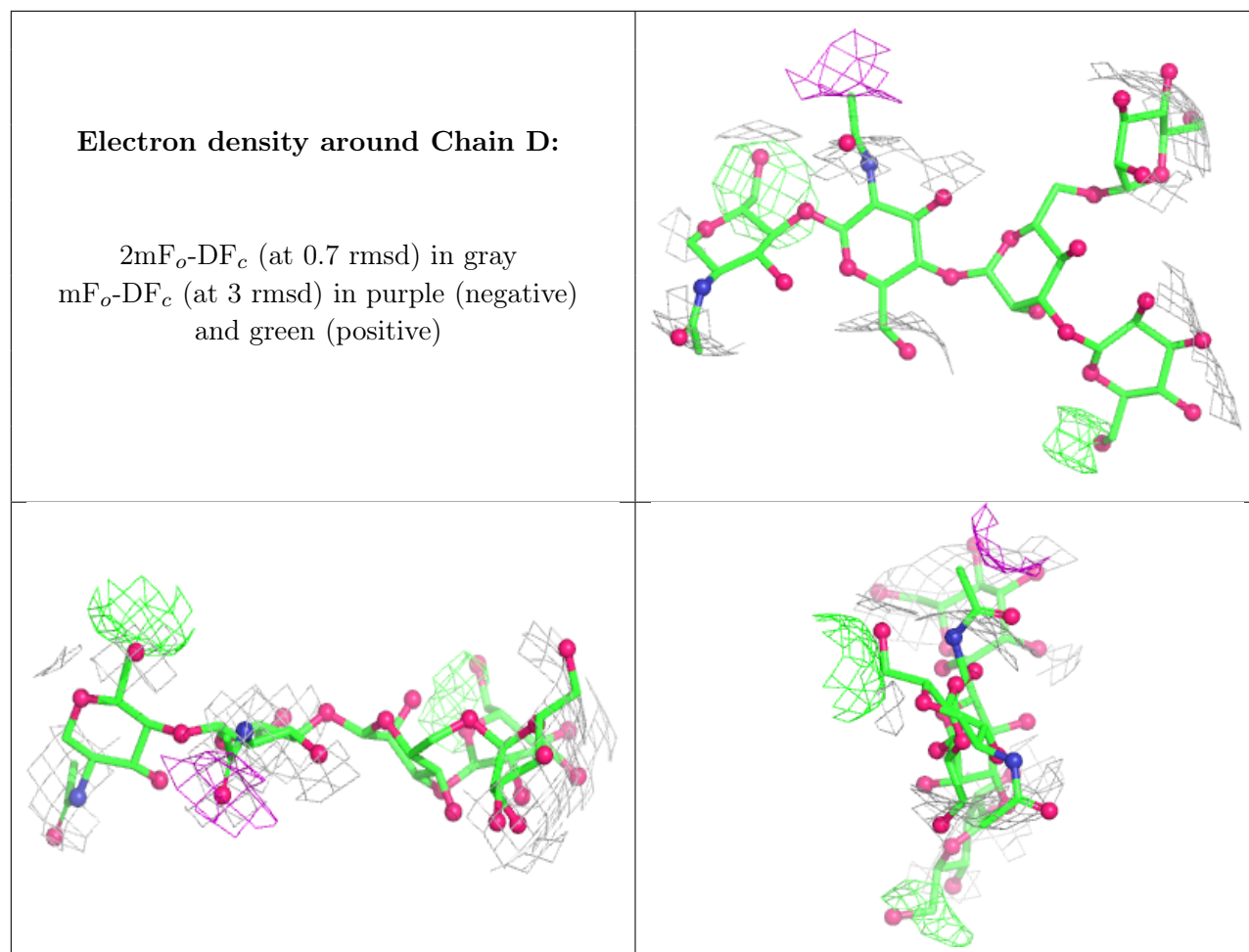
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	4	11/12	0.29	0.14	146,185,203,205	0
4	BMA	D	3	11/12	0.67	0.09	174,176,182,197	0
3	NAG	C	2	14/15	0.67	0.17	119,138,152,155	0
4	NAG	D	1	14/15	0.83	0.11	70,113,125,126	0
4	MAN	D	5	11/12	0.86	0.09	169,185,192,196	0
4	NAG	D	2	14/15	0.87	0.16	118,148,173,176	0
3	NAG	C	1	14/15	0.92	0.10	107,121,136,138	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)





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($\text{\AA}^2$)	Q<0.9
5	NAG	B	401	14/15	0.75	0.17	132,151,158,159	0
5	NAG	B	402	14/15	0.85	0.10	109,135,145,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.