



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 AM UTC

PDB ID : 3P70 / pdb_00003p70
Title : Structural basis of thrombin-mediated factor V activation: essential role of the hirudin-like sequence Glu666-Glu672 for processing at the heavy chain-B domain junction
Authors : Corral-Rodriguez, M.A.; Bock, P.E.; Hernandez-Carvajal, E.; Gutierrez-Gallego, R.; Fuentes-Prior, P.
Deposited on : 2010-10-11
Resolution : 2.55 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

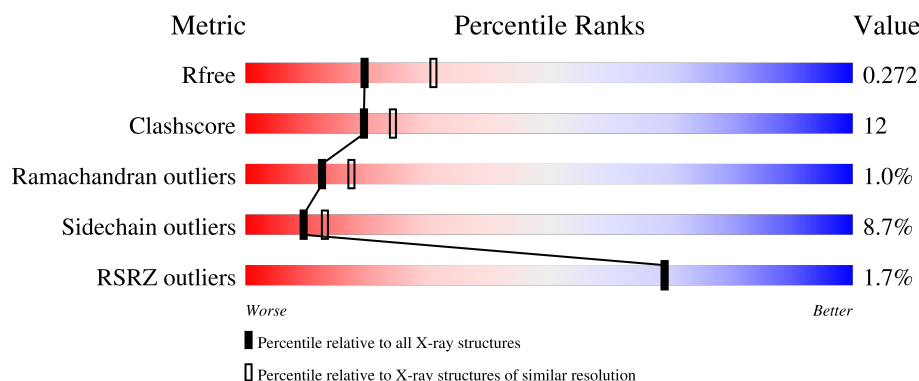
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	36	 3% 72% 6% 19%
1	C	36	 56% 22% 19%
1	E	36	 3% 50% 28% 19%
1	G	36	 3% 56% 22% 19%

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Mol	Chain	Length	Quality of chain
2	B	259	63%31%
2	D	259	2% 68%24%
2	F	259	2% 66%26%5%
2	H	259	% 67%29%
3	M	71	% 7% 92%
3	N	71	93%
3	O	71	% 93%
3	P	71	% 93%
4	I	2	100%
4	J	2	50%50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9477 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 HUMAN ALPHA-THROMBIN, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	C	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	E	29	Total	C	N	O	S	0	0	0
			234	146	38	49	1			
1	G	28	Total	C	N	O	S	0	0	0
			230	144	37	48	1			

- Molecule 2 is a protein called HUMAN ALPHA-THROMBIN, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	1	0
			2045	1302	364	365	14			
2	D	250	Total	C	N	O	S	0	1	0
			2031	1295	362	360	14			
2	F	252	Total	C	N	O	S	0	0	0
			2047	1309	361	363	14			
2	H	254	Total	C	N	O	S	0	0	0
			2056	1314	363	365	14			

- Molecule 3 is a protein called HUMAN FACTOR V, A2-B DOMAIN LINKER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	0	0	0
			51	35	6	10			
3	N	5	Total	C	N	O	0	0	0
			42	30	5	7			
3	O	5	Total	C	N	O	0	0	0
			42	30	5	7			
3	P	5	Total	C	N	O	0	0	0
			44	30	5	9			

There are 72 discrepancies between the modelled and reference sequences:

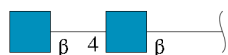
Chain	Residue	Modelled	Actual	Comment	Reference
M	639	ALA	-	expression tag	UNP P12259
M	640	HIS	-	expression tag	UNP P12259
M	641	HIS	-	expression tag	UNP P12259
M	642	HIS	-	expression tag	UNP P12259
M	643	HIS	-	expression tag	UNP P12259
M	644	HIS	-	expression tag	UNP P12259
M	645	HIS	-	expression tag	UNP P12259
M	646	VAL	-	expression tag	UNP P12259
M	647	GLY	-	expression tag	UNP P12259
M	648	THR	-	expression tag	UNP P12259
M	649	TRP	-	expression tag	UNP P12259
M	650	GLU	-	expression tag	UNP P12259
M	651	ASN	-	expression tag	UNP P12259
M	652	LEU	-	expression tag	UNP P12259
M	653	TYR	-	expression tag	UNP P12259
M	654	PHE	-	expression tag	UNP P12259
M	655	GLN	-	expression tag	UNP P12259
M	656	SER	-	expression tag	UNP P12259
N	639	ALA	-	expression tag	UNP P12259
N	640	HIS	-	expression tag	UNP P12259
N	641	HIS	-	expression tag	UNP P12259
N	642	HIS	-	expression tag	UNP P12259
N	643	HIS	-	expression tag	UNP P12259
N	644	HIS	-	expression tag	UNP P12259
N	645	HIS	-	expression tag	UNP P12259
N	646	VAL	-	expression tag	UNP P12259
N	647	GLY	-	expression tag	UNP P12259
N	648	THR	-	expression tag	UNP P12259
N	649	TRP	-	expression tag	UNP P12259
N	650	GLU	-	expression tag	UNP P12259
N	651	ASN	-	expression tag	UNP P12259
N	652	LEU	-	expression tag	UNP P12259
N	653	TYR	-	expression tag	UNP P12259
N	654	PHE	-	expression tag	UNP P12259
N	655	GLN	-	expression tag	UNP P12259
N	656	SER	-	expression tag	UNP P12259
O	639	ALA	-	expression tag	UNP P12259
O	640	HIS	-	expression tag	UNP P12259
O	641	HIS	-	expression tag	UNP P12259
O	642	HIS	-	expression tag	UNP P12259
O	643	HIS	-	expression tag	UNP P12259
O	644	HIS	-	expression tag	UNP P12259

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Chain	Residue	Modelled	Actual	Comment	Reference
O	645	HIS	-	expression tag	UNP P12259
O	646	VAL	-	expression tag	UNP P12259
O	647	GLY	-	expression tag	UNP P12259
O	648	THR	-	expression tag	UNP P12259
O	649	TRP	-	expression tag	UNP P12259
O	650	GLU	-	expression tag	UNP P12259
O	651	ASN	-	expression tag	UNP P12259
O	652	LEU	-	expression tag	UNP P12259
O	653	TYR	-	expression tag	UNP P12259
O	654	PHE	-	expression tag	UNP P12259
O	655	GLN	-	expression tag	UNP P12259
O	656	SER	-	expression tag	UNP P12259
P	639	ALA	-	expression tag	UNP P12259
P	640	HIS	-	expression tag	UNP P12259
P	641	HIS	-	expression tag	UNP P12259
P	642	HIS	-	expression tag	UNP P12259
P	643	HIS	-	expression tag	UNP P12259
P	644	HIS	-	expression tag	UNP P12259
P	645	HIS	-	expression tag	UNP P12259
P	646	VAL	-	expression tag	UNP P12259
P	647	GLY	-	expression tag	UNP P12259
P	648	THR	-	expression tag	UNP P12259
P	649	TRP	-	expression tag	UNP P12259
P	650	GLU	-	expression tag	UNP P12259
P	651	ASN	-	expression tag	UNP P12259
P	652	LEU	-	expression tag	UNP P12259
P	653	TYR	-	expression tag	UNP P12259
P	654	PHE	-	expression tag	UNP P12259
P	655	GLN	-	expression tag	UNP P12259
P	656	SER	-	expression tag	UNP P12259

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



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

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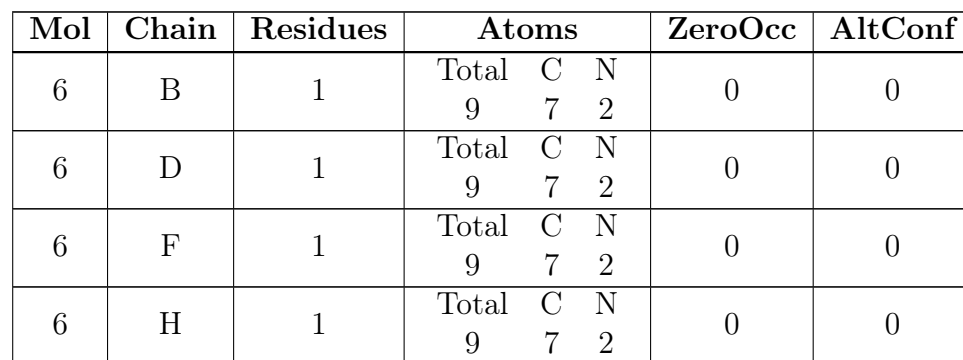
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



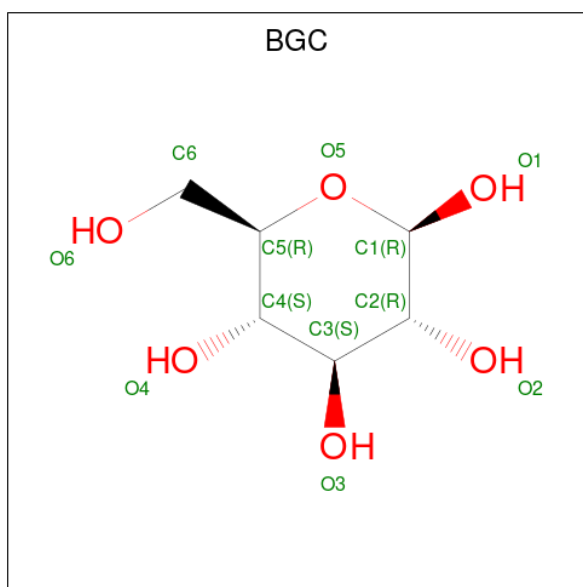
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7 | B | 2 | Total Na
2 2 | 0 | 0 |
| 7 | C | 1 | Total Na
1 1 | 0 | 0 |
| 7 | D | 1 | Total Na
1 1 | 0 | 0 |
| 7 | F | 1 | Total Na
1 1 | 0 | 0 |
| 7 | G | 1 | Total Na
1 1 | 0 | 0 |
| 7 | H | 1 | Total Na
1 1 | 0 | 0 |

- 



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			12	6	6		
8	F	1	Total	C	O	0	0
			12	6	6		
8	H	1	Total	C	O	0	0
			12	6	6		

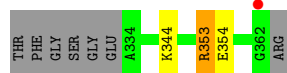
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O	0	0
			1	1		
9	B	11	Total	O	0	0
			11	11		
9	C	2	Total	O	0	0
			2	2		
9	F	6	Total	O	0	0
			6	6		
9	H	3	Total	O	0	0
			3	3		
9	N	1	Total	O	0	0
			1	1		

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: HUMAN ALPHA-THROMBIN, LIGHT CHAIN



- Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN



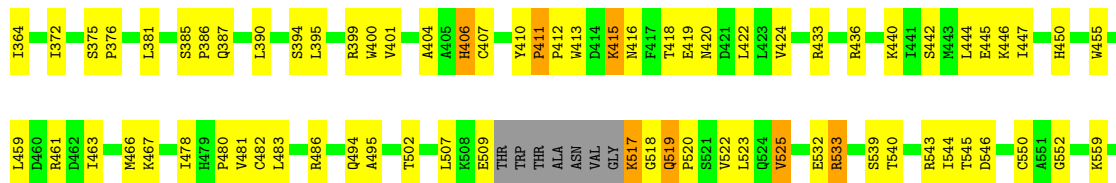
- Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN



- Molecule 1: HUMAN ALPHA-THROMBIN, LIGHT CHAIN

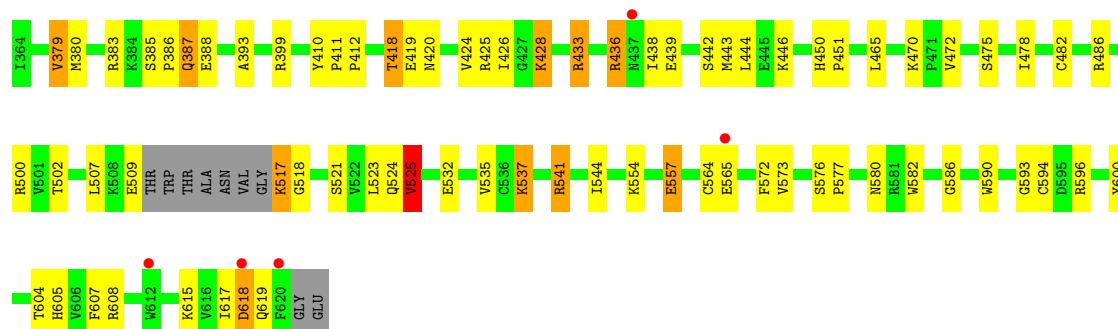


- Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

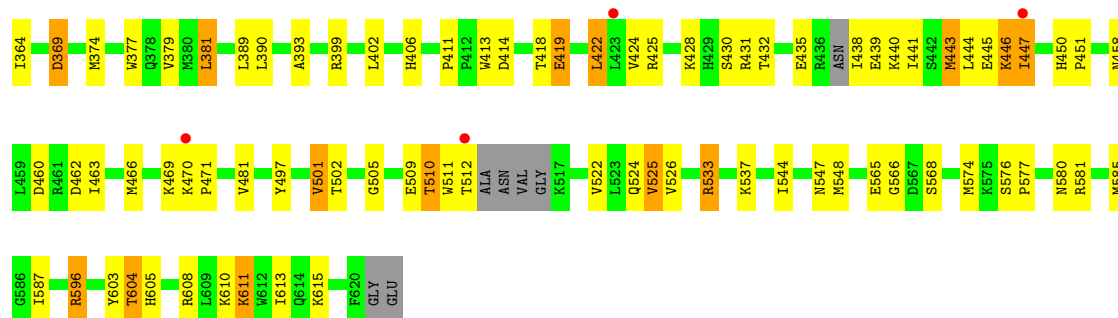




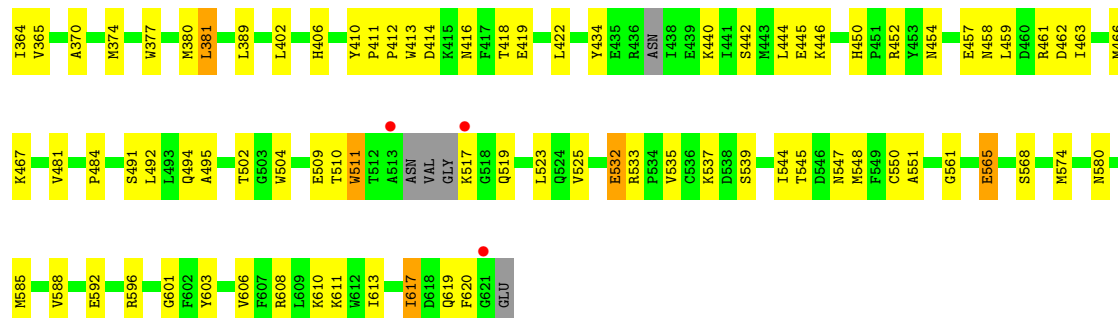
• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN



• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

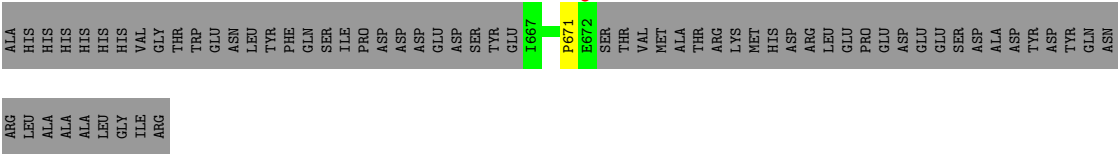


• Molecule 2: HUMAN ALPHA-THROMBIN, HEAVY CHAIN

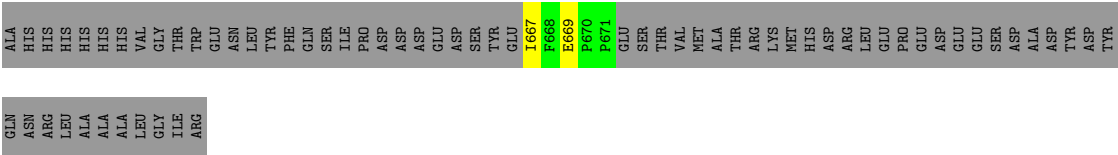


• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER

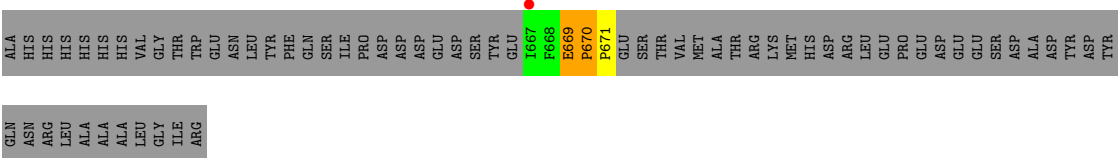




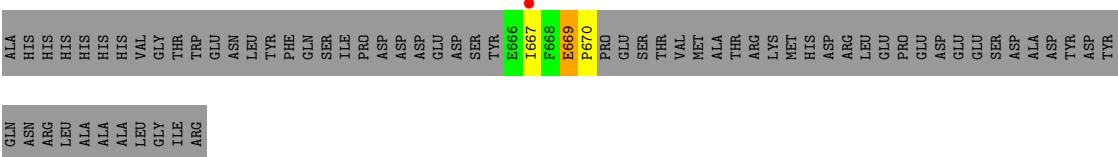
• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER



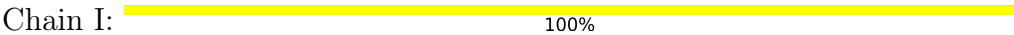
• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER



• Molecule 3: HUMAN FACTOR V, A2-B DOMAIN LINKER



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.24Å 68.23Å 98.97Å 72.57° 84.05° 80.45°	Depositor
Resolution (Å)	61.28 – 2.55 61.28 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.6 (61.28-2.55) 94.6 (61.28-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.55Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.279 (Not available) , 0.272	Depositor DCC
R_{free} test set	2384 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9477	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0360e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BEN, BGC, NAG, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	0/236	1.25	1/314 (0.3%)
1	C	0.97	0/236	1.17	2/314 (0.6%)
1	E	0.85	0/236	1.26	1/314 (0.3%)
1	G	1.02	0/232	1.14	1/309 (0.3%)
2	B	1.01	1/2104 (0.0%)	1.17	7/2838 (0.2%)
2	D	0.95	1/2090 (0.0%)	1.13	7/2821 (0.2%)
2	F	0.92	1/2100 (0.0%)	1.09	1/2836 (0.0%)
2	H	0.93	2/2109 (0.1%)	1.06	4/2848 (0.1%)
3	M	1.22	0/53	1.52	0/72
3	N	1.21	0/44	1.17	0/60
3	O	0.92	0/44	2.11	3/60 (5.0%)
3	P	1.22	0/45	1.54	0/60
All	All	0.96	5/9529 (0.1%)	1.14	27/12846 (0.2%)

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	D	0	1
2	F	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	551	ALA	CA-CB	-5.83	1.43	1.53
2	D	379	VAL	CA-CB	-5.72	1.46	1.55
2	B	617	ILE	CA-C	5.60	1.59	1.52
2	F	526	VAL	CA-CB	5.60	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	495	ALA	CA-CB	-5.17	1.44	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	669	GLU	CA-C-N	9.79	130.46	120.38
3	O	669	GLU	C-N-CA	9.79	130.46	120.38
2	D	617	ILE	N-CA-C	7.88	118.65	110.62
2	B	552	GLY	N-CA-C	-7.76	101.73	110.96
2	D	525	VAL	CB-CA-C	-6.95	99.80	110.50
2	B	411	PRO	N-CA-C	6.78	118.97	110.70
2	B	483	LEU	CA-C-N	-6.53	113.55	120.66
2	B	483	LEU	C-N-CA	-6.53	113.55	120.66
2	D	615	LYS	N-CA-C	-6.30	104.41	111.28
2	D	619	GLN	N-CA-C	-6.22	105.34	113.12
1	A	354	GLU	N-CA-C	-6.22	104.04	111.69
2	H	617	ILE	N-CA-C	5.98	116.76	110.72
2	H	606	VAL	N-CA-C	5.92	117.37	110.62
2	F	411	PRO	N-CA-C	5.83	117.81	110.70
2	H	588	VAL	CB-CA-C	-5.74	102.74	111.69
2	B	552	GLY	CA-C-O	-5.42	116.64	122.05
1	C	337	GLY	CA-C-N	-5.40	115.35	122.85
1	C	337	GLY	C-N-CA	-5.40	115.35	122.85
2	H	411	PRO	N-CA-C	5.38	117.27	110.70
1	E	354	GLU	N-CA-C	-5.22	105.76	111.82
2	B	606	VAL	N-CA-C	5.19	115.97	110.72
2	D	590	TRP	N-CA-C	5.18	116.72	108.79
3	O	670	PRO	N-CA-C	5.16	117.00	110.70
2	D	411	PRO	N-CA-C	5.13	116.96	110.70
1	G	354	GLU	N-CA-C	-5.11	105.79	111.36
2	D	475	SER	N-CA-C	-5.11	100.68	107.88
2	B	406	HIS	N-CA-C	-5.10	107.03	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	618	ASP	Peptide
2	F	431	ARG	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	234	0	229	1	0
1	C	234	0	229	7	0
1	E	234	0	229	5	0
1	G	230	0	226	4	0
2	B	2045	0	2016	52	0
2	D	2031	0	2006	42	0
2	F	2047	0	2023	54	0
2	H	2056	0	2031	47	0
3	M	51	0	45	0	0
3	N	42	0	39	1	0
3	O	42	0	39	3	0
3	P	44	0	38	9	0
4	I	28	0	25	0	0
4	J	28	0	25	2	0
5	B	14	0	13	2	0
5	D	14	0	13	0	0
6	B	9	0	7	0	0
6	D	9	0	7	0	0
6	F	9	0	7	0	0
6	H	9	0	7	1	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	B	12	0	12	1	0
8	F	12	0	12	0	0
8	H	12	0	12	1	0
9	A	1	0	0	0	0
9	B	11	0	0	0	0
9	C	2	0	0	0	0
9	F	6	0	0	0	0
9	H	3	0	0	0	0
9	N	1	0	0	2	0
All	All	9477	0	9290	218	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 12.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:502:THR:HG22	2:H:525:VAL:HG22	1.31	1.07
2:H:565:GLU:OE1	6:H:2001:BEN:H3	1.73	0.88
2:F:502:THR:HG22	2:F:525:VAL:HG13	1.55	0.87
2:D:541:ARG:HG3	2:D:541:ARG:HH21	1.41	0.83
2:F:502:THR:HG22	2:F:525:VAL:CG1	2.08	0.83
3:P:669:GLU:HG3	3:P:670:PRO:HD2	1.61	0.83
2:H:502:THR:CG2	2:H:525:VAL:HG22	2.14	0.77
4:J:1:NAG:H62	4:J:2:NAG:HN2	1.49	0.76
2:F:502:THR:CG2	2:F:525:VAL:CG1	2.65	0.74
2:F:502:THR:CG2	2:F:525:VAL:HG12	2.19	0.72
1:C:345:LYS:HE3	1:C:347:LEU:HD12	1.72	0.71
2:H:444:LEU:HD22	2:H:466:MET:HB3	1.74	0.69
2:F:533:ARG:NH2	2:F:548:MET:O	2.26	0.68
2:D:410:TYR:CE2	2:D:412:PRO:HG2	2.30	0.67
2:F:502:THR:HG23	2:F:525:VAL:HG12	1.76	0.67
2:H:610:LYS:HA	2:H:613:ILE:HD12	1.75	0.67
2:D:502:THR:HG22	2:D:525:VAL:HG13	1.77	0.66
2:B:364:ILE:N	2:B:567:ASP:OD2	2.29	0.66
1:E:352:GLU:HA	1:E:355:LEU:HD12	1.78	0.65
2:F:610:LYS:HA	2:F:613:ILE:HD12	1.78	0.65
1:C:340:PRO:HA	1:C:344:LYS:HG3	1.80	0.64
1:E:336:CYS:O	2:F:581:ARG:NH1	2.30	0.63
2:F:450:HIS:ND1	2:F:451:PRO:HD2	2.13	0.63
2:F:425:ARG:HG2	2:F:441:ILE:HG12	1.81	0.62
3:P:669:GLU:HB2	3:P:670:PRO:HD3	1.81	0.61
2:F:381:LEU:HD13	2:F:390:LEU:HD12	1.81	0.61
2:F:509:GLU:O	2:F:512:THR:HG22	2.01	0.61
2:D:410:TYR:C	2:D:412:PRO:HD2	2.25	0.61
2:D:428:LYS:HD2	2:D:439:GLU:OE2	2.00	0.61
2:D:537:LYS:HA	2:D:544:ILE:HD12	1.83	0.61
2:D:502:THR:HA	2:D:524:GLN:O	2.03	0.59
2:H:450:HIS:CE1	2:H:452:ARG:HB2	2.37	0.59
2:B:413:TRP:CH2	3:O:670:PRO:HD2	2.39	0.58
1:C:353:ARG:HG3	1:C:353:ARG:O	1.98	0.58
2:H:548:MET:HA	2:H:603:TYR:O	2.03	0.58
2:D:517:LYS:N	2:D:517:LYS:HE2	2.18	0.58
1:E:349:ASP:OD2	1:E:349:ASP:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:537:LYS:HA	2:H:544:ILE:HD12	1.83	0.58
3:P:669:GLU:CG	3:P:670:PRO:HD2	2.31	0.58
2:H:402:LEU:HD11	2:H:463:ILE:HD11	1.86	0.57
2:D:433:ARG:HG2	9:N:3509:HOH:O	2.03	0.57
2:D:554:LYS:H	2:D:557:GLU:HG3	1.70	0.57
2:F:364:ILE:HD12	2:F:501:VAL:HG12	1.87	0.57
2:B:461:ARG:HG2	2:B:609:LEU:HD21	1.87	0.57
2:H:454:ASN:HD21	2:H:457:GLU:HB3	1.70	0.57
1:C:338:LEU:HB3	1:C:344:LYS:HE3	1.87	0.57
3:P:669:GLU:CB	3:P:670:PRO:CD	2.82	0.56
3:P:669:GLU:CG	3:P:670:PRO:CD	2.84	0.56
2:F:444:LEU:HD22	2:F:466:MET:HB3	1.88	0.56
2:B:433[A]:ARG:HE	2:H:413:TRP:HA	1.68	0.56
2:B:519:GLN:N	2:B:519:GLN:OE1	2.39	0.56
2:H:419:GLU:HG2	2:H:446:LYS:HA	1.88	0.56
1:C:338:LEU:CB	1:C:344:LYS:HE3	2.36	0.55
2:F:447:ILE:HG12	2:F:466:MET:HG2	1.88	0.55
2:H:434:TYR:HB2	3:P:670:PRO:HD2	1.88	0.55
2:H:532:GLU:OE2	2:H:532:GLU:N	2.25	0.55
2:F:402:LEU:HD11	2:F:463:ILE:HD11	1.89	0.55
2:F:435:GLU:O	2:F:439:GLU:HB3	2.07	0.55
2:H:380:MET:HE2	2:H:389:LEU:HD12	1.88	0.55
2:D:424:VAL:HG13	2:D:444:LEU:HD21	1.89	0.55
2:B:546:ASP:HB2	2:B:608:ARG:HH12	1.72	0.54
5:B:1416:NAG:C1	5:B:1416:NAG:H82	2.35	0.54
2:H:410:TYR:C	2:H:412:PRO:HD2	2.33	0.54
2:H:459:LEU:O	2:H:462:ASP:HB2	2.08	0.54
2:F:379:VAL:HB	2:F:393:ALA:HB3	1.90	0.54
2:D:593:GLY:HA3	2:D:596:ARG:NH1	2.23	0.53
5:B:1416:NAG:C1	5:B:1416:NAG:C8	2.86	0.53
2:F:422:LEU:HD12	2:F:444:LEU:CD1	2.38	0.53
3:P:669:GLU:HB2	3:P:670:PRO:CD	2.37	0.53
2:D:502:THR:CG2	2:D:525:VAL:HG13	2.37	0.53
2:F:574:MET:SD	2:F:585:MET:HG3	2.48	0.53
2:B:387:GLN:HG2	2:H:511:TRP:CD1	2.44	0.53
2:D:500:ARG:O	2:D:572:PHE:HA	2.09	0.53
2:F:419:GLU:CG	2:F:446:LYS:HA	2.39	0.53
2:H:413:TRP:O	2:H:414:ASP:C	2.52	0.53
2:F:502:THR:HA	2:F:524:GLN:O	2.09	0.52
2:F:377:TRP:CG	2:F:481:VAL:HB	2.44	0.52
2:F:406:HIS:CE1	2:F:568:SER:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:ARG:NH2	2:B:545:THR:O	2.42	0.52
2:F:425:ARG:HG2	2:F:441:ILE:CG1	2.40	0.52
2:B:385:SER:HA	2:B:386:PRO:C	2.35	0.52
2:H:365:VAL:O	2:H:561:GLY:HA2	2.09	0.52
2:F:605:HIS:CG	2:F:608:ARG:HG3	2.45	0.51
2:B:522:VAL:O	2:B:523:LEU:C	2.54	0.51
2:D:541:ARG:HG3	2:D:541:ARG:NH2	2.18	0.51
2:H:434:TYR:H	3:P:669:GLU:CG	2.23	0.51
2:D:517:LYS:HE3	2:D:518:GLY:H	1.75	0.51
2:B:509:GLU:O	8:B:4202:BGC:H5	2.11	0.51
2:F:374:MET:O	2:F:374:MET:HG2	2.11	0.51
2:H:461:ARG:HE	2:H:547:ASN:ND2	2.09	0.51
2:D:482:CYS:HB2	2:D:582:TRP:O	2.12	0.50
2:F:399:ARG:HG3	2:F:471:PRO:HA	1.93	0.50
2:H:509:GLU:OE1	2:H:596:ARG:HD2	2.11	0.50
2:B:404:ALA:O	2:B:407:CYS:HB2	2.11	0.50
2:B:507:LEU:HD21	2:B:520:PRO:HB3	1.92	0.50
2:F:605:HIS:ND1	2:F:608:ARG:HG3	2.27	0.50
2:B:406:HIS:NE2	2:B:568:SER:HB3	2.27	0.50
2:B:390:LEU:CD1	2:B:422:LEU:HD22	2.42	0.49
2:F:369:ASP:OD2	2:F:522:VAL:HG21	2.12	0.49
2:H:617:ILE:O	2:H:620:PHE:O	2.31	0.49
2:H:532:GLU:H	2:H:532:GLU:CD	2.16	0.49
2:B:399:ARG:HB3	2:B:400:TRP:CD1	2.48	0.49
2:B:445:GLU:OE2	2:B:467:LYS:HE2	2.12	0.49
2:D:426:ILE:HG22	2:D:478:ILE:HG12	1.95	0.49
2:B:502:THR:HG22	2:B:525:VAL:HG13	1.95	0.48
2:D:436:ARG:O	2:D:438:ILE:HG12	2.13	0.48
3:O:669:GLU:HA	3:O:670:PRO:HD2	1.56	0.48
2:D:433:ARG:HD2	2:F:413:TRP:HA	1.96	0.48
2:F:419:GLU:HG2	2:F:446:LYS:HA	1.95	0.48
2:B:400:TRP:HH2	2:B:620:PHE:HB2	1.78	0.48
2:F:462:ASP:H	2:F:604:THR:HG21	1.79	0.48
2:H:484:PRO:HB3	2:H:585:MET:HE1	1.96	0.48
2:B:406:HIS:C	2:B:406:HIS:CD2	2.90	0.48
2:H:445:GLU:OE1	2:H:467:LYS:HE2	2.13	0.48
2:D:509:GLU:HB2	2:D:594:CYS:HB2	1.96	0.47
1:E:338:LEU:HD13	1:E:344:LYS:HE3	1.96	0.47
3:O:670:PRO:HA	3:O:671:PRO:HD2	1.75	0.47
2:B:539:SER:O	2:B:599:LYS:HE2	2.14	0.47
2:H:619:GLN:HG2	2:H:620:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PRO:HA	1:C:344:LYS:CG	2.44	0.47
2:H:377:TRP:CG	2:H:481:VAL:HB	2.50	0.47
2:B:410:TYR:H	2:B:415:LYS:HB3	1.80	0.47
2:D:379:VAL:HB	2:D:393:ALA:HB3	1.97	0.47
2:H:406:HIS:CE1	2:H:568:SER:HB3	2.50	0.47
2:B:400:TRP:HZ2	2:B:621:GLY:N	2.13	0.46
2:B:399:ARG:HD2	2:B:399:ARG:HA	1.49	0.46
2:B:406:HIS:CE1	2:B:568:SER:HB3	2.50	0.46
2:D:425:ARG:HB3	2:D:428:LYS:HD3	1.97	0.46
1:G:352:GLU:O	1:G:355:LEU:HB2	2.15	0.46
2:H:545:THR:OG1	2:H:548:MET:HE3	2.14	0.46
2:B:394:SER:O	2:B:401:VAL:HA	2.16	0.46
1:C:353:ARG:HE	1:C:353:ARG:HB2	1.57	0.45
2:D:554:LYS:HG2	2:D:600:TYR:OH	2.17	0.45
2:H:535:VAL:O	2:H:539:SER:HB3	2.16	0.45
2:D:532:GLU:HG2	2:D:535:VAL:HG23	1.98	0.45
2:H:510:THR:O	2:H:511:TRP:HB2	2.17	0.45
2:F:610:LYS:O	2:F:611:LYS:C	2.59	0.45
2:F:446:LYS:HD3	2:F:447:ILE:H	1.82	0.45
2:B:540:THR:HG21	2:B:544:ILE:HD11	1.98	0.45
2:D:379:VAL:HG12	2:D:380:MET:N	2.30	0.45
2:F:443:MET:HB2	2:F:469:LYS:HG3	1.99	0.44
2:B:532:GLU:H	2:B:532:GLU:CD	2.26	0.44
2:H:550:CYS:HA	2:H:601:GLY:O	2.18	0.44
4:J:1:NAG:H62	4:J:2:NAG:N2	2.27	0.44
2:D:554:LYS:N	2:D:557:GLU:HG3	2.32	0.44
2:F:509:GLU:OE2	2:F:596:ARG:HD2	2.17	0.44
2:H:491:SER:O	2:H:494:GLN:NE2	2.44	0.44
2:D:387:GLN:HG2	2:F:511:TRP:CD1	2.53	0.44
2:B:481:VAL:HG22	2:B:482:CYS:N	2.33	0.44
2:F:510:THR:O	2:F:511:TRP:HB2	2.18	0.44
2:F:537:LYS:HA	2:F:544:ILE:CD1	2.47	0.44
2:B:410:TYR:CD2	2:B:412:PRO:HD2	2.53	0.43
2:D:433:ARG:CG	9:N:3509:HOH:O	2.65	0.43
2:B:411:PRO:N	2:B:412:PRO:HD3	2.34	0.43
2:B:533:ARG:HH11	2:B:533:ARG:CG	2.30	0.43
2:F:389:LEU:C	2:F:389:LEU:HD23	2.42	0.43
2:B:381:LEU:HD11	2:B:422:LEU:HD13	1.99	0.43
2:D:450:HIS:HA	2:D:451:PRO:HD3	1.80	0.43
2:H:434:TYR:CB	3:P:670:PRO:HD2	2.47	0.43
2:B:494:GLN:O	2:B:495:ALA:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:381:LEU:HD21	2:H:422:LEU:HD13	2.00	0.43
2:H:444:LEU:CD2	2:H:466:MET:HB3	2.47	0.43
2:B:411:PRO:N	2:B:412:PRO:CD	2.81	0.43
2:B:543:ARG:HB3	2:B:543:ARG:HH11	1.84	0.43
2:D:586:GLY:HA2	2:D:604:THR:O	2.19	0.43
2:F:505:GLY:HA2	2:F:566:GLY:HA3	2.01	0.43
2:B:401:VAL:CG1	2:B:466:MET:HE3	2.49	0.43
2:D:576:SER:HA	2:D:577:PRO:HD3	1.89	0.43
2:H:380:MET:HE2	2:H:389:LEU:CD1	2.49	0.43
2:B:424:VAL:HG13	2:B:444:LEU:HD21	2.00	0.42
2:D:436:ARG:H	2:D:436:ARG:HG3	1.40	0.42
2:D:500:ARG:HB3	2:D:573:VAL:CG2	2.50	0.42
2:H:410:TYR:C	2:H:412:PRO:CD	2.92	0.42
2:H:533:ARG:HH11	8:H:4201:BGC:H4	1.83	0.42
2:F:576:SER:HA	2:F:577:PRO:HD3	1.89	0.42
2:F:587:ILE:O	2:F:603:TYR:HA	2.20	0.42
2:H:504:TRP:CE2	2:H:523:LEU:HD13	2.55	0.42
2:F:406:HIS:NE2	2:F:568:SER:HB3	2.34	0.42
2:B:440:LYS:HZ2	2:B:478:ILE:HD12	1.85	0.42
2:H:492:LEU:O	2:H:574:MET:HE1	2.20	0.42
1:E:359:TYR:HD2	2:F:497:TYR:CD2	2.38	0.42
2:D:433:ARG:HG3	3:N:669:GLU:OE2	2.20	0.42
2:B:401:VAL:HG12	2:B:466:MET:HE3	2.02	0.41
2:F:462:ASP:N	2:F:604:THR:HG21	2.35	0.41
2:F:501:VAL:O	2:F:525:VAL:HA	2.20	0.41
1:G:353:ARG:HA	1:G:353:ARG:HD3	1.92	0.41
1:A:353:ARG:HE	1:A:353:ARG:HB2	1.62	0.41
2:B:587:ILE:HB	2:B:604:THR:HB	2.02	0.41
2:F:445:GLU:HB2	2:F:469:LYS:HA	2.01	0.41
1:G:341:LEU:C	1:G:345:LYS:HD3	2.46	0.41
2:B:372:ILE:HD13	2:B:372:ILE:HA	1.86	0.41
2:D:418:THR:OG1	2:D:419:GLU:N	2.53	0.41
2:F:422:LEU:CD1	2:F:444:LEU:CD1	2.98	0.41
1:G:350:LYS:HE3	1:G:350:LYS:HB3	1.55	0.41
2:B:375:SER:N	2:B:376:PRO:HD3	2.35	0.41
2:B:517:LYS:HA	2:B:518:GLY:HA3	1.90	0.41
2:B:533:ARG:NH2	2:B:546:ASP:HA	2.36	0.41
2:F:381:LEU:HD23	2:F:424:VAL:HG12	2.01	0.41
2:B:450:HIS:HB2	2:B:463:ILE:CG2	2.50	0.41
2:D:385:SER:HA	2:D:386:PRO:C	2.45	0.41
2:F:460:ASP:OD1	2:F:547:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LEU:O	2:B:480:PRO:HA	2.20	0.41
2:B:486:ARG:HA	2:B:607:PHE:CZ	2.56	0.41
2:B:546:ASP:HB2	2:B:608:ARG:NH1	2.35	0.41
2:D:564:CYS:SG	2:D:565:GLU:N	2.91	0.41
2:F:381:LEU:HD13	2:F:390:LEU:CD1	2.48	0.41
2:H:510:THR:O	2:H:511:TRP:CB	2.69	0.41
2:H:370:ALA:HB2	2:H:525:VAL:HG23	2.02	0.41
2:H:458:ASN:OD1	2:H:458:ASN:N	2.51	0.41
2:H:523:LEU:HD12	2:H:523:LEU:HA	1.91	0.41
2:D:541:ARG:HH21	2:D:541:ARG:CG	2.22	0.40
2:D:486:ARG:HA	2:D:607:PHE:CZ	2.56	0.40
2:B:450:HIS:HB2	2:B:463:ILE:HG22	2.03	0.40
2:B:618:ASP:OD2	2:B:618:ASP:C	2.65	0.40
2:B:455:TRP:HA	2:B:459:LEU:HD23	2.03	0.40
2:D:383:ARG:HH11	2:D:383:ARG:HD2	1.72	0.40
2:F:428:LYS:HE3	2:F:430:SER:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	C	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	E	27/36 (75%)	25 (93%)	2 (7%)	0	100	100
1	G	26/36 (72%)	22 (85%)	4 (15%)	0	100	100
2	B	249/259 (96%)	236 (95%)	11 (4%)	2 (1%)	16	22
2	D	247/259 (95%)	231 (94%)	15 (6%)	1 (0%)	30	39
2	F	246/259 (95%)	233 (95%)	10 (4%)	3 (1%)	10	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	248/259 (96%)	229 (92%)	16 (6%)	3 (1%)	10	13
3	M	4/71 (6%)	3 (75%)	0	1 (25%)	0	0
3	N	3/71 (4%)	3 (100%)	0	0	100	100
3	O	3/71 (4%)	2 (67%)	1 (33%)	0	100	100
3	P	3/71 (4%)	2 (67%)	0	1 (33%)	0	0
All	All	1110/1464 (76%)	1036 (93%)	63 (6%)	11 (1%)	12	17

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	669	GLU
2	F	458	ASN
2	H	511	TRP
2	H	608	ARG
3	M	671	PRO
2	B	559	LYS
2	D	523	LEU
2	H	416	ASN
2	B	416	ASN
2	F	419	GLU
2	F	580	ASN

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	26/31 (84%)	24 (92%)	2 (8%)	12	17
1	C	26/31 (84%)	23 (88%)	3 (12%)	5	6
1	E	26/31 (84%)	22 (85%)	4 (15%)	2	2
1	G	26/31 (84%)	25 (96%)	1 (4%)	29	44
2	B	221/225 (98%)	203 (92%)	18 (8%)	11	15
2	D	220/225 (98%)	195 (89%)	25 (11%)	5	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	221/225 (98%)	200 (90%)	21 (10%)	8	9
2	H	221/225 (98%)	208 (94%)	13 (6%)	18	27
3	M	6/63 (10%)	6 (100%)	0	100	100
3	N	5/63 (8%)	4 (80%)	1 (20%)	1	1
3	O	5/63 (8%)	5 (100%)	0	100	100
3	P	5/63 (8%)	4 (80%)	1 (20%)	1	1
All	All	1008/1276 (79%)	919 (91%)	89 (9%)	9	12

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	LYS
1	A	353	ARG
2	B	415	LYS
2	B	418	THR
2	B	419	GLU
2	B	420	ASN
2	B	436	ARG
2	B	442	SER
2	B	446	LYS
2	B	447	ILE
2	B	517	LYS
2	B	519	GLN
2	B	525	VAL
2	B	533	ARG
2	B	550	CYS
2	B	565	GLU
2	B	580	ASN
2	B	617	ILE
2	B	618	ASP
2	B	622	GLU
1	C	350	LYS
1	C	353	ARG
1	C	357	GLU
2	D	387	GLN
2	D	388	GLU
2	D	399	ARG
2	D	418	THR
2	D	420	ASN
2	D	428	LYS

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Mol	Chain	Res	Type
2	D	433	ARG
2	D	436	ARG
2	D	442	SER
2	D	443	MET
2	D	446	LYS
2	D	465	LEU
2	D	470	LYS
2	D	472	VAL
2	D	507	LEU
2	D	517	LYS
2	D	521	SER
2	D	525	VAL
2	D	537	LYS
2	D	541	ARG
2	D	557	GLU
2	D	580	ASN
2	D	608[A]	ARG
2	D	608[B]	ARG
2	D	618	ASP
1	E	341	LEU
1	E	345	LYS
1	E	349	ASP
1	E	360	ILE
2	F	369	ASP
2	F	381	LEU
2	F	414	ASP
2	F	418	THR
2	F	422	LEU
2	F	432	THR
2	F	438	ILE
2	F	440	LYS
2	F	443	MET
2	F	446	LYS
2	F	447	ILE
2	F	470	LYS
2	F	501	VAL
2	F	510	THR
2	F	525	VAL
2	F	533	ARG
2	F	565	GLU
2	F	596	ARG
2	F	604	THR

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Mol	Chain	Res	Type
2	F	611	LYS
2	F	615	LYS
1	G	346	SER
2	H	364	ILE
2	H	374	MET
2	H	381	LEU
2	H	418	THR
2	H	440	LYS
2	H	442	SER
2	H	517	LYS
2	H	519	GLN
2	H	532	GLU
2	H	565	GLU
2	H	580	ASN
2	H	592	GLU
2	H	611	LYS
3	N	667	ILE
3	P	667	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	429	HIS
2	D	524	GLN
2	D	614	GLN
2	H	454	ASN

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](#)

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	1	4,2	14,14,15	0.58	0	17,19,21	2.54	5 (29%)
4	NAG	I	2	4	14,14,15	1.19	1 (7%)	17,19,21	1.22	2 (11%)
4	NAG	J	1	4,2	14,14,15	0.64	0	17,19,21	2.87	6 (35%)
4	NAG	J	2	4	14,14,15	0.66	0	17,19,21	0.95	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
4	NAG	I	1	4,2	-	5/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	O5-C1	-3.98	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C2-N2-C7	6.75	131.95	122.90
4	J	1	NAG	C1-O5-C5	6.52	120.92	112.19
4	I	1	NAG	C2-N2-C7	5.98	130.91	122.90
4	I	1	NAG	C1-O5-C5	5.50	119.56	112.19
4	J	1	NAG	C8-C7-N2	3.86	122.52	116.12
4	I	1	NAG	C1-C2-N2	3.65	116.18	110.43
4	J	1	NAG	O7-C7-C8	-3.04	116.65	122.05
4	J	1	NAG	C3-C4-C5	2.96	115.60	110.23
4	I	1	NAG	O5-C1-C2	-2.94	106.75	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	O5-C1-C2	-2.93	106.76	111.29
4	I	2	NAG	C1-C2-N2	2.82	114.87	110.43
4	I	1	NAG	C8-C7-N2	2.65	120.51	116.12
4	J	1	NAG	O5-C5-C4	2.21	116.19	110.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

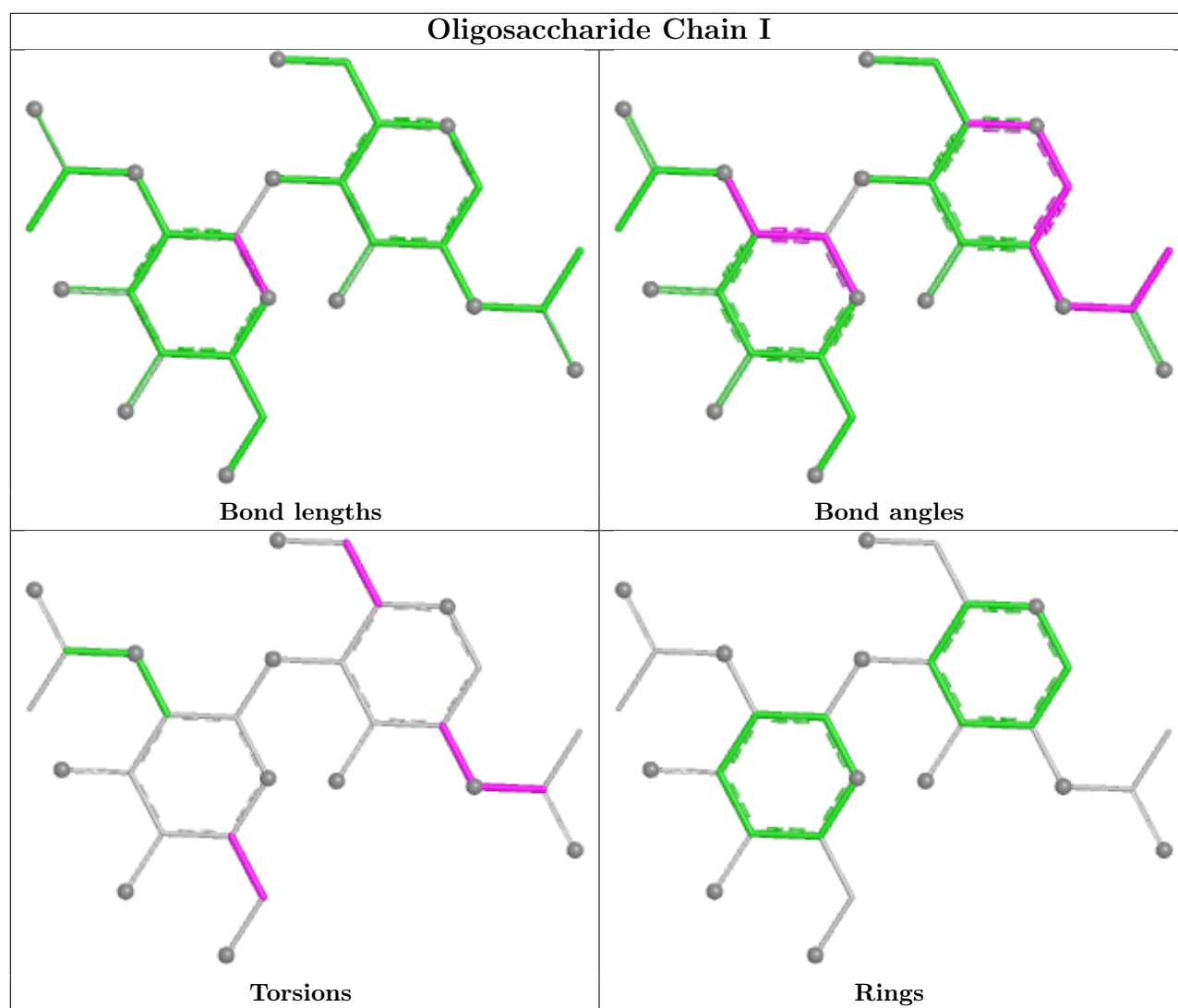
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C8-C7-N2-C2
4	I	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C3-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	J	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7

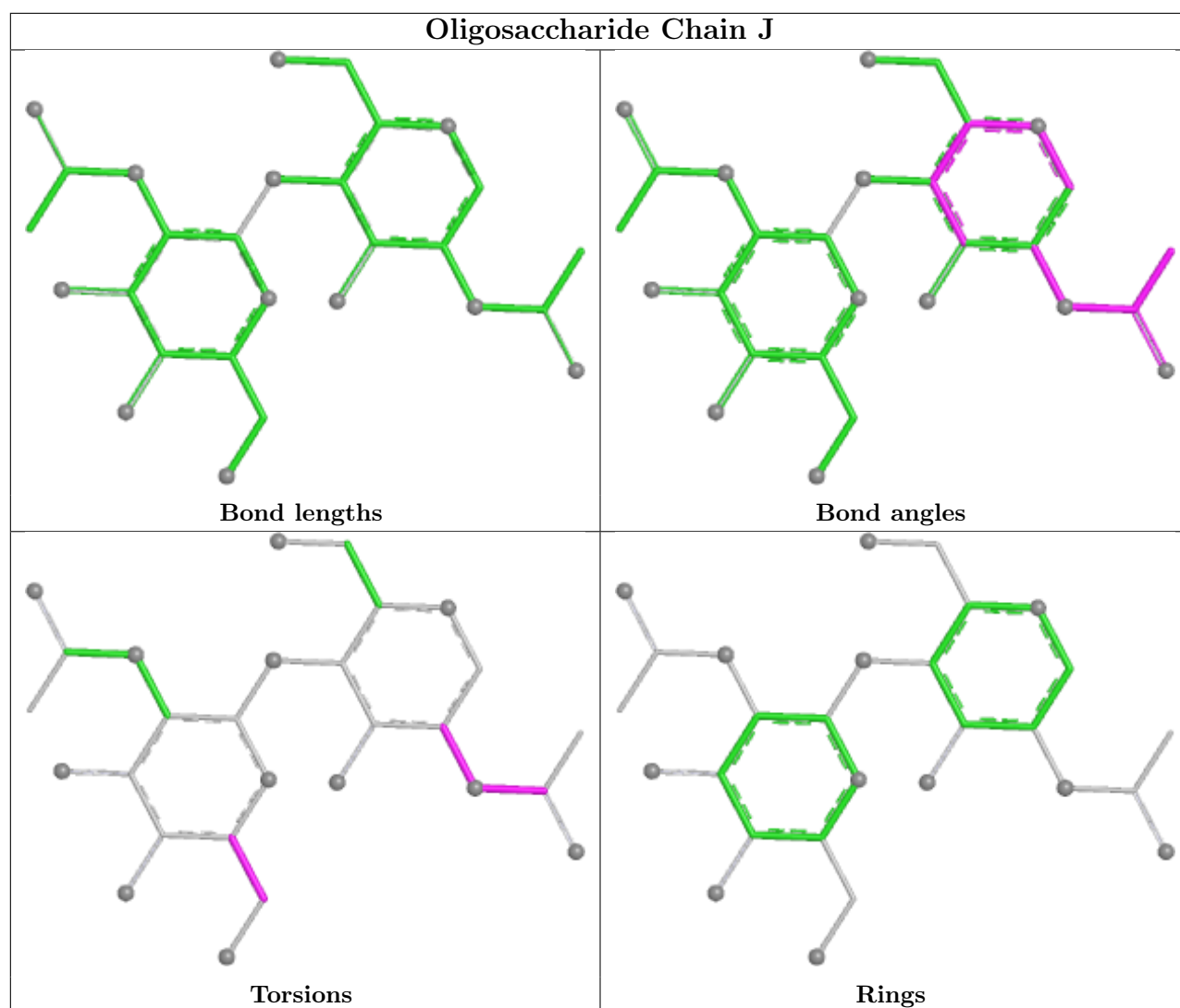
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	2	NAG	2	0
4	J	1	NAG	2	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](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	$\# Z > 2$
5	NAG	B	1416	2	14,14,15	0.71	0	17,19,21	1.79	4 (23%)
8	BGC	H	4201	-	12,12,12	0.83	0	17,17,17	2.95	7 (41%)
8	BGC	F	4203	-	12,12,12	0.94	0	17,17,17	2.89	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BEN	D	2001	-	9,9,9	1.78	1 (11%)	7,11,11	1.33	0
6	BEN	F	2001	-	9,9,9	1.35	1 (11%)	7,11,11	0.69	0
6	BEN	H	2001	-	9,9,9	1.30	1 (11%)	7,11,11	1.66	1 (14%)
8	BGC	B	4202	-	12,12,12	0.81	0	17,17,17	1.78	5 (29%)
6	BEN	B	2001	-	9,9,9	1.60	1 (11%)	7,11,11	0.95	0
5	NAG	D	1416	2	14,14,15	0.70	0	17,19,21	2.68	6 (35%)

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	1416	2	-	3/6/23/26	0/1/1/1
8	BGC	H	4201	-	-	1/2/22/22	0/1/1/1
8	BGC	F	4203	-	-	1/2/22/22	0/1/1/1
6	BEN	D	2001	-	-	4/4/4/4	0/1/1/1
6	BEN	F	2001	-	-	4/4/4/4	0/1/1/1
6	BEN	H	2001	-	-	4/4/4/4	0/1/1/1
8	BGC	B	4202	-	-	2/2/22/22	0/1/1/1
6	BEN	B	2001	-	-	4/4/4/4	0/1/1/1
5	NAG	D	1416	2	-	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2001	BEN	C1-C	-4.27	1.39	1.47
6	B	2001	BEN	C1-C	-4.08	1.39	1.47
6	H	2001	BEN	C1-C	-3.22	1.41	1.47
6	F	2001	BEN	C1-C	-2.58	1.42	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1416	NAG	C2-N2-C7	7.77	133.31	122.90
8	F	4203	BGC	C4-C3-C2	-7.33	97.97	110.83
8	H	4201	BGC	C4-C3-C2	-6.63	99.19	110.83
8	H	4201	BGC	C1-O5-C5	6.22	125.68	113.65
5	B	1416	NAG	C2-N2-C7	4.16	128.48	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	4203	BGC	O3-C3-C4	4.13	120.11	110.38
5	D	1416	NAG	C8-C7-N2	4.00	122.74	116.12
5	D	1416	NAG	O5-C1-C2	-3.80	105.41	111.29
6	H	2001	BEN	C1-C-N2	3.68	123.60	118.01
8	F	4203	BGC	C1-C2-C3	-3.64	102.94	110.36
8	H	4201	BGC	O4-C4-C5	3.58	118.15	109.32
8	H	4201	BGC	O3-C3-C2	3.57	118.80	110.38
5	B	1416	NAG	C8-C7-N2	3.51	121.95	116.12
8	F	4203	BGC	O5-C5-C4	3.51	116.02	109.70
8	H	4201	BGC	C3-C4-C5	-3.50	103.89	110.23
8	B	4202	BGC	C4-C3-C2	-3.38	104.91	110.83
8	H	4201	BGC	C1-C2-C3	-3.32	103.59	110.36
5	D	1416	NAG	C4-C3-C2	3.00	115.41	111.02
8	F	4203	BGC	O4-C4-C3	2.98	117.40	110.38
8	B	4202	BGC	C3-C4-C5	-2.93	104.92	110.23
8	B	4202	BGC	O5-C5-C6	2.85	113.50	106.44
5	D	1416	NAG	C3-C4-C5	2.85	115.39	110.23
5	D	1416	NAG	O7-C7-C8	-2.82	117.03	122.05
8	H	4201	BGC	O2-C2-C3	2.70	116.75	110.38
8	F	4203	BGC	O5-C1-C2	-2.68	105.59	110.30
8	F	4203	BGC	O2-C2-C1	2.55	115.13	109.25
8	F	4203	BGC	C1-O5-C5	2.52	118.52	113.65
8	B	4202	BGC	O4-C4-C5	2.45	115.36	109.32
8	F	4203	BGC	O2-C2-C3	2.41	116.05	110.38
5	B	1416	NAG	O5-C1-C2	2.27	114.80	111.29
5	B	1416	NAG	O7-C7-C8	-2.24	118.06	122.05
8	B	4202	BGC	O3-C3-C2	2.16	115.48	110.38

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1416	NAG	C1-C2-N2-C7
8	B	4202	BGC	O5-C5-C6-O6
8	B	4202	BGC	C4-C5-C6-O6
5	D	1416	NAG	C4-C5-C6-O6
5	B	1416	NAG	C8-C7-N2-C2
5	B	1416	NAG	O7-C7-N2-C2
5	D	1416	NAG	C8-C7-N2-C2
5	D	1416	NAG	O7-C7-N2-C2
5	D	1416	NAG	O5-C5-C6-O6
8	F	4203	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	1416	NAG	C3-C2-N2-C7
8	H	4201	BGC	C4-C5-C6-O6
6	B	2001	BEN	N2-C-C1-C2
6	B	2001	BEN	N2-C-C1-C6
6	D	2001	BEN	N2-C-C1-C2
6	D	2001	BEN	N2-C-C1-C6
6	F	2001	BEN	N2-C-C1-C2
6	F	2001	BEN	N2-C-C1-C6
6	H	2001	BEN	N2-C-C1-C2
6	H	2001	BEN	N2-C-C1-C6
6	B	2001	BEN	N1-C-C1-C2
6	B	2001	BEN	N1-C-C1-C6
6	D	2001	BEN	N1-C-C1-C2
6	D	2001	BEN	N1-C-C1-C6
6	F	2001	BEN	N1-C-C1-C2
6	F	2001	BEN	N1-C-C1-C6
6	H	2001	BEN	N1-C-C1-C2
6	H	2001	BEN	N1-C-C1-C6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1416	NAG	2	0
8	H	4201	BGC	1	0
6	H	2001	BEN	1	0
8	B	4202	BGC	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	29/36 (80%)	-0.18	1 (3%) 48 49	32, 43, 61, 65	0
1	C	29/36 (80%)	-0.13	0 100 100	34, 50, 68, 79	0
1	E	29/36 (80%)	0.12	1 (3%) 48 49	37, 57, 77, 88	0
1	G	28/36 (77%)	-0.04	1 (3%) 46 47	33, 50, 76, 85	0
2	B	252/259 (97%)	-0.15	1 (0%) 88 90	24, 44, 70, 91	1 (0%)
2	D	250/259 (96%)	0.15	5 (2%) 65 65	28, 56, 97, 132	1 (0%)
2	F	252/259 (97%)	0.12	4 (1%) 70 71	31, 54, 79, 90	0
2	H	254/259 (98%)	-0.12	3 (1%) 76 77	25, 49, 79, 90	0
3	M	6/71 (8%)	1.47	1 (16%) 4 3	35, 54, 54, 58	1 (16%)
3	N	5/71 (7%)	0.51	0 100 100	51, 52, 54, 57	0
3	O	5/71 (7%)	0.74	1 (20%) 3 2	60, 61, 63, 64	0
3	P	5/71 (7%)	1.08	1 (20%) 3 2	63, 64, 66, 69	0
All	All	1144/1464 (78%)	0.01	19 (1%) 69 69	24, 51, 82, 132	3 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	672	GLU	7.9
2	D	620	PHE	4.2
1	G	334	ALA	3.5
1	E	334	ALA	3.4
2	H	513	ALA	3.2
2	H	621	GLY	3.0
2	F	470	LYS	2.8
2	F	423	LEU	2.6
2	D	618	ASP	2.5
2	F	512	THR	2.4
2	B	622	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	667	ILE	2.4
2	D	437	ASN	2.4
2	H	517	LYS	2.3
2	D	612	TRP	2.3
2	D	565	GLU	2.2
3	O	667	ILE	2.1
1	A	362	GLY	2.1
2	F	447	ILE	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](#)

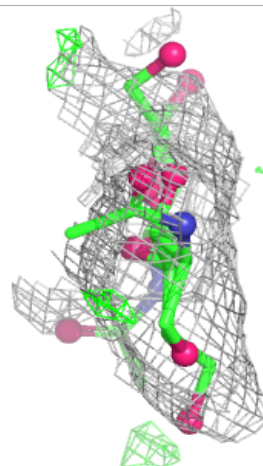
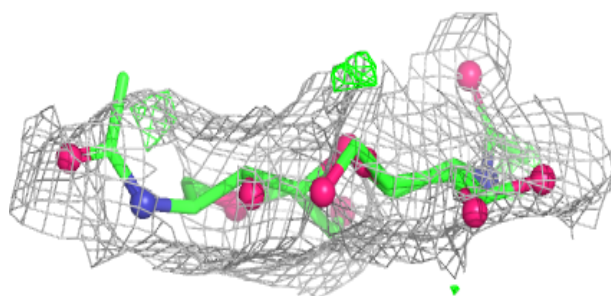
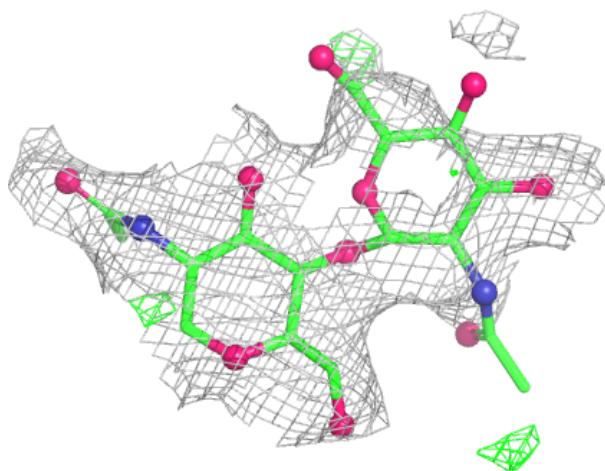
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

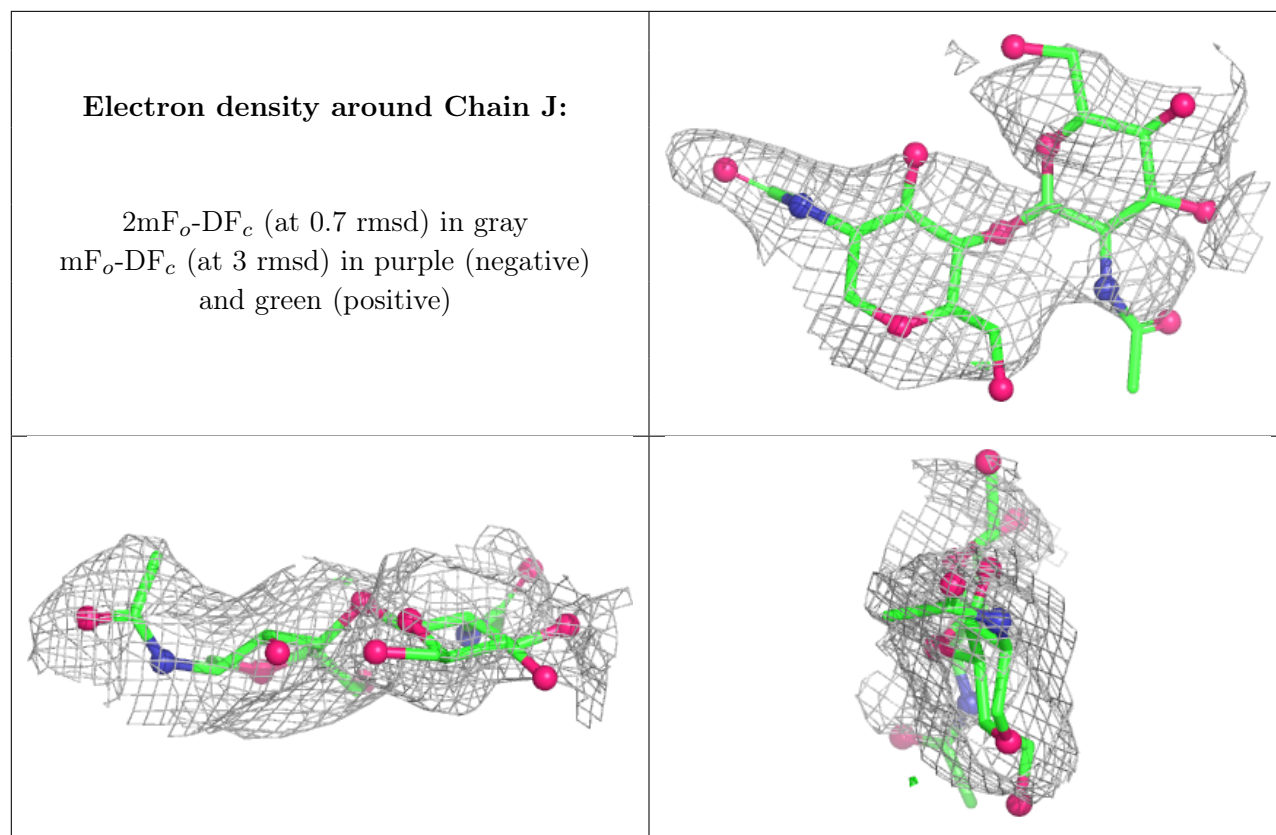
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	-	-	98,106,116,121	0
4	NAG	I	2	14/15	-	-	129,135,145,148	0
4	NAG	J	1	14/15	-	-	100,109,122,126	0
4	NAG	J	2	14/15	-	-	135,142,153,158	0

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 I:

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





6.4 Ligands ⓘ

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
5	NAG	D	1416	14/15	0.65	0.17	127,133,141,147	0
7	NA	B	1500	1/1	0.68	0.25	49,49,49,49	0
8	BGC	B	4202	12/12	0.72	0.24	136,139,143,144	0
5	NAG	B	1416	14/15	0.75	0.13	92,101,110,112	0
8	BGC	F	4203	12/12	0.85	0.18	93,98,109,111	0
8	BGC	H	4201	12/12	0.86	0.15	77,84,88,92	0
7	NA	G	1501	1/1	0.87	0.18	50,50,50,50	0
7	NA	C	3200	1/1	0.90	0.12	65,65,65,65	0
7	NA	H	1500	1/1	0.92	0.19	48,48,48,48	0
7	NA	D	1500	1/1	0.92	0.08	28,28,28,28	0
6	BEN	B	2001	9/9	0.94	0.10	38,41,42,44	0
6	BEN	D	2001	9/9	0.95	0.09	42,45,47,48	0
7	NA	F	1500	1/1	0.96	0.08	42,42,42,42	0
7	NA	B	1501	1/1	0.97	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BEN	H	2001	9/9	0.97	0.08	33,36,38,39	0
6	BEN	F	2001	9/9	0.97	0.08	41,43,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.