



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:41 PM UTC

PDB ID : 1Z68 / pdb_00001z68
Title : Crystal Structure Of Human Fibroblast Activation Protein alpha
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Deposited on : 2005-03-21
Resolution : 2.60 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

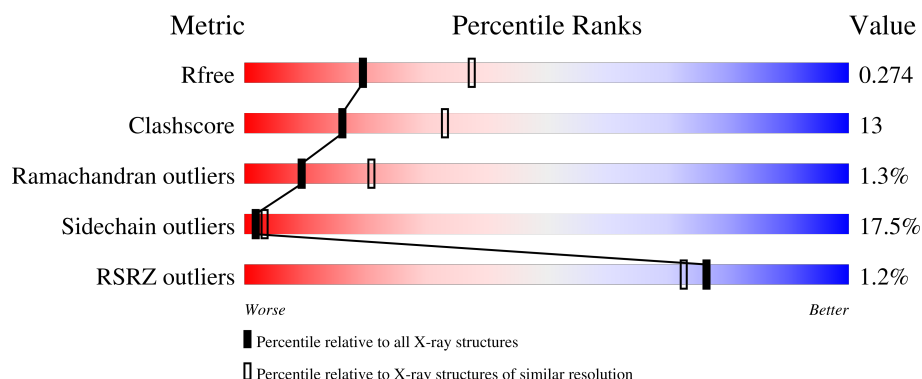
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	719	2% 65% 28% 7%
1	B	719	62% 31% 6%
2	C	2	50% 50%
2	E	2	100%
3	D	2	100%

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	NAG	C	1	X	-	-	-
3	NAG	D	1	X	-	-	-
4	NAG	B	4903	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12600 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 fibroblast activation protein, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5889	3812	961	1094	22			
1	B	719	Total	C	N	O	S	0	6	0
			5915	3825	965	1103	22			

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

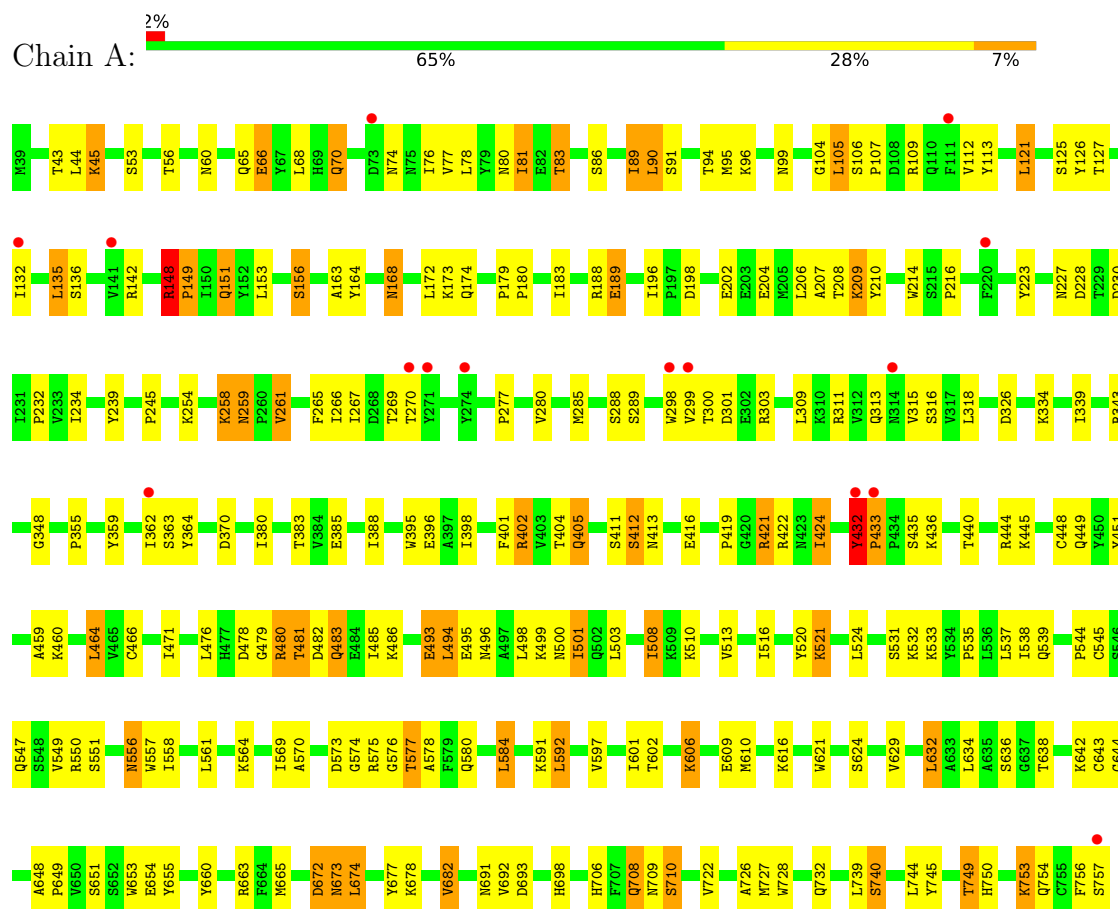
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	422	Total	O	0	0
			422	422		

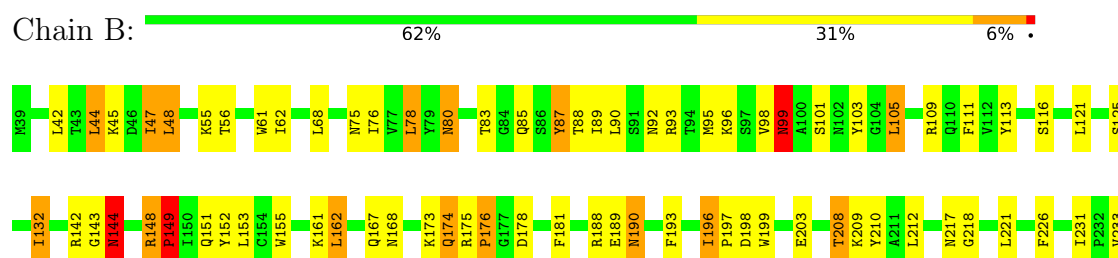
3 Residue-property plots

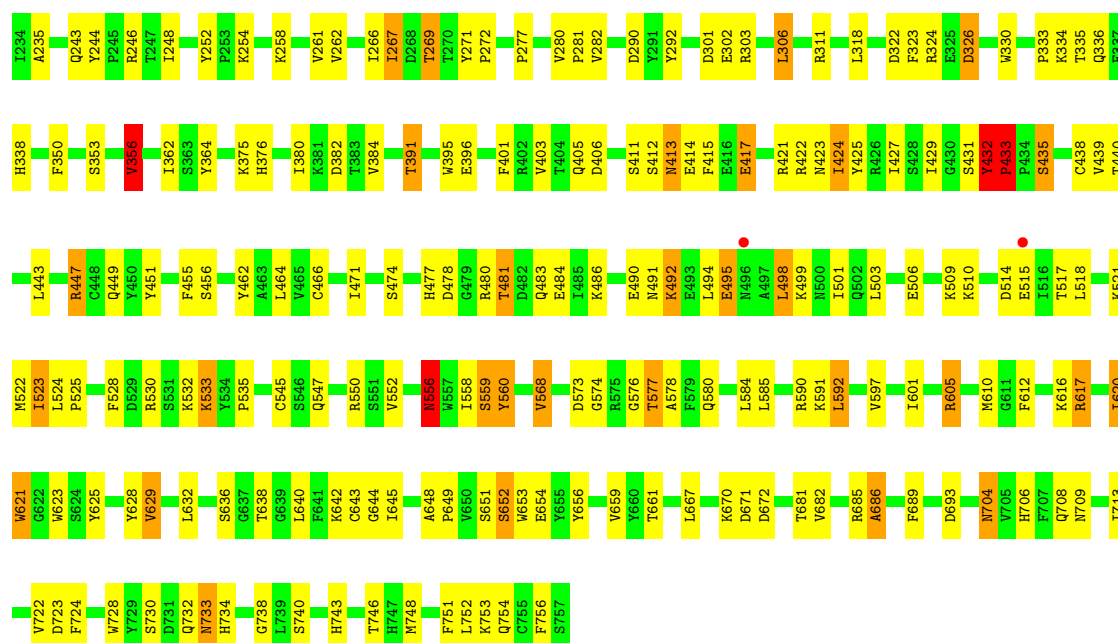
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: fibroblast activation protein, alpha subunit



- Molecule 1: fibroblast activation protein, alpha subunit





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

Chain C: 50% 50%

NAG1
NAG2

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

Chain E: 100%

NAG1
NAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.30Å 152.58Å 214.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.60) 97.8 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.283 0.222 , 0.274	Depositor DCC
R_{free} test set	3558 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12600	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

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	0.50	0/6065	0.88	3/8250 (0.0%)
1	B	0.63	0/6119	0.98	9/8322 (0.1%)
All	All	0.57	0/12184	0.94	12/16572 (0.1%)

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	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	ARG	N-CA-C	-9.91	101.29	113.97
1	B	417	GLU	N-CA-C	7.06	121.28	112.24
1	B	196	ILE	N-CA-C	-6.43	103.92	109.19
1	A	412	SER	N-CA-C	6.41	118.60	108.79
1	B	556	ASN	N-CA-C	6.20	116.63	108.07
1	B	149	PRO	N-CD-CG	-6.17	93.94	103.20
1	A	677	TYR	N-CA-C	-5.61	105.07	111.07
1	B	515	GLU	N-CA-C	-5.47	105.83	112.88
1	B	432	TYR	CA-C-N	5.22	125.75	120.38
1	B	432	TYR	C-N-CA	5.22	125.75	120.38
1	B	356	VAL	CB-CA-C	5.16	118.27	110.63
1	B	433	PRO	N-CA-C	5.13	116.96	110.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Peptide
1	A	432	TYR	Peptide
1	B	148	ARG	Peptide
1	B	432	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5889	0	5660	135	0
1	B	5915	0	5674	179	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	56	0	52	0	0
5	A	206	0	0	4	0
5	B	422	0	0	6	0
All	All	12600	0	11487	307	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 13.

All (307) 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:148:ARG:HB3	1:A:149:PRO:HD2	1.34	1.07
1:B:376:HIS:ND1	1:B:391:THR:HG22	1.72	1.05
1:B:254:LYS:NZ	1:B:706:HIS:HD2	1.65	0.93
1:B:651:SER:H	1:B:709:ASN:HD22	1.14	0.93
1:A:651:SER:H	1:A:709:ASN:HD22	0.97	0.92
1:B:151:GLN:HE22	1:B:168:ASN:H	1.22	0.88
1:A:651:SER:H	1:A:709:ASN:ND2	1.70	0.88
1:B:396:GLU:H	1:B:413:ASN:HD21	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HB2	1:A:449:GLN:O	1.78	0.82
1:A:745:TYR:O	1:A:749:THR:CG2	2.30	0.81
1:B:44:LEU:HD13	1:B:48:LEU:HD11	1.64	0.79
1:A:574:GLY:O	1:A:577:THR:HB	1.82	0.79
1:A:43:THR:HG22	1:A:45:LYS:NZ	1.96	0.79
1:A:148:ARG:HB3	1:A:149:PRO:CD	2.13	0.78
1:B:132:ILE:HD11	1:B:176:PRO:HB3	1.66	0.77
1:A:43:THR:HG22	1:A:45:LYS:HZ2	1.48	0.76
1:B:55:LYS:H	1:B:491:ASN:HD21	1.34	0.76
1:B:645:ILE:HG21	1:B:748:MET:HE3	1.68	0.74
1:B:197:PRO:HA	1:B:226:PHE:CE2	2.23	0.74
1:B:254:LYS:HZ3	1:B:706:HIS:HD2	1.32	0.74
1:B:218:GLY:O	1:B:269:THR:HG21	1.87	0.74
1:A:651:SER:N	1:A:709:ASN:HD22	1.79	0.73
1:B:173:LYS:HE3	1:B:178:ASP:O	1.88	0.73
1:B:638:THR:HG23	1:B:640:LEU:H	1.53	0.73
1:B:704:ASN:C	1:B:704:ASN:HD22	1.97	0.73
1:B:421:ARG:HD3	1:B:449:GLN:HE21	1.54	0.72
1:A:254:LYS:NZ	1:A:706:HIS:HD2	1.88	0.72
1:B:254:LYS:HZ1	1:B:706:HIS:HD2	1.38	0.70
1:A:539:GLN:HE21	1:A:621:TRP:HE1	1.41	0.68
1:A:745:TYR:O	1:A:749:THR:HG23	1.92	0.68
1:A:727:MET:HE1	1:B:724:PHE:CZ	2.29	0.68
1:A:521:LYS:NZ	1:A:550:ARG:O	2.27	0.67
1:B:391:THR:HG23	1:B:395:TRP:CH2	2.29	0.67
1:B:432:TYR:CD2	1:B:433:PRO:HD3	2.29	0.66
1:B:254:LYS:HZ3	1:B:706:HIS:CD2	2.11	0.66
1:A:597:VAL:HG21	1:A:632:LEU:HB3	1.78	0.66
1:B:732:GLN:HG3	1:B:740:SER:OG	1.95	0.66
1:B:573:ASP:HB3	1:B:577:THR:HG21	1.77	0.65
1:A:727:MET:HE3	1:A:728:TRP:O	1.96	0.65
1:B:175:ARG:HG2	1:B:176:PRO:HD2	1.78	0.65
1:A:254:LYS:HE3	1:A:655:TYR:HA	1.79	0.65
1:B:734:HIS:CD2	5:B:5083:HOH:O	2.50	0.64
1:B:254:LYS:NZ	1:B:706:HIS:CD2	2.57	0.64
1:A:404:THR:HG22	1:A:405:GLN:H	1.62	0.64
1:B:132:ILE:CD1	1:B:176:PRO:HB3	2.26	0.64
1:B:254:LYS:HZ2	1:B:708:GLN:HE22	1.45	0.64
1:A:481:THR:CG2	1:A:483:GLN:HB2	2.28	0.63
1:B:208:THR:CG2	1:B:210:TYR:O	2.47	0.63
1:A:575:ARG:HA	1:A:584:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:HH12	1:B:547:GLN:NE2	1.97	0.63
1:A:105:LEU:HD11	1:A:109:ARG:HG2	1.81	0.62
1:B:651:SER:HB3	1:B:713:ILE:HD11	1.81	0.62
1:B:208:THR:HG23	1:B:210:TYR:H	1.64	0.62
1:A:513:VAL:HG11	1:A:606:LYS:HD3	1.82	0.62
1:B:621:TRP:CE3	1:B:748:MET:HE1	2.35	0.61
1:A:745:TYR:O	1:A:749:THR:HG22	1.98	0.61
1:B:221:LEU:HB3	1:B:267:ILE:HD11	1.82	0.61
1:B:396:GLU:H	1:B:413:ASN:ND2	1.96	0.61
1:A:245:PRO:HD3	1:B:708:GLN:OE1	2.01	0.60
1:B:221:LEU:HB3	1:B:267:ILE:CD1	2.33	0.59
1:B:652:SER:HB2	1:B:681:THR:HG22	1.85	0.59
1:B:208:THR:HG23	1:B:210:TYR:O	2.02	0.59
1:B:55:LYS:H	1:B:491:ASN:ND2	2.01	0.58
1:B:254:LYS:NZ	1:B:708:GLN:HE22	2.01	0.58
1:A:148:ARG:CB	1:A:149:PRO:HD2	2.23	0.58
1:A:76:ILE:HD11	1:A:95:MET:HE2	1.85	0.58
1:A:223:TYR:CZ	1:A:265:PHE:HB2	2.39	0.58
1:B:292:TYR:CZ	1:B:659:VAL:HG22	2.39	0.58
1:A:422:ARG:NH2	1:A:547:GLN:OE1	2.33	0.57
1:A:432:TYR:O	1:A:433:PRO:C	2.45	0.57
1:B:432:TYR:CD2	1:B:433:PRO:CD	2.87	0.57
1:A:498:LEU:HD22	1:A:503:LEU:HD11	1.85	0.57
1:B:80:ASN:ND2	1:B:83:THR:H	2.02	0.57
1:B:75:ASN:ND2	1:B:92:ASN:H	2.02	0.57
1:A:577:THR:CG2	5:A:5002:HOH:O	2.52	0.57
1:B:324:ARG:NH2	1:B:326:ASP:OD1	2.38	0.57
1:B:547:GLN:O	1:B:550:ARG:NH2	2.37	0.56
1:A:544:PRO:HA	1:A:576:GLY:O	2.06	0.56
1:B:651:SER:H	1:B:709:ASN:ND2	1.94	0.56
1:A:254:LYS:NZ	1:A:708:GLN:HE22	2.04	0.56
1:B:535:PRO:HB3	1:B:617:ARG:HB3	1.88	0.56
1:B:161:LYS:HE2	1:B:174:GLN:HE21	1.71	0.55
1:B:574:GLY:O	1:B:577:THR:HB	2.06	0.55
1:B:423:ASN:HD21	1:B:449:GLN:NE2	2.04	0.55
1:B:620:ILE:O	1:B:644:GLY:HA2	2.07	0.55
1:B:733:ASN:HD22	1:B:733:ASN:H	1.53	0.55
1:A:81:ILE:HD12	1:A:476:LEU:HD21	1.88	0.55
1:A:634:LEU:HG	1:A:692:VAL:HG21	1.88	0.55
1:B:148:ARG:HB3	1:B:149:PRO:HD2	1.88	0.55
1:A:478:ASP:HB3	1:A:481:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASP:OD1	1:B:311:ARG:NH2	2.39	0.55
1:A:107:PRO:HG2	1:A:156:SER:O	2.07	0.55
1:A:481:THR:HG23	1:A:483:GLN:HB2	1.89	0.54
1:B:217:ASN:HB2	1:B:301:ASP:OD1	2.07	0.54
1:A:227:ASN:HB3	1:A:261:VAL:HG22	1.90	0.54
1:A:508:ILE:HG13	1:A:508:ILE:O	2.06	0.54
1:A:673:ASN:O	1:A:674:LEU:C	2.51	0.54
1:B:303:ARG:HD2	1:B:322:ASP:OD1	2.08	0.54
1:A:285:MET:HE1	1:A:339:ILE:HD11	1.90	0.54
1:A:538:ILE:HD13	1:A:570:ALA:HB3	1.90	0.54
1:A:749:THR:O	1:A:753:LYS:HB2	2.08	0.54
1:A:592:LEU:HD22	1:A:665:MET:HG2	1.89	0.53
1:B:111:PHE:CE1	1:B:176:PRO:HG2	2.43	0.53
1:A:45:LYS:HZ2	1:A:45:LYS:H	1.56	0.53
1:A:654:GLU:HG2	1:B:243:GLN:HG3	1.89	0.53
1:A:70:GLN:HE22	1:A:74:ASN:HD22	1.56	0.52
1:A:267:ILE:HD12	1:A:277:PRO:HG3	1.91	0.52
1:B:447:ARG:HD3	1:B:471:ILE:O	2.09	0.52
1:B:111:PHE:CD1	1:B:176:PRO:HG2	2.44	0.52
1:B:651:SER:N	1:B:709:ASN:HD22	1.96	0.52
1:B:375:LYS:H	1:B:396:GLU:HG2	1.75	0.52
1:A:722:VAL:O	1:B:743:HIS:HE1	1.93	0.51
1:B:401:PHE:HE1	1:B:411:SER:HB3	1.74	0.51
1:B:601:ILE:HG23	1:B:640:LEU:HD11	1.91	0.51
1:A:70:GLN:NE2	1:A:74:ASN:HD22	2.08	0.51
1:A:479:GLY:H	1:A:482:ASP:H	1.59	0.51
1:B:592:LEU:HG	1:B:625:TYR:OH	2.11	0.51
1:A:580:GLN:HB2	1:A:584:LEU:HD12	1.93	0.51
1:B:643:CYS:HB3	1:B:693:ASP:HB2	1.92	0.51
1:A:557:TRP:CE2	1:A:561:LEU:HD11	2.46	0.50
1:B:226:PHE:CD1	1:B:262:VAL:HG12	2.47	0.50
1:B:380:ILE:HD13	1:B:384:VAL:HG23	1.93	0.50
1:B:421:ARG:HD3	1:B:449:GLN:HB3	1.94	0.50
1:B:212:LEU:HD13	1:B:221:LEU:HD11	1.92	0.50
1:B:455:PHE:CD1	1:B:462:TYR:HB3	2.47	0.50
1:B:625:TYR:O	1:B:629:VAL:HG23	2.11	0.50
1:A:643:CYS:HB3	1:A:693:ASP:HB2	1.94	0.50
1:B:656:TYR:CE2	1:B:704:ASN:ND2	2.80	0.50
1:B:280:VAL:HG11	1:B:306:LEU:HD13	1.93	0.50
1:B:292:TYR:CE2	1:B:659:VAL:HG22	2.47	0.50
1:A:636:SER:HB3	1:A:638:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:GLN:NE2	5:B:5006:HOH:O	2.44	0.50
1:B:645:ILE:CG2	1:B:748:MET:HE3	2.39	0.50
1:A:309:LEU:HD22	1:A:313:GLN:HG2	1.94	0.50
1:A:601:ILE:HD13	1:A:638:THR:HG21	1.94	0.49
1:B:545:CYS:HB3	5:B:5178:HOH:O	2.11	0.49
1:A:432:TYR:CD2	1:A:433:PRO:HD3	2.47	0.49
1:A:148:ARG:CB	1:A:149:PRO:CD	2.88	0.49
1:A:395:TRP:HB2	1:A:413:ASN:HB3	1.94	0.49
1:B:391:THR:CG2	1:B:395:TRP:CH2	2.95	0.49
1:B:68:LEU:HD23	1:B:78:LEU:HB2	1.93	0.49
1:A:216:PRO:HD3	1:A:298:TRP:HB3	1.95	0.49
1:A:401:PHE:CE2	1:A:424:ILE:HD11	2.48	0.49
1:A:254:LYS:HG2	1:A:655:TYR:O	2.11	0.48
1:B:427:ILE:HA	1:B:435:SER:O	2.13	0.48
1:B:61:TRP:CE3	1:B:456:SER:HB3	2.48	0.48
1:A:89:ILE:HG13	1:A:135:LEU:HD21	1.96	0.48
1:B:623:TRP:HZ2	1:B:734:HIS:O	1.96	0.48
1:B:47:ILE:HD13	1:B:560:TYR:HB2	1.94	0.48
1:B:556:ASN:ND2	1:B:559:SER:OG	2.47	0.48
1:A:43:THR:HG22	1:A:45:LYS:HZ3	1.77	0.48
1:B:391:THR:HG23	1:B:395:TRP:HH2	1.77	0.48
1:A:448:CYS:HB3	1:A:451:TYR:CE2	2.49	0.47
1:A:732:GLN:HG3	1:A:740:SER:OG	2.14	0.47
1:B:267:ILE:HG23	1:B:277:PRO:HA	1.96	0.47
1:B:522:MET:HE3	1:B:522:MET:HB2	1.85	0.47
1:B:590:ARG:NH2	1:B:672:ASP:OD2	2.45	0.47
1:A:239:TYR:HA	1:A:245:PRO:HB3	1.97	0.47
1:B:425:TYR:CE2	1:B:438:CYS:HB2	2.49	0.47
1:B:481:THR:HG23	1:B:483:GLN:H	1.80	0.47
1:A:364:TYR:CE2	1:A:380:ILE:HD12	2.50	0.47
1:B:356:VAL:CG2	1:B:403:VAL:HG23	2.45	0.47
1:A:66:GLU:HG2	1:A:78:LEU:HD21	1.96	0.47
1:B:311:ARG:HG2	5:B:5013:HOH:O	2.15	0.47
1:A:556:ASN:HD22	1:A:556:ASN:H	1.62	0.47
1:A:81:ILE:HG21	1:A:476:LEU:HD21	1.96	0.46
1:A:188:ARG:O	1:A:189:GLU:C	2.58	0.46
1:B:656:TYR:HE2	1:B:704:ASN:ND2	2.13	0.46
1:A:90:LEU:HG	1:A:112:VAL:HG11	1.97	0.46
1:A:402:ARG:HG2	1:A:459:ALA:HB2	1.96	0.46
1:A:493:GLU:CD	1:A:493:GLU:N	2.73	0.46
1:B:155:TRP:CE3	1:B:162:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ARG:O	1:B:686:ALA:C	2.57	0.46
1:B:494:LEU:O	1:B:495:GLU:C	2.57	0.46
1:B:254:LYS:HZ1	1:B:706:HIS:CD2	2.26	0.46
1:B:302[A]:GLU:HG2	1:B:323:PHE:HB3	1.98	0.46
1:A:60:ASN:HB3	1:A:68:LEU:O	2.15	0.46
1:B:413:ASN:ND2	1:B:413:ASN:H	2.13	0.46
1:A:202:GLU:O	1:A:207:ALA:HA	2.16	0.46
1:B:376:HIS:ND1	1:B:391:THR:CG2	2.61	0.46
1:B:506:GLU:HG2	1:B:523:ILE:HD13	1.98	0.46
1:A:573:ASP:HB3	1:A:577:THR:HG21	1.97	0.46
1:B:556:ASN:H	1:B:559:SER:HG	1.62	0.46
1:A:501:ILE:HG22	1:A:503:LEU:HG	1.97	0.45
1:B:478:ASP:HB3	1:B:481:THR:HG22	1.98	0.45
1:A:80:ASN:HB3	1:A:83:THR:HG22	1.98	0.45
1:A:396:GLU:H	1:A:413:ASN:HB3	1.81	0.45
1:B:80:ASN:HD22	1:B:83:THR:H	1.61	0.45
1:B:98:VAL:O	1:B:99:ASN:C	2.58	0.45
1:A:125:SER:HA	1:A:209:LYS:HB2	1.98	0.45
1:A:496:ASN:O	1:A:499:LYS:HB2	2.16	0.45
1:B:55:LYS:N	1:B:491:ASN:HD21	2.08	0.45
1:B:439:VAL:HG13	1:B:440:THR:HG23	1.98	0.45
1:B:751:PHE:O	1:B:754:GLN:HB3	2.16	0.45
1:A:313:GLN:OE1	1:A:663:ARG:HD2	2.16	0.45
1:A:698:HIS:CD2	1:A:710:SER:HB2	2.52	0.45
1:A:153:LEU:HD12	1:A:164:TYR:HB3	1.99	0.45
1:A:168:ASN:HD22	1:A:168:ASN:N	2.14	0.45
1:A:493:GLU:CD	1:A:493:GLU:H	2.24	0.45
1:B:545:CYS:HA	1:B:578:ALA:HB2	1.98	0.45
1:B:638:THR:HG23	1:B:640:LEU:N	2.27	0.45
1:A:513:VAL:CG1	1:A:606:LYS:HD3	2.45	0.45
1:B:490:GLU:HB3	1:B:492:LYS:HE3	1.99	0.45
1:B:61:TRP:CZ3	1:B:456:SER:HB3	2.52	0.44
1:B:318:LEU:HB3	1:B:338:HIS:HB2	1.98	0.44
1:B:576:GLY:HA2	1:B:585:LEU:O	2.17	0.44
1:A:259:ASN:HD22	1:A:259:ASN:HA	1.60	0.44
1:B:533:LYS:HA	1:B:612:PHE:O	2.17	0.44
1:A:440:THR:HG22	1:A:464:LEU:HD21	1.99	0.44
1:B:75:ASN:HD22	1:B:92:ASN:H	1.63	0.44
1:B:580:GLN:HB2	1:B:584:LEU:HD23	2.00	0.44
1:B:85:GLN:HB3	1:B:87:TYR:CZ	2.52	0.44
1:A:535:PRO:HB2	1:A:756:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG11	1:B:306:LEU:CD1	2.47	0.44
1:A:104:GLY:HA3	1:A:113:TYR:CE1	2.53	0.44
1:A:547:GLN:HB3	1:A:550:ARG:HE	1.82	0.44
1:B:413:ASN:H	1:B:413:ASN:HD22	1.66	0.44
1:B:752:LEU:HD23	1:B:752:LEU:HA	1.50	0.44
1:A:198:ASP:HB2	1:A:228:ASP:OD2	2.17	0.44
1:A:471:ILE:HG12	1:A:494:LEU:HD13	1.99	0.44
1:B:364:TYR:CE1	1:B:380:ILE:HD12	2.53	0.43
1:B:424:ILE:O	1:B:439:VAL:HG12	2.18	0.43
1:A:401:PHE:HE2	1:A:411:SER:HB3	1.82	0.43
1:B:181:PHE:CE1	1:B:272:PRO:HB2	2.53	0.43
1:A:520:TYR:HA	1:A:549:VAL:HG21	1.98	0.43
1:A:556:ASN:O	1:A:557:TRP:C	2.61	0.43
1:A:651:SER:HA	1:A:682:VAL:CG1	2.48	0.43
1:A:756:PHE:O	1:A:757:SER:C	2.61	0.43
1:B:477:HIS:NE2	1:B:484:GLU:HB3	2.32	0.43
1:A:126:TYR:CD1	1:A:126:TYR:C	2.97	0.43
1:B:198:ASP:OD2	1:B:198:ASP:C	2.61	0.43
1:B:481:THR:CG2	1:B:483:GLN:H	2.32	0.43
1:B:524:LEU:HD23	1:B:568:VAL:HG22	2.01	0.43
1:B:648:ALA:N	1:B:649:PRO:CD	2.82	0.43
1:A:230:ASP:HB3	1:A:258:LYS:HD2	2.00	0.43
1:A:232:PRO:HB2	1:B:244:TYR:CZ	2.53	0.43
1:B:203:GLU:HB2	5:B:5179:HOH:O	2.17	0.43
1:B:689:PHE:HB2	1:B:722:VAL:HG11	2.00	0.43
1:A:78:LEU:O	1:A:86:SER:HA	2.19	0.43
1:B:125:SER:HA	1:B:209:LYS:HB2	2.00	0.43
1:B:440:THR:HB	1:B:451:TYR:CE1	2.54	0.43
1:B:636:SER:OG	1:B:638:THR:HB	2.18	0.43
1:B:113:TYR:C	1:B:113:TYR:CD2	2.96	0.43
1:B:422:ARG:HH22	1:B:547:GLN:HE22	1.67	0.43
1:A:254:LYS:NZ	1:A:706:HIS:CD2	2.77	0.43
1:A:577:THR:HG21	5:A:5002:HOH:O	2.19	0.43
1:B:103:TYR:HA	1:B:113:TYR:O	2.18	0.43
1:B:190:ASN:HA	1:B:193:PHE:CZ	2.54	0.43
1:B:199:TRP:CZ2	1:B:704:ASN:HA	2.53	0.42
1:A:545:CYS:HA	1:A:578:ALA:HB2	2.00	0.42
1:A:592:LEU:HD23	1:A:653:TRP:CE2	2.54	0.42
1:A:300:THR:OG1	1:A:303:ARG:HB2	2.19	0.42
1:B:266:ILE:HD12	1:B:330:TRP:CE2	2.55	0.42
1:B:704:ASN:C	1:B:704:ASN:ND2	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLY:HA2	5:A:5010:HOH:O	2.18	0.42
1:A:643:CYS:CB	1:A:693:ASP:HB2	2.50	0.42
1:A:556:ASN:HD22	1:A:556:ASN:N	2.16	0.42
1:B:494:LEU:HG	1:B:498:LEU:HD22	2.01	0.42
1:B:653:TRP:HB3	1:B:661:THR:CG2	2.49	0.42
1:A:537:LEU:HD23	1:A:569:ILE:HD12	2.01	0.42
1:A:148:ARG:HD3	1:A:148:ARG:HA	1.83	0.42
1:A:206:LEU:HB3	1:A:208:THR:HG22	2.00	0.42
1:A:404:THR:HG22	5:A:5083:HOH:O	2.19	0.42
1:A:726:ALA:HB1	1:B:728:TRP:CZ3	2.55	0.42
1:B:254:LYS:NZ	1:B:708:GLN:NE2	2.68	0.42
1:B:143:GLY:O	1:B:144:ASN:C	2.62	0.42
1:B:271:TYR:N	1:B:272:PRO:CD	2.83	0.42
1:A:163:ALA:HB2	1:A:214:TRP:CZ2	2.55	0.42
1:B:267:ILE:HG23	1:B:277:PRO:CA	2.50	0.42
1:B:415:PHE:C	1:B:417:GLU:H	2.27	0.42
1:A:413:ASN:OD1	1:A:419:PRO:HA	2.20	0.42
1:A:660:TYR:CD2	1:A:660:TYR:C	2.97	0.41
1:A:208:THR:HG23	1:A:210:TYR:O	2.20	0.41
1:A:648:ALA:N	1:A:649:PRO:CD	2.83	0.41
1:B:176:PRO:O	5:B:5001:HOH:O	2.22	0.41
1:B:188:ARG:O	1:B:189:GLU:C	2.63	0.41
1:A:634:LEU:HD22	1:A:644:GLY:HA3	2.03	0.41
1:B:152:TYR:HD2	1:B:209:LYS:HE2	1.85	0.41
1:B:656:TYR:HE2	1:B:704:ASN:HD22	1.68	0.41
1:A:318:LEU:HD11	1:A:355:PRO:HG3	2.02	0.41
1:B:68:LEU:CD2	1:B:78:LEU:HB2	2.49	0.41
1:B:252:TYR:C	1:B:252:TYR:CD2	2.98	0.41
1:A:416:GLU:OE2	1:A:421:ARG:NH2	2.54	0.41
1:B:161:LYS:HZ3	1:B:269:THR:HG23	1.85	0.41
1:B:235:ALA:HA	1:B:248:ILE:O	2.20	0.41
1:B:395:TRP:CD2	1:B:414:GLU:HB2	2.56	0.41
1:B:423:ASN:HD21	1:B:449:GLN:HE22	1.66	0.41
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.77	0.41
1:B:605:ARG:HH21	1:B:605:ARG:CG	2.34	0.41
1:B:617:ARG:HG2	1:B:756:PHE:CD2	2.56	0.41
1:B:148:ARG:HB3	1:B:149:PRO:CD	2.49	0.41
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.86	0.41
1:B:280:VAL:HA	1:B:281:PRO:HD3	1.93	0.41
1:B:733:ASN:C	1:B:733:ASN:ND2	2.78	0.41
1:A:179:PRO:HA	1:A:180:PRO:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:HIS:CD2	1:B:723:ASP:OD1	2.75	0.40
1:B:333:PRO:HG2	1:B:336:GLN:HG3	2.03	0.40
1:A:413:ASN:CG	1:A:419:PRO:HA	2.47	0.40
1:B:95:MET:HE1	1:B:103:TYR:HB3	2.02	0.40
1:B:628:TYR:CE1	1:B:632:LEU:HD11	2.56	0.40
1:B:350:PHE:HD2	1:B:545:CYS:HB2	1.86	0.40
1:A:362:ILE:HG23	1:A:363:SER:N	2.36	0.40
1:A:672:ASP:HB3	1:A:673:ASN:H	1.65	0.40
1:B:62:ILE:HG21	1:B:105:LEU:HD12	2.04	0.40
1:B:524:LEU:HA	1:B:525:PRO:HD3	1.94	0.40
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.98	0.40
1:B:47:ILE:HG12	1:B:556:ASN:C	2.47	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	717/719 (100%)	652 (91%)	58 (8%)	7 (1%)	12	28
1	B	723/719 (101%)	656 (91%)	56 (8%)	11 (2%)	8	18
All	All	1440/1438 (100%)	1308 (91%)	114 (8%)	18 (1%)	9	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	432	TYR
1	B	149	PRO
1	B	433	PRO
1	A	99	ASN
1	A	433	PRO

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Mol	Chain	Res	Type
1	B	99	ASN
1	B	144	ASN
1	B	190	ASN
1	A	151	GLN
1	B	335	THR
1	B	382	ASP
1	A	674	LEU
1	B	76	ILE
1	B	528	PHE
1	B	686	ALA
1	A	370	ASP
1	B	738	GLY

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	634/634 (100%)	516 (81%)	118 (19%)	1	3
1	B	640/634 (101%)	534 (83%)	106 (17%)	2	4
All	All	1274/1268 (100%)	1050 (82%)	224 (18%)	2	3

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	LYS
1	A	53	SER
1	A	56	THR
1	A	65	GLN
1	A	66	GLU
1	A	70	GLN
1	A	77	VAL
1	A	81	ILE
1	A	83	THR
1	A	89	ILE

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Mol	Chain	Res	Type
1	A	90	LEU
1	A	91	SER
1	A	94	THR
1	A	96	LYS
1	A	105	LEU
1	A	106	SER
1	A	121	LEU
1	A	127	THR
1	A	132	ILE
1	A	135	LEU
1	A	136	SER
1	A	142	ARG
1	A	148	ARG
1	A	151	GLN
1	A	156	SER
1	A	168	ASN
1	A	172	LEU
1	A	173	LYS
1	A	174	GLN
1	A	183	ILE
1	A	189	GLU
1	A	196	ILE
1	A	204	GLU
1	A	209	LYS
1	A	234	ILE
1	A	258	LYS
1	A	259	ASN
1	A	261	VAL
1	A	266	ILE
1	A	269	THR
1	A	270	THR
1	A	280	VAL
1	A	288	SER
1	A	289	SER
1	A	299	VAL
1	A	301	ASP
1	A	311	ARG
1	A	315	VAL
1	A	316	SER
1	A	326	ASP
1	A	334	LYS
1	A	343	ARG

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Mol	Chain	Res	Type
1	A	359	TYR
1	A	383	THR
1	A	385	GLU
1	A	388	ILE
1	A	398	ILE
1	A	402	ARG
1	A	405	GLN
1	A	412	SER
1	A	421	ARG
1	A	424	ILE
1	A	435	SER
1	A	436	LYS
1	A	444	ARG
1	A	445	LYS
1	A	460	LYS
1	A	464	LEU
1	A	466	CYS
1	A	480	ARG
1	A	481	THR
1	A	483	GLN
1	A	485	ILE
1	A	486	LYS
1	A	493	GLU
1	A	494	LEU
1	A	495	GLU
1	A	500	ASN
1	A	501	ILE
1	A	508	ILE
1	A	510	LYS
1	A	516	ILE
1	A	521	LYS
1	A	524	LEU
1	A	531	SER
1	A	532	LYS
1	A	533	LYS
1	A	551	SER
1	A	556	ASN
1	A	558	ILE
1	A	564	LYS
1	A	577	THR
1	A	584	LEU
1	A	591	LYS

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Mol	Chain	Res	Type
1	A	592	LEU
1	A	602	THR
1	A	606	LYS
1	A	609	GLU
1	A	610	MET
1	A	616	LYS
1	A	624	SER
1	A	629	VAL
1	A	632	LEU
1	A	642	LYS
1	A	672	ASP
1	A	673	ASN
1	A	678	LYS
1	A	682	VAL
1	A	691	ASN
1	A	708	GLN
1	A	710	SER
1	A	739	LEU
1	A	740	SER
1	A	744	LEU
1	A	749	THR
1	A	753	LYS
1	A	754	GLN
1	B	42	LEU
1	B	44	LEU
1	B	45	LYS
1	B	47	ILE
1	B	48	LEU
1	B	56	THR
1	B	78	LEU
1	B	80	ASN
1	B	87	TYR
1	B	88	THR
1	B	89	ILE
1	B	90	LEU
1	B	93	ARG
1	B	96	LYS
1	B	99	ASN
1	B	101	SER
1	B	105	LEU
1	B	109	ARG
1	B	116	SER

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Mol	Chain	Res	Type
1	B	121	LEU
1	B	132	ILE
1	B	142	ARG
1	B	144	ASN
1	B	153	LEU
1	B	162	LEU
1	B	174	GLN
1	B	176	PRO
1	B	196	ILE
1	B	208	THR
1	B	231	ILE
1	B	233	VAL
1	B	246[A]	ARG
1	B	246[B]	ARG
1	B	258	LYS
1	B	261	VAL
1	B	267	ILE
1	B	269	THR
1	B	282	VAL
1	B	306	LEU
1	B	326	ASP
1	B	334	LYS
1	B	353	SER
1	B	356	VAL
1	B	362	ILE
1	B	391	THR
1	B	405	GLN
1	B	406	ASP
1	B	412	SER
1	B	413	ASN
1	B	424	ILE
1	B	429	ILE
1	B	431	SER
1	B	435	SER
1	B	443	LEU
1	B	447	ARG
1	B	466	CYS
1	B	474	SER
1	B	480	ARG
1	B	481	THR
1	B	486	LYS
1	B	492	LYS

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Mol	Chain	Res	Type
1	B	495	GLU
1	B	498	LEU
1	B	499	LYS
1	B	501	ILE
1	B	503	LEU
1	B	509	LYS
1	B	510	LYS
1	B	514	ASP
1	B	517	THR
1	B	518	LEU
1	B	521	LYS
1	B	523	ILE
1	B	530	ARG
1	B	532	LYS
1	B	533	LYS
1	B	552	VAL
1	B	556	ASN
1	B	558	ILE
1	B	559	SER
1	B	560	TYR
1	B	568	VAL
1	B	577	THR
1	B	591	LYS
1	B	592	LEU
1	B	597	VAL
1	B	605	ARG
1	B	610	MET
1	B	616	LYS
1	B	617	ARG
1	B	620	ILE
1	B	621	TRP
1	B	629	VAL
1	B	642	LYS
1	B	652	SER
1	B	654[A]	GLU
1	B	654[B]	GLU
1	B	667	LEU
1	B	670	LYS
1	B	671	ASP
1	B	682	VAL
1	B	704	ASN
1	B	730	SER

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Mol	Chain	Res	Type
1	B	733	ASN
1	B	746	THR
1	B	753	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	74	ASN
1	A	85	GLN
1	A	151	GLN
1	A	168	ASN
1	A	182	GLN
1	A	243	GLN
1	A	259	ASN
1	A	423	ASN
1	A	449	GLN
1	A	483	GLN
1	A	502	GLN
1	A	539	GLN
1	A	556	ASN
1	A	673	ASN
1	A	676	HIS
1	A	691	ASN
1	A	698	HIS
1	A	704	ASN
1	A	706	HIS
1	A	708	GLN
1	A	709	ASN
1	A	719	ASN
1	A	721	GLN
1	A	732	GLN
1	A	742	ASN
1	A	754	GLN
1	B	60	ASN
1	B	69	HIS
1	B	75	ASN
1	B	80	ASN
1	B	102	ASN
1	B	144	ASN
1	B	151	GLN
1	B	167	GLN

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Mol	Chain	Res	Type
1	B	168	ASN
1	B	174	GLN
1	B	182	GLN
1	B	194	ASN
1	B	243	GLN
1	B	249	ASN
1	B	259	ASN
1	B	313	GLN
1	B	378	HIS
1	B	413	ASN
1	B	423	ASN
1	B	442	HIS
1	B	449	GLN
1	B	477	HIS
1	B	491	ASN
1	B	527	GLN
1	B	547	GLN
1	B	556	ASN
1	B	704	ASN
1	B	706	HIS
1	B	708	GLN
1	B	709	ASN
1	B	719	ASN
1	B	733	ASN
1	B	742	ASN
1	B	743	HIS
1	B	754	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	1,2	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
2	NAG	C	2	2	14,14,15	0.50	0	17,19,21	0.81	0
3	NAG	D	1	1,3	14,14,15	0.67	0	17,19,21	1.38	3 (17%)
3	NAG	D	2	3	14,14,15	0.63	0	17,19,21	0.97	1 (5%)
2	NAG	E	1	1,2	14,14,15	1.16	1 (7%)	17,19,21	1.58	4 (23%)
2	NAG	E	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.37	2 (11%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	-3.77	1.37	1.43
2	E	2	NAG	C1-C2	2.31	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-C2-N2	3.85	116.50	110.43
2	E	1	NAG	C1-O5-C5	3.24	116.53	112.19
3	D	1	NAG	C2-N2-C7	3.16	127.14	122.90
2	E	2	NAG	C4-C3-C2	3.08	115.53	111.02
3	D	1	NAG	O3-C3-C4	2.67	116.66	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	O5-C5-C6	2.58	112.69	107.66
2	C	1	NAG	C1-O5-C5	2.52	115.57	112.19
2	E	1	NAG	O5-C1-C2	-2.50	107.42	111.29
3	D	2	NAG	O5-C5-C6	2.19	111.93	107.66
2	E	1	NAG	C2-N2-C7	2.14	125.77	122.90
3	D	1	NAG	C1-C2-N2	-2.09	107.13	110.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
3	D	1	NAG	C1

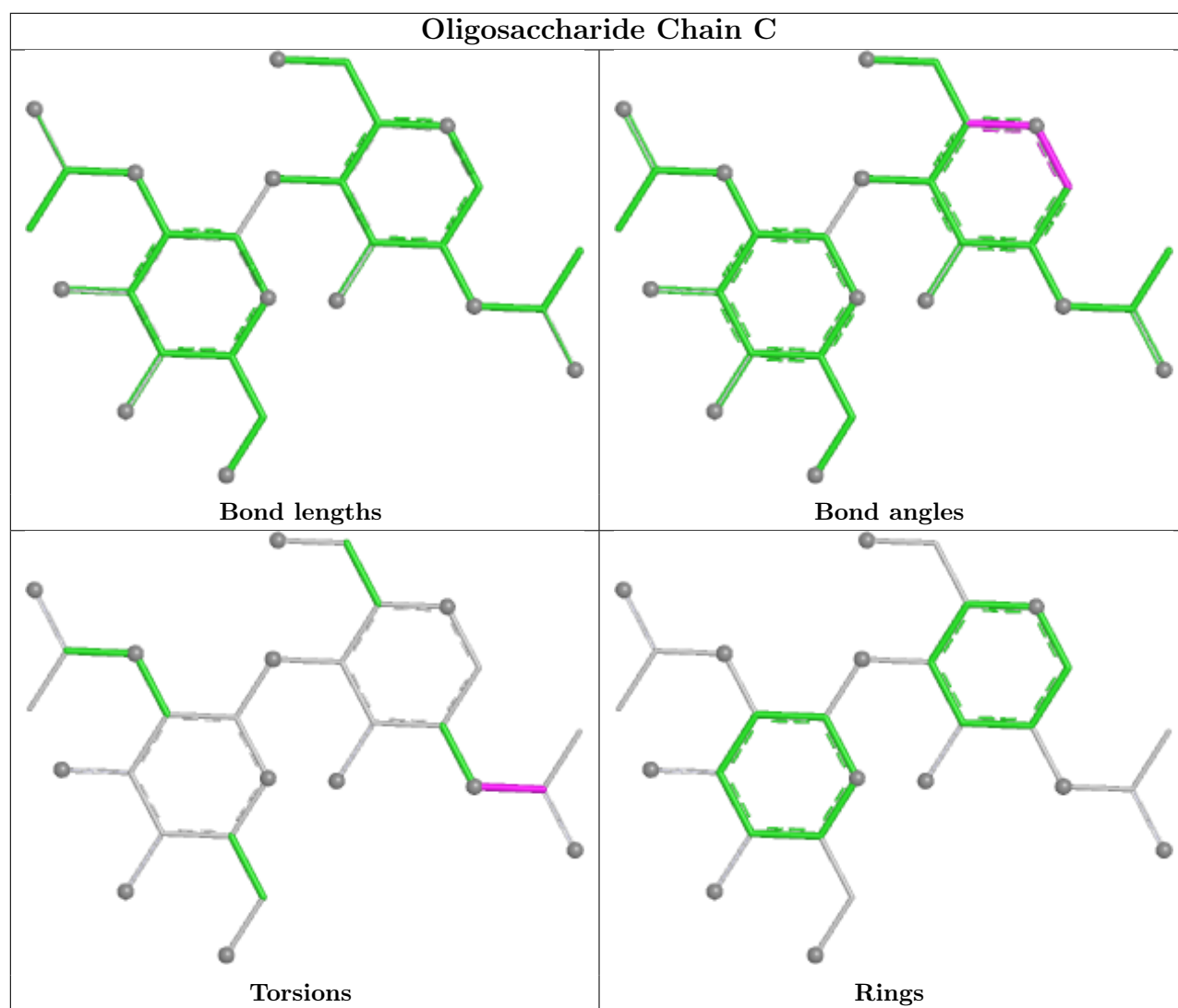
All (16) torsion outliers are listed below:

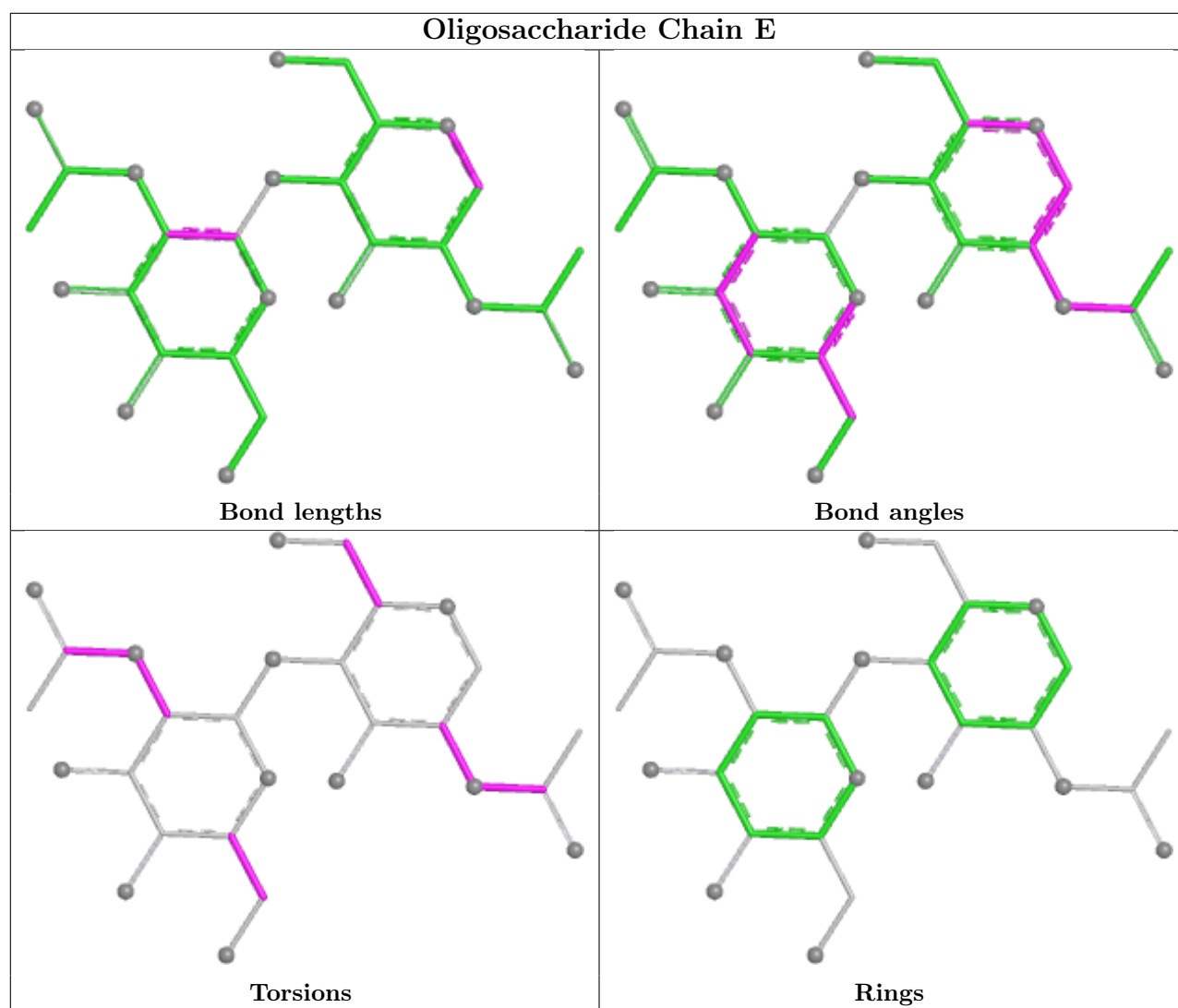
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

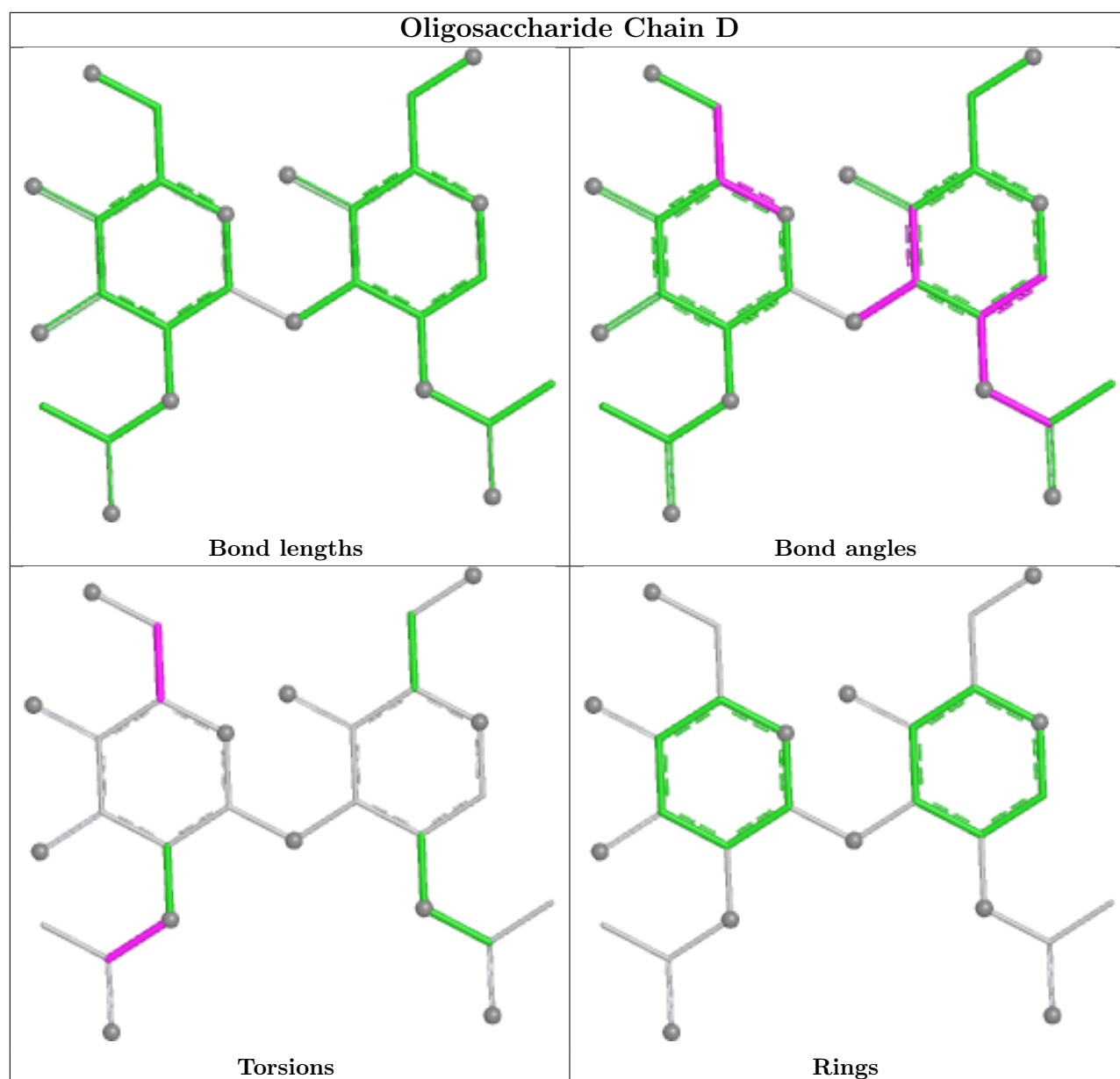
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

6 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
4	NAG	B	4901	1	14,14,15	0.61	0	17,19,21	2.01	3 (17%)
4	NAG	B	4902	1	14,14,15	0.59	0	17,19,21	1.37	2 (11%)
4	NAG	B	4903	1	14,14,15	0.64	0	17,19,21	1.41	2 (11%)
4	NAG	B	4904	1	14,14,15	0.48	0	17,19,21	1.89	2 (11%)
4	NAG	A	4901	1	14,14,15	0.87	1 (7%)	17,19,21	1.57	4 (23%)
4	NAG	A	4902	1	14,14,15	0.64	0	17,19,21	1.31	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4901	1	-	5/6/23/26	0/1/1/1
4	NAG	B	4902	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4903	1	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	B	4904	1	-	5/6/23/26	0/1/1/1
4	NAG	A	4901	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4902	1	-	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)
4	A	4901	NAG	C1-C2	2.59	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4904	NAG	C1-O5-C5	6.58	121.00	112.19
4	B	4901	NAG	C1-O5-C5	6.32	120.66	112.19
4	A	4902	NAG	C4-C3-C2	3.97	116.83	111.02
4	A	4901	NAG	C2-N2-C7	3.90	128.13	122.90
4	B	4902	NAG	C1-O5-C5	3.52	116.90	112.19
4	B	4901	NAG	C2-N2-C7	2.99	126.91	122.90
4	B	4903	NAG	C2-N2-C7	2.80	126.66	122.90
4	A	4901	NAG	C1-C2-N2	2.80	114.84	110.43
4	B	4901	NAG	C1-C2-N2	2.68	114.66	110.43
4	A	4901	NAG	O5-C1-C2	-2.66	107.18	111.29
4	B	4902	NAG	O5-C1-C2	-2.62	107.24	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4901	NAG	C1-O5-C5	2.46	115.48	112.19
4	B	4904	NAG	C2-N2-C7	-2.14	120.03	122.90
4	B	4903	NAG	C1-O5-C5	-2.12	109.34	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	4903	NAG	C1

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4901	NAG	C3-C2-N2-C7
4	A	4901	NAG	C8-C7-N2-C2
4	A	4901	NAG	O7-C7-N2-C2
4	A	4902	NAG	C3-C2-N2-C7
4	A	4902	NAG	C8-C7-N2-C2
4	A	4902	NAG	O7-C7-N2-C2
4	B	4901	NAG	C1-C2-N2-C7
4	B	4901	NAG	O7-C7-N2-C2
4	B	4902	NAG	C8-C7-N2-C2
4	B	4902	NAG	O7-C7-N2-C2
4	B	4903	NAG	C8-C7-N2-C2
4	B	4903	NAG	O7-C7-N2-C2
4	B	4901	NAG	C8-C7-N2-C2
4	B	4904	NAG	C8-C7-N2-C2
4	B	4904	NAG	O7-C7-N2-C2
4	B	4903	NAG	O5-C5-C6-O6
4	B	4903	NAG	C4-C5-C6-O6
4	B	4904	NAG	O5-C5-C6-O6
4	B	4904	NAG	C4-C5-C6-O6
4	B	4901	NAG	C4-C5-C6-O6
4	B	4901	NAG	O5-C5-C6-O6
4	B	4902	NAG	C4-C5-C6-O6
4	B	4903	NAG	C3-C2-N2-C7
4	B	4904	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	719/719 (100%)	0.35	15 (2%) 63 58	7, 27, 40, 67	0
1	B	719/719 (100%)	0.03	2 (0%) 90 88	9, 23, 35, 47	6 (0%)
All	All	1438/1438 (100%)	0.19	17 (1%) 76 73	7, 25, 39, 67	6 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	3.3
1	A	141	VAL	3.1
1	A	271	TYR	2.8
1	A	220	PHE	2.7
1	B	496	ASN	2.5
1	A	314	ASN	2.4
1	A	274	TYR	2.4
1	A	299	VAL	2.3
1	A	757	SER	2.3
1	A	111	PHE	2.2
1	A	270	THR	2.2
1	A	432	TYR	2.1
1	B	515	GLU	2.0
1	A	298	TRP	2.0
1	A	433	PRO	2.0
1	A	362	ILE	2.0
1	A	73	ASP	2.0

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

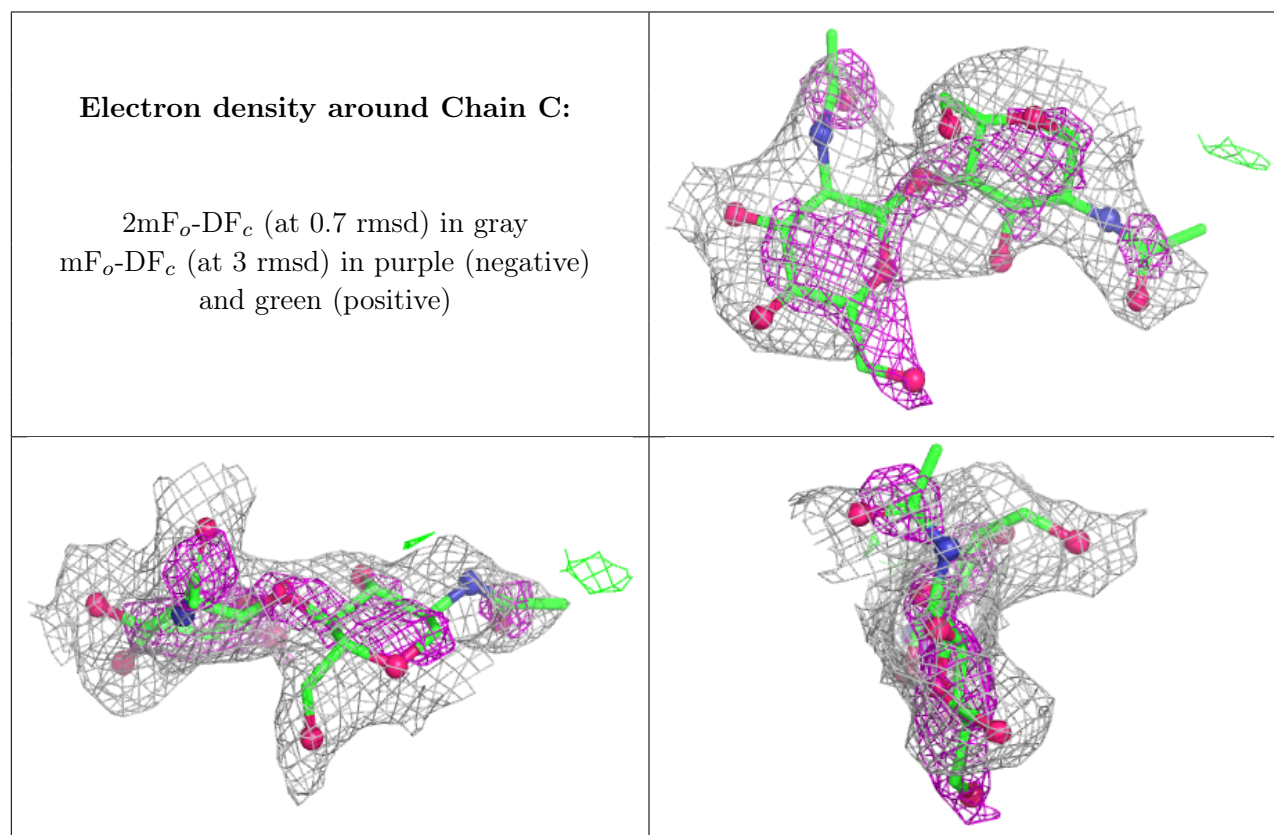
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

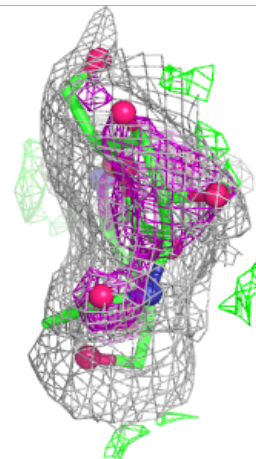
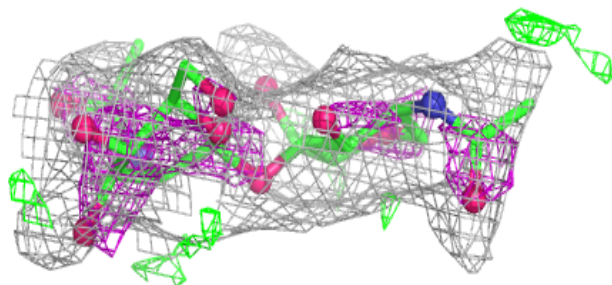
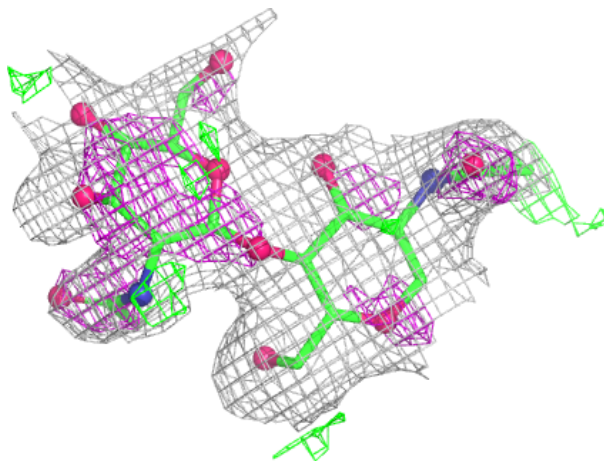
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.41	0.18	57,57,57,57	0
3	NAG	D	2	14/15	0.45	0.18	50,51,52,52	0
2	NAG	C	1	14/15	0.60	0.16	55,56,57,57	0
2	NAG	E	2	14/15	0.61	0.16	50,51,51,52	0
2	NAG	E	1	14/15	0.64	0.15	43,45,46,48	0
3	NAG	D	1	14/15	0.73	0.13	44,47,48,48	0

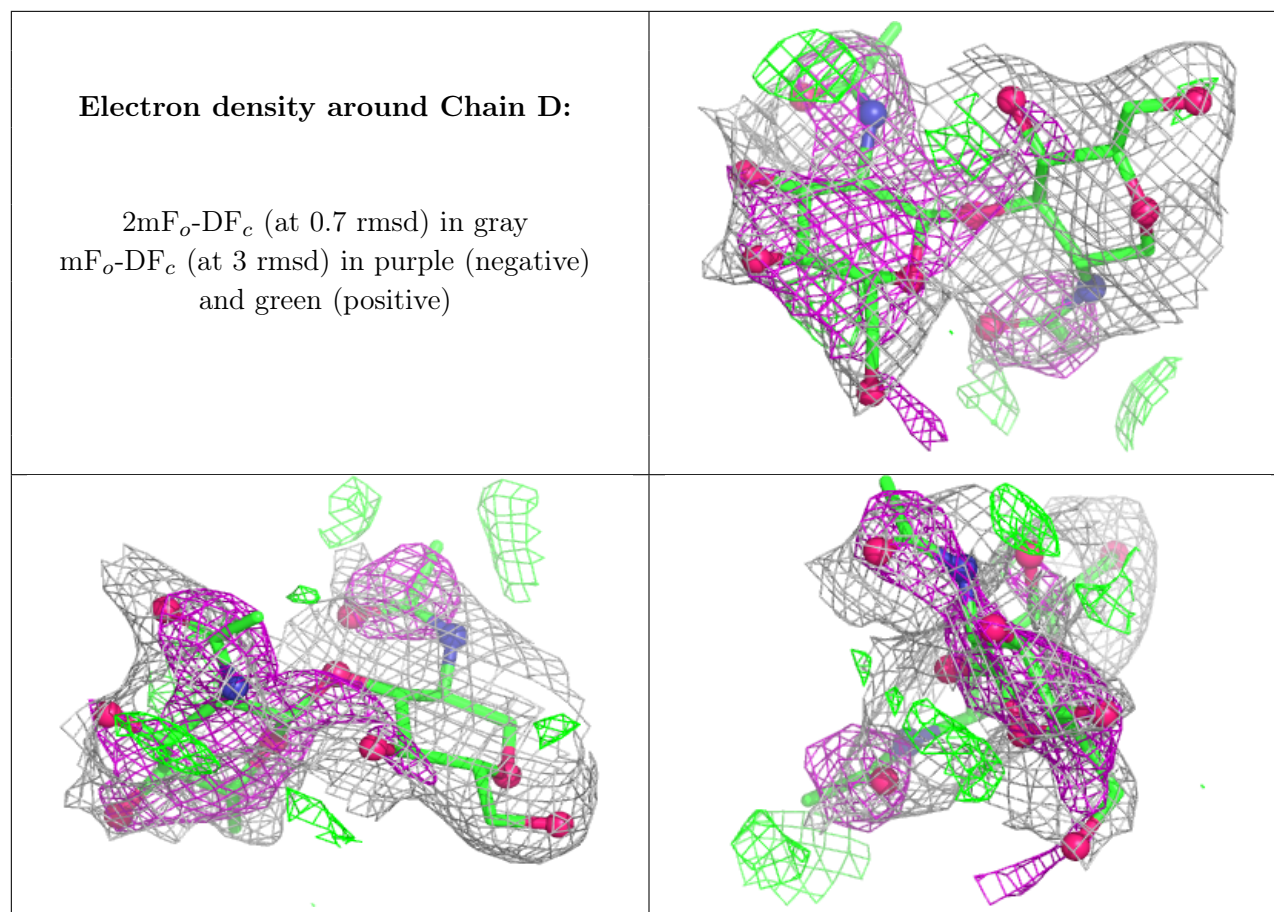
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

$2mF_o-DF_c$ (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
4	NAG	B	4904	14/15	0.63	0.16	53,56,59,59	0
4	NAG	A	4902	14/15	0.68	0.19	105,115,121,121	0
4	NAG	B	4901	14/15	0.69	0.11	36,38,39,39	0
4	NAG	A	4901	14/15	0.69	0.12	49,51,52,52	0
4	NAG	B	4902	14/15	0.81	0.11	38,42,44,44	0
4	NAG	B	4903	14/15	0.84	0.12	47,51,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.