



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 PM UTC

PDB ID : 1P8J / pdb_00001p8j
Title : CRYSTAL STRUCTURE OF THE PROPROTEIN CONVERTASE FURIN
Authors : Henrich, S.; Cameron, A.; Bourenkov, G.P.; Kiefersauer, R.; Huber, R.; Lindberg, I.; Bode, W.; Than, M.E.
Deposited on : 2003-05-07
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

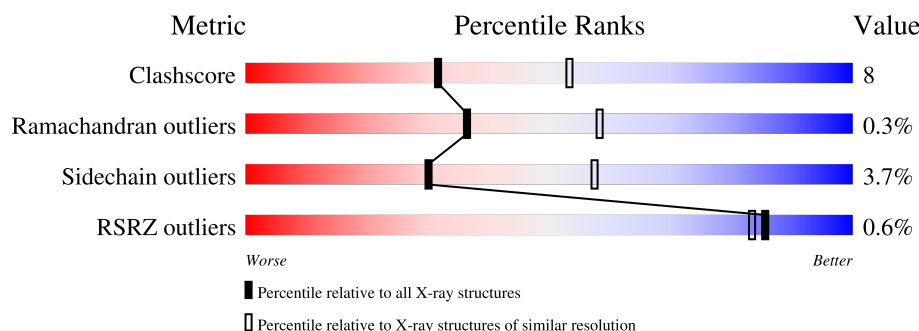
1 Overall quality at a glance

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.



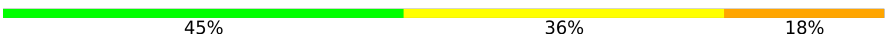
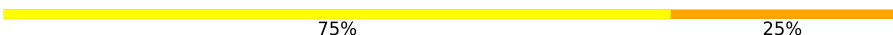
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	471	
1	B	471	
1	C	471	
1	D	471	
1	E	471	
1	F	471	

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Mol	Chain	Length	Quality of chain
1	G	471	
1	H	471	
2	J	6	
2	K	6	
2	L	6	
2	M	6	
2	N	6	
2	P	6	
2	Q	6	
2	R	6	
3	I	11	
4	O	4	

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
4	FUC	O	4	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31923 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 Furin precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	44	0	0
			3591	2227	640	710	14			
1	B	468	Total	C	N	O	S	39	0	0
			3578	2219	638	707	14			
1	C	467	Total	C	N	O	S	56	0	0
			3569	2214	637	704	14			
1	D	467	Total	C	N	O	S	51	0	0
			3569	2214	637	704	14			
1	E	467	Total	C	N	O	S	45	0	0
			3569	2214	637	704	14			
1	F	468	Total	C	N	O	S	40	0	0
			3577	2218	638	707	14			
1	G	467	Total	C	N	O	S	43	0	0
			3569	2214	637	704	14			
1	H	466	Total	C	N	O	S	60	0	0
			3562	2209	636	703	14			

- Molecule 2 is a protein called DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR.

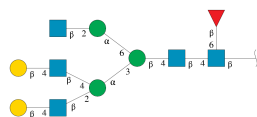
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	K	6	Total	C	N	O	2	0	1
			50	34	11	5			
2	L	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	M	6	Total	C	N	O	1	0	1
			50	34	11	5			
2	N	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	P	6	Total	C	N	O	0	0	1
			50	34	11	5			

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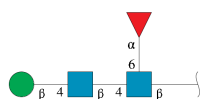
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	6	Total	C	N	O	0	0	1
			50	34	11	5			
2	R	6	Total	C	N	O	0	0	1
			50	34	11	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	4	0	0
			135	76	5	54			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	O	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	3	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ca	0	0
			2	2		
6	B	2	Total	Ca	0	0
			2	2		
6	C	2	Total	Ca	0	0
			2	2		
6	D	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		
6	F	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Ca	0	0
			2	2		
6	H	2	Total	Ca	0	0
			2	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	F	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	J	1	Total	O	S	0	0
			5	4	1		
7	K	1	Total	O	S	0	0
			5	4	1		
7	L	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	N	1	Total	O	S	0	0
			5	4	1		
7	P	1	Total	O	S	0	0
			5	4	1		
7	Q	1	Total	O	S	0	0
			5	4	1		
7	R	1	Total	O	S	0	0
			5	4	1		

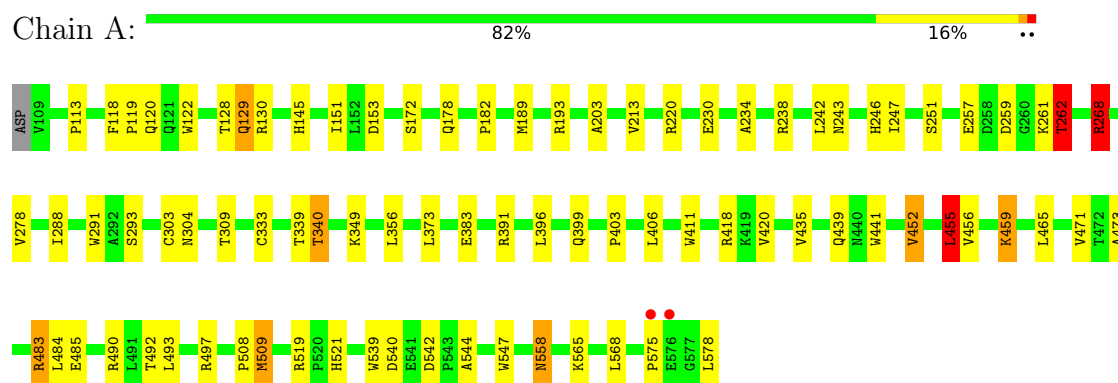
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	352	Total 352	O 352	0	0
8	B	291	Total 291	O 291	0	0
8	C	292	Total 292	O 292	0	0
8	D	181	Total 181	O 181	0	0
8	E	270	Total 270	O 270	0	0
8	F	325	Total 325	O 325	0	0
8	G	319	Total 319	O 319	0	0
8	H	231	Total 231	O 231	0	0
8	J	6	Total 6	O 6	0	0
8	K	7	Total 7	O 7	0	0
8	L	5	Total 5	O 5	0	0
8	M	5	Total 5	O 5	0	0
8	N	8	Total 8	O 8	0	0
8	P	6	Total 6	O 6	0	0
8	Q	3	Total 3	O 3	0	0
8	R	4	Total 4	O 4	0	0

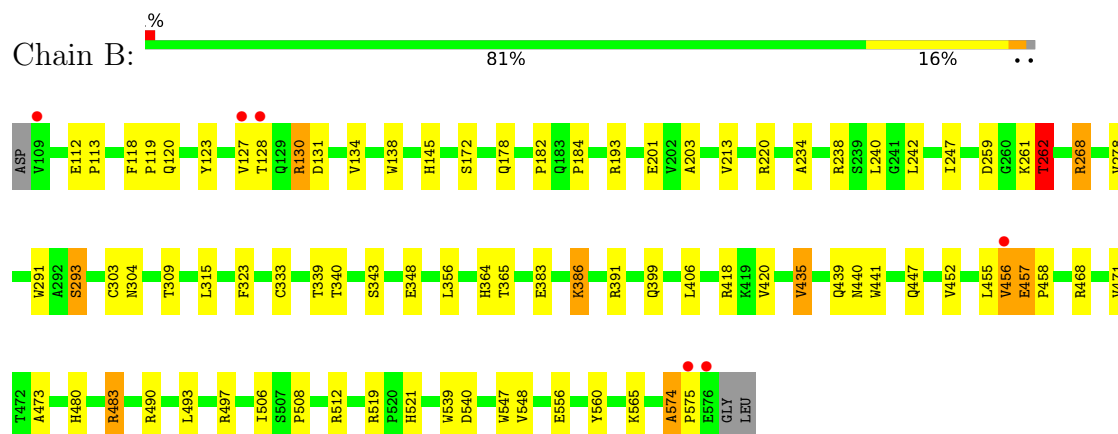
3 Residue-property plots

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.

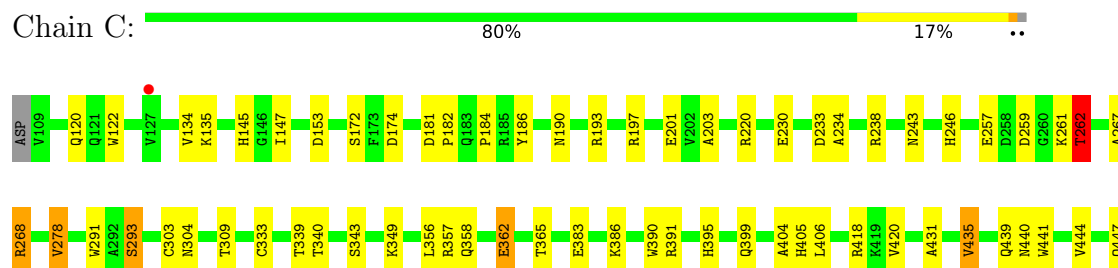
- Molecule 1: Furin precursor



- Molecule 1: Furin precursor

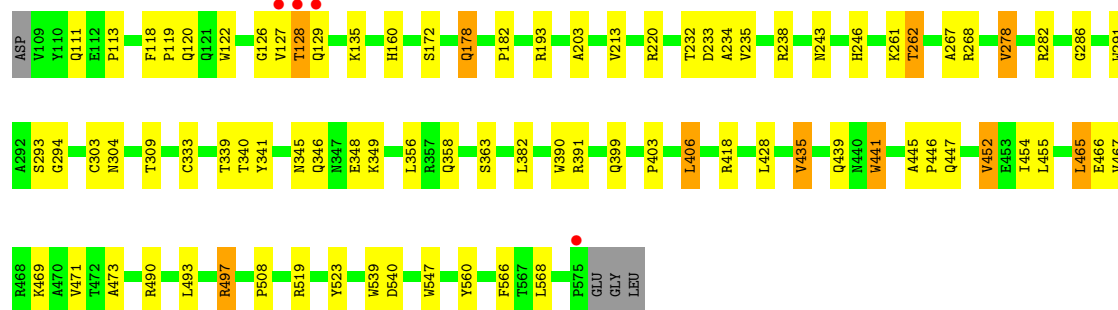
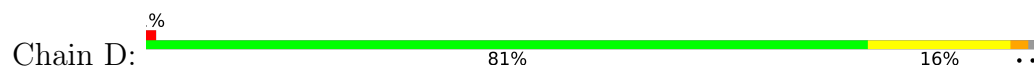


- Molecule 1: Furin precursor

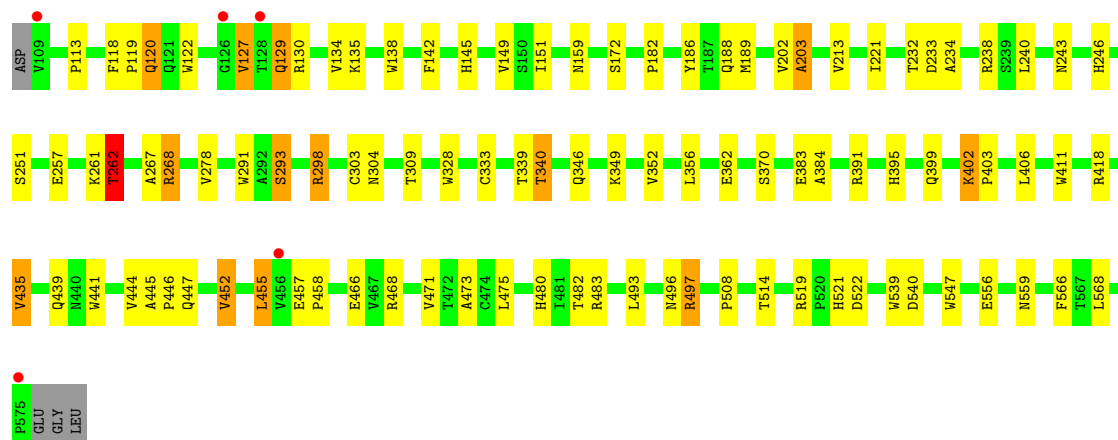
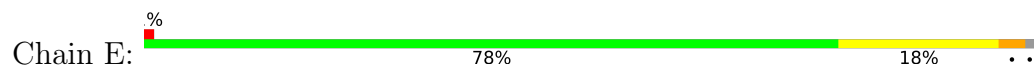




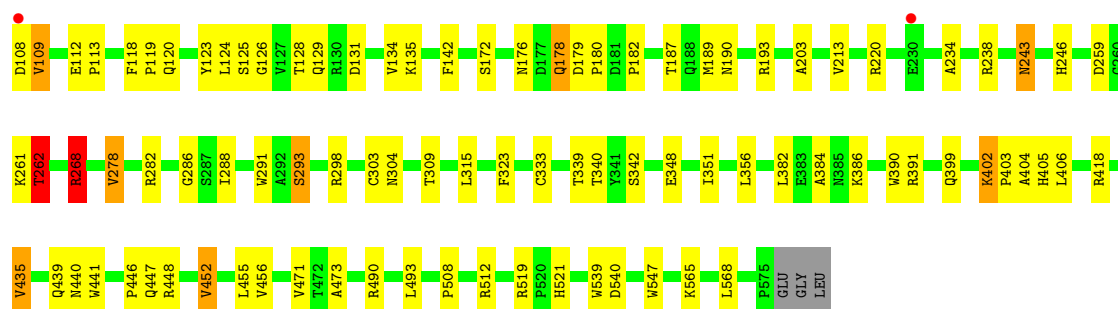
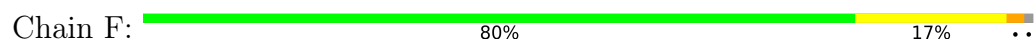
- Molecule 1: Furin precursor



- Molecule 1: Furin precursor

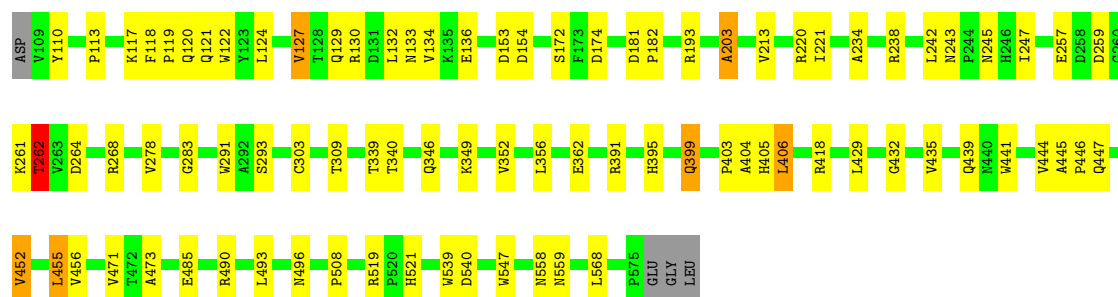


- Molecule 1: Furin precursor



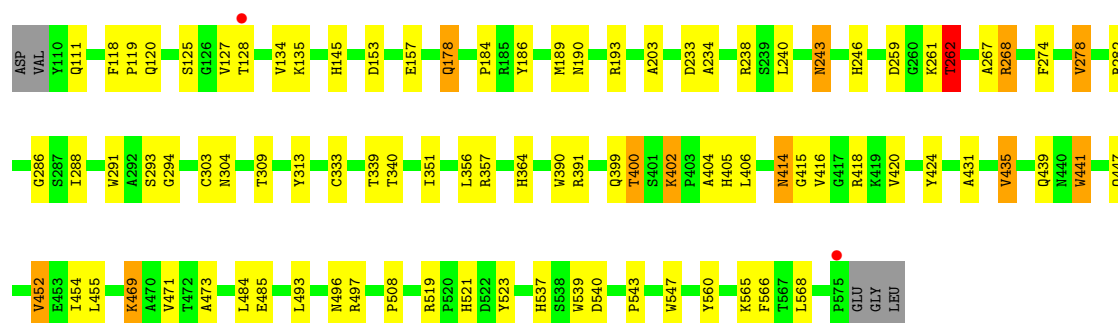
- Molecule 1: Furin precursor

Chain G:  81% 17% ..

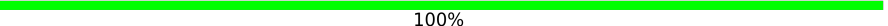


- Molecule 1: Furin precursor

Chain H:  79% 17% ..



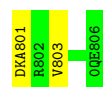
- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain J:  100%

There are no outlier residues recorded for this chain.

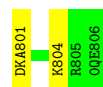
- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain K:  67% 33%



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain L:  67% 33%



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain M:  83% 17%



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain Q:  50% 50%



- Molecule 2: DECANOYL-ARG-VAL-LYS-ARG-CHLOROMETHYLKETONE INHIBITOR

Chain R:  67% 33%



- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  45% 36% 18%



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 135.39Å 137.81Å 103.56° 98.98° 107.09°	Depositor
Resolution (Å)	18.82 – 2.60 18.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (18.82-2.60) 97.7 (18.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.219 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31923	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, AR7, SO4, BMA, DKA, OQE, FUC, GAL, MAN, FUL, CA

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	0.48	0/3674	0.93	6/5007 (0.1%)
1	B	0.47	0/3661	0.95	8/4991 (0.2%)
1	C	0.48	0/3652	0.94	7/4979 (0.1%)
1	D	0.44	0/3652	0.92	6/4979 (0.1%)
1	E	0.45	0/3652	0.93	8/4979 (0.2%)
1	F	0.48	0/3660	0.93	6/4990 (0.1%)
1	G	0.48	0/3652	0.95	7/4979 (0.1%)
1	H	0.45	0/3645	0.94	10/4969 (0.2%)
2	J	0.46	0/26	0.92	0/32
2	K	0.42	0/26	0.85	0/32
2	L	0.50	0/26	0.94	0/32
2	M	0.39	0/26	0.97	0/32
2	N	0.43	0/26	0.87	0/32
2	P	0.36	0/26	0.90	0/32
2	Q	0.43	0/26	0.93	0/32
2	R	0.50	0/26	0.86	0/32
All	All	0.47	0/29456	0.94	58/40129 (0.1%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	439	GLN	N-CA-C	9.93	123.35	111.33
1	G	203	ALA	N-CA-C	7.05	119.42	110.61
1	B	574	ALA	CA-C-N	6.94	128.52	119.84
1	B	574	ALA	C-N-CA	6.94	128.52	119.84
1	H	268	ARG	N-CA-C	6.87	118.42	111.07
1	E	203	ALA	N-CA-C	6.79	119.10	110.61
1	G	262	THR	N-CA-C	6.69	120.94	110.17
1	D	268	ARG	N-CA-C	6.69	118.23	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	415	GLY	N-CA-C	-6.64	107.37	114.67
1	G	268	ARG	N-CA-C	6.49	118.94	111.02
1	A	268	ARG	N-CA-C	6.49	118.94	111.02
1	A	262	THR	N-CA-C	6.33	120.36	110.17
1	D	262	THR	N-CA-C	6.29	120.30	110.17
1	C	203	ALA	N-CA-C	6.26	119.01	110.06
1	A	203	ALA	N-CA-C	6.24	118.98	110.06
1	H	262	THR	N-CA-C	6.22	119.84	109.95
1	C	457	GLU	CA-C-N	6.21	126.22	119.89
1	C	457	GLU	C-N-CA	6.21	126.22	119.89
1	C	268	ARG	N-CA-C	6.08	118.43	111.02
1	B	262	THR	N-CA-C	6.04	119.89	110.17
1	D	203	ALA	N-CA-C	5.91	118.51	110.06
1	E	268	ARG	N-CA-C	5.89	118.21	111.02
1	H	203	ALA	N-CA-C	5.89	118.49	110.06
1	F	203	ALA	N-CA-C	5.89	118.48	110.06
1	H	454	ILE	N-CA-C	5.88	117.41	111.00
1	D	454	ILE	N-CA-C	5.87	116.51	110.82
1	C	456	VAL	N-CA-C	-5.84	107.81	113.53
1	F	268	ARG	N-CA-C	5.81	118.11	111.02
1	B	203	ALA	N-CA-C	5.81	118.37	110.06
1	H	441	TRP	N-CA-C	5.80	118.41	109.07
1	A	455	LEU	N-CA-C	5.70	117.73	108.26
1	F	262	THR	N-CA-C	5.62	119.22	110.17
1	E	262	THR	N-CA-C	5.61	119.21	110.17
1	H	400	THR	N-CA-C	5.52	120.17	113.38
1	C	262	THR	N-CA-C	5.51	119.04	110.17
1	E	457	GLU	CA-C-N	5.50	126.72	119.84
1	E	457	GLU	C-N-CA	5.50	126.72	119.84
1	B	268	ARG	N-CA-C	5.47	117.70	111.02
1	D	128	THR	N-CA-C	-5.47	106.61	113.28
1	H	402	LYS	N-CA-C	5.41	118.19	109.15
1	E	402	LYS	N-CA-C	5.38	117.21	109.04
1	E	293	SER	N-CA-C	5.37	119.09	112.54
1	C	293	SER	N-CA-C	5.32	119.03	112.54
1	B	293	SER	N-CA-C	5.32	118.87	112.38
1	G	399	GLN	N-CA-C	5.32	117.16	111.36
1	F	243	ASN	CB-CA-C	-5.26	106.42	111.00
1	G	456	VAL	N-CA-C	-5.21	106.72	111.67
1	B	112	GLU	CA-C-N	5.20	125.19	119.89
1	B	112	GLU	C-N-CA	5.20	125.19	119.89
1	A	439	GLN	N-CA-C	5.19	119.88	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	243	ASN	CB-CA-C	-5.18	106.49	111.00
1	D	441	TRP	N-CA-C	5.17	117.97	109.76
1	F	293	SER	N-CA-C	5.14	118.81	112.54
1	A	484	LEU	N-CA-C	5.09	117.24	110.53
1	F	402	LYS	N-CA-C	5.04	117.57	109.15
1	H	455	LEU	N-CA-C	5.04	118.33	110.32
1	E	129	GLN	N-CA-C	-5.03	104.48	111.52
1	H	243	ASN	CB-CA-C	-5.01	106.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3591	0	3406	60	0
1	B	3578	0	3393	51	0
1	C	3569	0	3388	56	0
1	D	3569	0	3388	49	0
1	E	3569	0	3387	73	0
1	F	3577	0	3389	55	0
1	G	3569	0	3387	52	0
1	H	3562	0	3378	56	0
2	J	50	0	66	0	0
2	K	50	0	66	2	0
2	L	50	0	66	2	0
2	M	50	0	66	1	0
2	N	50	0	66	0	0
2	P	50	0	66	0	0
2	Q	50	0	66	3	0
2	R	50	0	66	2	0
3	I	135	0	115	3	0
4	O	49	0	43	3	0
5	A	14	0	13	0	0
5	B	14	0	13	1	0
5	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	28	0	26	1	0
5	H	14	0	13	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
7	A	55	0	0	1	0
7	B	30	0	0	1	0
7	C	30	0	0	0	0
7	D	45	0	0	1	0
7	E	45	0	0	2	0
7	F	45	0	0	1	0
7	G	30	0	0	1	0
7	H	30	0	0	0	0
7	J	5	0	0	0	0
7	K	5	0	0	0	0
7	L	5	0	0	1	0
7	M	5	0	0	0	0
7	N	5	0	0	0	0
7	P	5	0	0	0	0
7	Q	5	0	0	0	0
7	R	5	0	0	0	0
8	A	352	0	0	12	0
8	B	291	0	0	9	0
8	C	292	0	0	6	0
8	D	181	0	0	6	0
8	E	270	0	0	5	0
8	F	325	0	0	10	0
8	G	319	0	0	6	0
8	H	231	0	0	4	0
8	J	6	0	0	0	0
8	K	7	0	0	1	0
8	L	5	0	0	0	0
8	M	5	0	0	0	0
8	N	8	0	0	0	0
8	P	6	0	0	0	0
8	Q	3	0	0	0	0
8	R	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31923	0	27880	458	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 8.

All (458) 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:E:298:ARG:HH21	1:E:298:ARG:HB2	1.02	1.11
1:A:509:MET:HE2	1:A:542:ASP:H	1.18	1.05
1:E:298:ARG:HH21	1:E:298:ARG:CB	1.74	0.99
1:E:475:LEU:HA	1:E:480:HIS:CD2	1.99	0.98
1:E:475:LEU:HA	1:E:480:HIS:HD2	1.28	0.95
1:F:125:SER:HA	1:F:135:LYS:HE2	1.49	0.92
1:E:298:ARG:HB2	1:E:298:ARG:NH2	1.83	0.91
1:H:304:ASN:OD1	1:H:333:CYS:HB2	1.72	0.89
1:C:190:ASN:HD21	1:C:357:ARG:HE	1.26	0.83
1:D:304:ASN:OD1	1:D:333:CYS:HB2	1.79	0.81
1:C:120:GLN:NE2	1:C:362:GLU:HG2	1.96	0.81
4:O:2:NAG:H4	4:O:3:BMA:O2	1.77	0.80
1:D:519:ARG:HD3	8:D:4069:HOH:O	1.82	0.78
1:H:178:GLN:HE21	1:H:178:GLN:C	1.92	0.77
1:A:519:ARG:HD3	8:A:4225:HOH:O	1.85	0.77
1:A:509:MET:HE2	1:A:542:ASP:N	1.99	0.75
1:F:304:ASN:OD1	1:F:333:CYS:HB2	1.85	0.75
1:E:257:GLU:HB3	1:E:262:THR:HG21	1.70	0.73
1:G:519:ARG:HD3	8:G:4176:HOH:O	1.89	0.72
1:C:440:ASN:HB3	8:C:4282:HOH:O	1.90	0.71
1:G:455:LEU:HD12	1:G:455:LEU:O	1.90	0.71
1:E:120:GLN:H	1:E:120:GLN:HE21	1.36	0.71
1:C:257:GLU:HB3	1:C:262:THR:HG21	1.74	0.70
1:D:111:GLN:HG3	8:D:4217:HOH:O	1.92	0.70
1:C:483:ARG:HD3	1:C:540:ASP:OD2	1.92	0.70
4:O:2:NAG:O3	4:O:3:BMA:H2	1.92	0.70
1:A:304:ASN:OD1	1:A:333:CYS:HB2	1.92	0.69
1:E:519:ARG:HD3	8:E:4068:HOH:O	1.92	0.69
1:F:298:ARG:HD2	8:F:4242:HOH:O	1.92	0.69
1:B:304:ASN:OD1	1:B:333:CYS:HB2	1.92	0.69
1:G:127:VAL:HA	1:G:133:ASN:ND2	2.08	0.69
1:B:220:ARG:HG3	8:B:4140:HOH:O	1.92	0.68
1:C:519:ARG:HD3	8:C:4065:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG23	1:A:130:ARG:H	1.59	0.68
1:A:257:GLU:HB3	1:A:262:THR:HG21	1.76	0.67
1:E:120:GLN:H	1:E:120:GLN:NE2	1.92	0.67
1:H:519:ARG:HD3	8:H:4074:HOH:O	1.94	0.67
1:H:560:TYR:CE1	2:Q:801:DKA:H102	2.30	0.67
1:A:220:ARG:HD3	8:A:4119:HOH:O	1.95	0.66
1:D:493:LEU:HD12	1:D:493:LEU:C	2.21	0.65
1:C:468:ARG:HG2	1:C:548:VAL:HG22	1.79	0.65
1:H:399:GLN:HE22	1:H:441:TRP:HZ3	1.44	0.65
1:H:261:LYS:HG2	1:H:521:HIS:O	1.97	0.65
1:H:189:MET:HA	1:H:189:MET:HE2	1.79	0.65
8:A:4162:HOH:O	1:B:565:LYS:HE2	1.96	0.64
1:G:124:LEU:HD22	1:G:134:VAL:HG21	1.79	0.64
1:H:414:ASN:ND2	1:H:537:HIS:O	2.27	0.64
1:A:128:THR:O	1:A:129:GLN:HB2	1.98	0.64
1:E:399:GLN:HE22	1:E:441:TRP:HZ3	1.46	0.64
1:G:136:GLU:OE1	1:G:432:GLY:HA3	1.98	0.63
1:B:440:ASN:HB3	8:B:4307:HOH:O	1.98	0.63
1:C:304:ASN:OD1	1:C:333:CYS:HB2	1.99	0.63
1:A:544:ALA:HB2	8:A:4330:HOH:O	1.99	0.62
1:G:403:PRO:O	1:G:406:LEU:HB2	1.99	0.62
1:G:418:ARG:NH1	1:G:540:ASP:OD1	2.32	0.62
1:B:323:PHE:CD1	1:B:348:GLU:HG2	2.35	0.62
1:C:399:GLN:HE22	1:C:441:TRP:HZ3	1.46	0.61
1:D:465:LEU:HD22	1:D:466:GLU:N	2.16	0.61
1:G:245:ASN:ND2	1:G:283:GLY:H	1.97	0.61
1:E:418:ARG:NH1	1:E:540:ASP:OD1	2.33	0.61
1:F:234:ALA:O	1:F:238:ARG:HG3	2.01	0.61
1:A:455:LEU:HA	8:A:4318:HOH:O	2.00	0.61
1:H:418:ARG:NH1	1:H:540:ASP:OD1	2.33	0.61
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.66	0.61
1:B:493:LEU:HD12	1:B:493:LEU:C	2.26	0.60
1:F:399:GLN:HE22	1:F:441:TRP:HZ3	1.46	0.60
1:F:418:ARG:NH1	1:F:540:ASP:OD1	2.34	0.60
1:E:340:THR:HG21	1:E:370:SER:HA	1.83	0.60
1:F:493:LEU:C	1:F:493:LEU:HD12	2.25	0.60
1:G:493:LEU:C	1:G:493:LEU:HD12	2.26	0.60
1:E:120:GLN:NE2	1:E:120:GLN:N	2.50	0.60
1:F:440:ASN:HB3	5:F:951:NAG:O7	2.01	0.59
1:E:475:LEU:HD12	1:E:480:HIS:CD2	2.37	0.58
1:E:232:THR:HB	7:E:4060:SO4:O1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:TRP:NE1	1:E:349:LYS:HB3	2.18	0.58
1:E:298:ARG:HH21	1:E:298:ARG:CG	2.16	0.58
1:E:493:LEU:C	1:E:493:LEU:HD12	2.29	0.57
1:G:257:GLU:HB3	1:G:262:THR:HG21	1.86	0.57
1:C:493:LEU:C	1:C:493:LEU:HD12	2.29	0.57
1:C:234:ALA:O	1:C:238:ARG:HG3	2.05	0.57
1:B:418:ARG:NH1	1:B:540:ASP:OD1	2.36	0.57
1:D:399:GLN:NE2	1:D:441:TRP:CH2	2.73	0.57
1:E:339:THR:HG22	1:E:340:THR:N	2.20	0.57
1:A:220:ARG:NH1	1:A:246:HIS:HE1	2.03	0.57
1:A:418:ARG:NH1	1:A:540:ASP:OD1	2.37	0.57
1:D:345:ASN:OD1	1:D:348:GLU:HG3	2.04	0.57
1:E:145:HIS:HB2	1:E:383:GLU:OE2	2.04	0.57
1:C:471:VAL:HG12	1:C:473:ALA:H	1.69	0.56
1:A:455:LEU:HD23	1:A:455:LEU:O	2.05	0.56
1:B:145:HIS:HB2	1:B:383:GLU:OE2	2.05	0.56
1:C:418:ARG:NH1	1:C:540:ASP:OD1	2.39	0.56
1:F:193:ARG:HA	1:F:356:LEU:HG	1.86	0.56
1:A:493:LEU:C	1:A:493:LEU:HD12	2.31	0.56
1:D:418:ARG:NH1	1:D:540:ASP:OD1	2.39	0.56
5:B:901:NAG:H61	8:B:4336:HOH:O	2.05	0.56
1:E:539:TRP:O	1:E:540:ASP:HB2	2.04	0.56
1:A:456:VAL:N	8:A:4318:HOH:O	2.34	0.56
1:H:493:LEU:C	1:H:493:LEU:HD12	2.31	0.56
1:B:234:ALA:O	1:B:238:ARG:HG3	2.06	0.56
1:E:304:ASN:OD1	1:E:333:CYS:HB2	2.06	0.56
1:F:512:ARG:NH2	8:F:4222:HOH:O	2.39	0.56
1:C:483:ARG:HG2	1:C:540:ASP:HA	1.88	0.55
1:E:556:GLU:OE2	1:E:556:GLU:HA	2.06	0.55
1:A:288:ILE:HA	8:A:4113:HOH:O	2.06	0.55
1:E:497:ARG:NH2	1:E:522:ASP:O	2.39	0.55
1:A:122:TRP:NE1	1:A:349:LYS:HB3	2.21	0.55
1:A:340:THR:HG21	1:A:373:LEU:HB2	1.89	0.55
1:B:512:ARG:NH2	8:B:4289:HOH:O	2.39	0.55
1:C:333:CYS:HA	8:C:4169:HOH:O	2.06	0.55
1:F:435:VAL:O	1:F:439:GLN:HG3	2.06	0.55
1:F:124:LEU:HD22	1:F:134:VAL:HG21	1.88	0.54
1:G:539:TRP:O	1:G:540:ASP:HB2	2.07	0.54
1:B:455:LEU:HD12	1:B:455:LEU:C	2.32	0.54
1:A:396:LEU:HD21	1:A:441:TRP:CE3	2.42	0.54
1:A:483:ARG:HD3	1:A:540:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:4279:HOH:O	2:K:803:VAL:HB	2.06	0.54
1:D:193:ARG:HA	1:D:356:LEU:HG	1.89	0.54
1:H:414:ASN:HB3	1:H:416:VAL:H	1.72	0.54
1:C:190:ASN:ND2	1:C:357:ARG:HE	2.01	0.54
1:E:497:ARG:HH21	1:E:497:ARG:HG3	1.72	0.54
1:C:468:ARG:NH2	1:C:546:GLU:OE2	2.41	0.54
1:H:178:GLN:HE21	1:H:178:GLN:CA	2.18	0.54
1:C:145:HIS:HB2	1:C:383:GLU:OE2	2.06	0.54
1:E:471:VAL:HG12	1:E:473:ALA:H	1.73	0.54
1:A:339:THR:HG22	1:A:340:THR:N	2.23	0.54
1:E:234:ALA:O	1:E:238:ARG:HG3	2.08	0.54
1:F:490:ARG:NH1	7:F:4070:SO4:O1	2.41	0.54
1:C:339:THR:HG22	1:C:340:THR:N	2.23	0.54
1:H:234:ALA:O	1:H:238:ARG:HG3	2.07	0.54
1:A:193:ARG:HA	1:A:356:LEU:HG	1.90	0.54
1:A:418:ARG:HD3	8:A:4124:HOH:O	2.08	0.54
1:C:435:VAL:O	1:C:439:GLN:HG3	2.08	0.54
1:A:145:HIS:HB2	1:A:383:GLU:OE2	2.07	0.53
1:B:128:THR:HG22	1:B:130:ARG:HB2	1.90	0.53
1:E:293:SER:HA	1:E:309:THR:HG21	1.90	0.53
1:H:193:ARG:HA	1:H:356:LEU:HG	1.90	0.53
1:A:459:LYS:HG2	1:A:465:LEU:HD11	1.90	0.53
1:D:445:ALA:HB1	1:D:446:PRO:HD2	1.89	0.53
1:H:145:HIS:HB3	8:H:4262:HOH:O	2.07	0.53
1:H:400:THR:O	1:H:402:LYS:HE3	2.08	0.53
1:A:565:LYS:HE3	8:A:4300:HOH:O	2.08	0.53
1:F:539:TRP:O	1:F:540:ASP:HB2	2.08	0.53
1:A:558:ASN:C	1:A:558:ASN:ND2	2.67	0.53
1:F:399:GLN:NE2	1:F:441:TRP:CZ3	2.76	0.53
1:B:519:ARG:HD3	8:B:4082:HOH:O	2.08	0.53
1:B:201:GLU:OE2	1:B:364:HIS:ND1	2.40	0.53
2:K:801:DKA:H82	8:K:780:HOH:O	2.08	0.52
1:D:399:GLN:NE2	1:D:441:TRP:CZ3	2.75	0.52
1:E:188:GLN:HG2	1:E:189:MET:HE2	1.92	0.52
1:G:234:ALA:O	1:G:238:ARG:HG3	2.08	0.52
2:R:801:DKA:H82	8:R:587:HOH:O	2.09	0.52
1:D:471:VAL:HG12	1:D:473:ALA:H	1.73	0.52
1:E:159:ASN:HB2	8:E:4298:HOH:O	2.08	0.52
1:F:261:LYS:HG2	1:F:521:HIS:O	2.09	0.52
1:H:452:VAL:HG13	1:H:568:LEU:HB3	1.91	0.52
1:B:508:PRO:HD3	1:B:547:TRP:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:GLN:NE2	1:C:441:TRP:CZ3	2.78	0.52
1:D:435:VAL:O	1:D:439:GLN:HG3	2.10	0.52
1:G:245:ASN:HD21	1:G:283:GLY:H	1.58	0.52
1:A:259:ASP:OD2	1:A:262:THR:HG22	2.10	0.52
1:A:399:GLN:NE2	1:A:441:TRP:CH2	2.78	0.51
1:C:261:LYS:HG2	1:C:521:HIS:O	2.10	0.51
1:E:445:ALA:HB1	1:E:446:PRO:HD2	1.92	0.51
1:F:178:GLN:HA	1:F:178:GLN:OE1	2.10	0.51
1:C:455:LEU:HD12	1:C:455:LEU:O	2.10	0.51
1:F:220:ARG:HG3	8:F:4344:HOH:O	2.10	0.51
1:H:539:TRP:O	1:H:540:ASP:HB2	2.08	0.51
1:C:293:SER:HA	1:C:309:THR:HG21	1.93	0.51
1:C:497:ARG:HD2	1:C:523:TYR:HA	1.92	0.51
1:B:457:GLU:CD	1:B:457:GLU:H	2.18	0.51
1:B:480:HIS:HE1	8:B:4173:HOH:O	1.94	0.51
1:D:346:GLN:HA	8:D:4232:HOH:O	2.11	0.51
1:A:471:VAL:HG12	1:A:473:ALA:H	1.75	0.51
1:B:399:GLN:HE22	1:B:441:TRP:HZ3	1.58	0.51
1:C:147:ILE:HD11	1:C:386:LYS:HD3	1.93	0.51
1:F:508:PRO:HD3	1:F:547:TRP:CE2	2.46	0.51
1:G:418:ARG:HD3	8:G:4279:HOH:O	2.09	0.51
1:C:220:ARG:HD3	8:C:4218:HOH:O	2.11	0.51
1:E:480:HIS:HE1	1:E:482:THR:HG22	1.75	0.51
1:G:399:GLN:HE22	1:G:441:TRP:HZ3	1.58	0.51
1:D:508:PRO:HD3	1:D:547:TRP:CE2	2.46	0.51
1:B:172:SER:HB3	1:B:182:PRO:HG3	1.93	0.51
1:B:574:ALA:HB2	8:B:4321:HOH:O	2.11	0.51
1:D:391:ARG:CZ	1:D:447:GLN:HB2	2.40	0.51
1:D:539:TRP:O	1:D:540:ASP:HB2	2.11	0.50
1:G:220:ARG:HG3	8:G:4276:HOH:O	2.12	0.50
1:H:288:ILE:HA	8:H:4060:HOH:O	2.11	0.50
1:B:539:TRP:O	1:B:540:ASP:HB2	2.10	0.50
1:D:220:ARG:HG3	8:D:4113:HOH:O	2.10	0.50
1:F:268:ARG:NE	8:F:4230:HOH:O	2.44	0.50
1:H:293:SER:HA	1:H:309:THR:HG21	1.92	0.50
1:E:483:ARG:HD3	1:E:540:ASP:OD2	2.11	0.50
1:A:234:ALA:O	1:A:238:ARG:HG3	2.11	0.50
1:F:128:THR:O	1:F:129:GLN:HB2	2.11	0.50
1:A:558:ASN:C	1:A:558:ASN:HD22	2.18	0.50
1:E:130:ARG:HD3	8:E:4256:HOH:O	2.11	0.50
4:O:2:NAG:H4	4:O:3:BMA:HO2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:PHE:HD1	1:B:348:GLU:HG2	1.75	0.50
1:D:120:GLN:OE1	1:D:120:GLN:N	2.44	0.50
1:E:186:TYR:CE2	1:E:356:LEU:HD22	2.46	0.50
1:B:339:THR:HG22	1:B:340:THR:N	2.25	0.50
1:C:465:LEU:HD12	1:C:466:GLU:N	2.27	0.50
1:G:391:ARG:HD2	1:G:485:GLU:OE2	2.11	0.50
1:H:471:VAL:HG12	1:H:473:ALA:H	1.77	0.50
1:C:455:LEU:HD12	1:C:455:LEU:C	2.37	0.49
1:G:293:SER:HA	1:G:309:THR:HG21	1.94	0.49
1:F:176:ASN:ND2	8:F:4151:HOH:O	2.40	0.49
1:F:339:THR:HG22	1:F:340:THR:N	2.27	0.49
1:H:508:PRO:HD3	1:H:547:TRP:CE2	2.47	0.49
1:B:134:VAL:HG12	1:B:138:TRP:CE2	2.48	0.49
1:A:452:VAL:HG13	1:A:568:LEU:HB3	1.95	0.49
1:D:234:ALA:O	1:D:238:ARG:HG3	2.13	0.49
1:D:363:SER:HB2	8:D:4181:HOH:O	2.12	0.49
1:C:193:ARG:HA	1:C:356:LEU:HG	1.95	0.49
1:E:483:ARG:HG2	1:E:540:ASP:HA	1.94	0.49
1:G:193:ARG:HA	1:G:356:LEU:HG	1.95	0.49
1:F:519:ARG:HD3	8:F:4105:HOH:O	2.13	0.49
1:A:539:TRP:O	1:A:540:ASP:HB2	2.13	0.48
1:C:358:GLN:NE2	8:C:4220:HOH:O	2.39	0.48
1:H:178:GLN:CA	1:H:178:GLN:NE2	2.76	0.48
1:D:339:THR:HG22	1:D:340:THR:N	2.27	0.48
1:G:471:VAL:HG12	1:G:473:ALA:H	1.78	0.48
1:B:123:TYR:O	1:B:131:ASP:HB2	2.13	0.48
1:B:468:ARG:HG2	1:B:548:VAL:HG22	1.95	0.48
1:B:471:VAL:HG12	1:B:473:ALA:H	1.78	0.48
1:A:293:SER:HA	1:A:309:THR:HG21	1.95	0.48
1:D:126:GLY:C	1:D:128:THR:H	2.21	0.48
1:E:458:PRO:HD2	1:G:558:ASN:HD22	1.77	0.48
1:G:339:THR:HG22	1:G:340:THR:N	2.28	0.48
1:A:230:GLU:HA	1:D:560:TYR:CE2	2.49	0.48
1:C:452:VAL:HG13	1:C:568:LEU:HB3	1.96	0.48
1:D:490:ARG:NH1	7:D:4012:SO4:O4	2.46	0.48
1:G:154:ASP:HB3	2:Q:804:LYS:HE2	1.96	0.48
1:C:539:TRP:O	1:C:540:ASP:HB2	2.12	0.48
1:F:323:PHE:CD1	1:F:348:GLU:HG2	2.48	0.48
1:A:508:PRO:HD3	1:A:547:TRP:CE2	2.49	0.48
1:D:293:SER:HA	1:D:309:THR:HG21	1.96	0.48
1:F:404:ALA:O	1:F:405:HIS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:391:ARG:CZ	1:H:447:GLN:HB2	2.44	0.48
1:A:172:SER:HB3	1:A:182:PRO:HG3	1.96	0.48
1:C:122:TRP:NE1	1:C:349:LYS:HB3	2.29	0.48
1:H:189:MET:O	1:H:190:ASN:HB2	2.13	0.48
1:H:339:THR:HG22	1:H:340:THR:N	2.29	0.48
1:G:259:ASP:OD2	1:G:262:THR:CG2	2.62	0.47
1:G:508:PRO:HD3	1:G:547:TRP:CE2	2.49	0.47
1:A:189:MET:HG2	8:D:4088:HOH:O	2.14	0.47
1:E:261:LYS:HG2	1:E:521:HIS:O	2.14	0.47
1:E:435:VAL:O	1:E:439:GLN:HG3	2.15	0.47
1:H:125:SER:OG	1:H:135:LYS:HD3	2.14	0.47
1:H:190:ASN:OD1	1:H:357:ARG:NE	2.43	0.47
1:B:193:ARG:HA	1:B:356:LEU:HG	1.96	0.47
1:H:268:ARG:HG3	1:H:268:ARG:HH11	1.78	0.47
1:D:465:LEU:HD22	1:D:466:GLU:H	1.78	0.47
1:G:130:ARG:HA	1:G:404:ALA:HB1	1.97	0.47
1:E:340:THR:CG2	1:E:370:SER:HA	2.44	0.47
1:E:508:PRO:HD3	1:E:547:TRP:CE2	2.50	0.47
1:F:259:ASP:OD2	1:F:262:THR:CG2	2.62	0.47
1:F:391:ARG:CZ	1:F:447:GLN:HB2	2.45	0.47
1:H:128:THR:HG22	1:H:128:THR:O	2.14	0.47
1:B:259:ASP:OD2	1:B:262:THR:CG2	2.62	0.47
1:H:399:GLN:NE2	1:H:441:TRP:CZ3	2.79	0.47
3:I:4:MAN:H61	3:I:7:NAG:H82	1.96	0.47
1:C:508:PRO:HD3	1:C:547:TRP:CE2	2.49	0.47
1:G:496:ASN:OD1	1:G:559:ASN:HB3	2.14	0.47
1:H:469:LYS:HE3	1:H:469:LYS:HA	1.96	0.47
1:G:127:VAL:HA	1:G:133:ASN:HD22	1.79	0.47
1:F:323:PHE:HD1	1:F:348:GLU:HG2	1.78	0.47
1:B:506:ILE:N	1:B:506:ILE:HD12	2.30	0.46
1:C:259:ASP:OD2	1:C:262:THR:CG2	2.63	0.46
3:I:1:NAG:H62	3:I:2:NAG:H82	1.97	0.46
1:A:399:GLN:NE2	1:A:441:TRP:HH2	2.13	0.46
1:A:490:ARG:NH1	7:A:4069:SO4:O3	2.49	0.46
1:D:178:GLN:C	1:D:178:GLN:HE21	2.24	0.46
1:D:243:ASN:HB3	1:D:246:HIS:HB3	1.98	0.46
1:E:120:GLN:HE21	1:E:120:GLN:N	2.07	0.46
1:G:264:ASP:OD2	2:Q:802:ARG:NH2	2.44	0.46
1:D:282:ARG:NH1	1:D:286:GLY:O	2.44	0.46
1:D:399:GLN:HE22	1:D:441:TRP:HZ3	1.60	0.46
1:A:459:LYS:HG2	1:A:465:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:LEU:HD12	1:C:466:GLU:H	1.80	0.46
1:G:395:HIS:CD2	1:G:444:VAL:HG11	2.51	0.46
1:G:404:ALA:O	1:G:405:HIS:HB2	2.15	0.46
1:E:391:ARG:CZ	1:E:447:GLN:HB2	2.45	0.46
1:F:471:VAL:HG12	1:F:473:ALA:H	1.79	0.46
1:G:129:GLN:HA	7:G:4029:SO4:O2	2.16	0.46
1:B:490:ARG:NH1	7:B:4027:SO4:O4	2.47	0.46
1:E:452:VAL:HG13	1:E:568:LEU:HB3	1.97	0.46
1:E:268:ARG:HB2	8:H:4097:HOH:O	2.16	0.46
1:F:108:ASP:O	1:F:109:VAL:HB	2.16	0.46
1:D:452:VAL:HG13	1:D:568:LEU:HB3	1.98	0.45
1:F:259:ASP:OD2	1:F:262:THR:HG22	2.15	0.45
1:C:184:PRO:HG3	1:C:356:LEU:HD21	1.96	0.45
1:E:127:VAL:C	1:E:129:GLN:N	2.74	0.45
1:E:399:GLN:NE2	1:E:441:TRP:CZ3	2.79	0.45
1:B:113:PRO:HB3	1:B:213:VAL:HG11	1.98	0.45
1:D:497:ARG:NH2	1:D:523:TYR:CE2	2.85	0.45
1:B:456:VAL:O	1:B:456:VAL:HG13	2.15	0.45
1:B:323:PHE:CE1	1:B:348:GLU:HG2	2.51	0.45
1:B:391:ARG:CZ	1:B:447:GLN:HB2	2.46	0.45
1:D:465:LEU:HD11	1:D:467:VAL:HG23	1.99	0.45
1:H:496:ASN:O	1:H:497:ARG:HD2	2.17	0.45
1:A:497:ARG:HH21	1:A:497:ARG:HG3	1.81	0.45
1:C:197:ARG:O	1:C:201:GLU:HG3	2.16	0.45
1:F:452:VAL:HG13	1:F:568:LEU:HB3	1.99	0.45
1:G:172:SER:HB3	1:G:182:PRO:HG3	1.99	0.45
1:A:391:ARG:HD2	1:A:485:GLU:OE2	2.17	0.45
1:F:172:SER:HB3	1:F:182:PRO:HG3	1.98	0.45
1:A:268:ARG:HB2	8:B:4071:HOH:O	2.17	0.44
1:E:352:VAL:HG22	1:E:362:GLU:HG2	1.99	0.44
1:A:113:PRO:HB3	1:A:213:VAL:HG11	1.99	0.44
1:G:242:LEU:O	1:G:247:ILE:HD12	2.17	0.44
1:H:414:ASN:HD22	1:H:414:ASN:HA	1.53	0.44
1:E:298:ARG:NH2	1:E:328:TRP:CE3	2.85	0.44
1:B:184:PRO:HG3	1:B:356:LEU:HD21	1.99	0.44
1:E:328:TRP:HD1	8:E:4267:HOH:O	1.99	0.44
1:G:391:ARG:CZ	1:G:447:GLN:HB2	2.48	0.44
1:B:268:ARG:HH11	1:B:268:ARG:CG	2.30	0.44
1:A:459:LYS:HD3	8:A:4220:HOH:O	2.17	0.44
1:D:118:PHE:N	1:D:119:PRO:CD	2.81	0.44
1:G:118:PHE:N	1:G:119:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASP:OD2	1:A:262:THR:CG2	2.66	0.44
1:F:118:PHE:N	1:F:119:PRO:CD	2.81	0.44
1:G:132:LEU:HD23	1:G:429:LEU:O	2.18	0.44
1:G:261:LYS:HG2	1:G:521:HIS:O	2.18	0.44
1:H:404:ALA:O	1:H:405:HIS:HB2	2.18	0.44
1:A:243:ASN:HA	8:A:4409:HOH:O	2.17	0.44
1:E:402:LYS:HA	1:E:403:PRO:HD2	1.92	0.43
1:G:445:ALA:HB1	1:G:446:PRO:HD2	1.99	0.43
1:A:242:LEU:O	1:A:247:ILE:HD12	2.18	0.43
1:B:242:LEU:O	1:B:247:ILE:HD12	2.18	0.43
1:C:343:SER:OG	1:C:365:THR:HB	2.19	0.43
1:D:294:GLY:HA2	2:M:805:AR7:HD1	1.99	0.43
1:F:382:LEU:HD23	1:F:382:LEU:HA	1.84	0.43
1:F:402:LYS:HA	1:F:403:PRO:HD3	1.81	0.43
1:D:455:LEU:HG	1:D:566:PHE:HB3	2.00	0.43
1:H:157:GLU:HG3	1:H:186:TYR:OH	2.18	0.43
1:A:220:ARG:NH1	1:A:246:HIS:CE1	2.85	0.43
1:B:118:PHE:N	1:B:119:PRO:CD	2.82	0.43
1:D:391:ARG:NH1	1:D:445:ALA:O	2.44	0.43
1:F:565:LYS:HE3	8:F:4270:HOH:O	2.17	0.43
1:G:122:TRP:NE1	1:G:349:LYS:HB3	2.34	0.43
1:G:113:PRO:HB3	1:G:213:VAL:HG11	1.99	0.43
1:C:391:ARG:CZ	1:C:447:GLN:HB2	2.48	0.43
1:E:149:VAL:HG11	1:E:202:VAL:HG11	2.00	0.43
1:G:110:TYR:HA	8:G:4189:HOH:O	2.17	0.43
1:E:233:ASP:CG	1:E:267:ALA:HB3	2.44	0.43
1:E:496:ASN:OD1	1:E:559:ASN:HB3	2.19	0.43
1:C:404:ALA:O	1:C:405:HIS:HB2	2.19	0.43
1:B:293:SER:HA	1:B:309:THR:HG21	2.01	0.43
1:F:189:MET:O	1:F:190:ASN:HB2	2.19	0.43
1:F:243:ASN:HB3	1:F:246:HIS:HB3	2.01	0.43
1:G:352:VAL:HG22	1:G:362:GLU:HG2	2.01	0.43
1:H:268:ARG:HG3	1:H:268:ARG:NH1	2.33	0.43
1:H:497:ARG:HH22	1:H:523:TYR:HB3	1.84	0.43
1:C:278:VAL:HG13	1:C:390:TRP:NE1	2.34	0.42
1:G:121:GLN:HG2	1:G:352:VAL:HB	2.01	0.42
1:G:203:ALA:HB3	1:G:221:ILE:HB	2.01	0.42
1:A:230:GLU:HG3	1:D:560:TYR:CZ	2.55	0.42
1:B:343:SER:OG	1:B:365:THR:HB	2.19	0.42
1:B:386:LYS:NZ	1:B:386:LYS:HB3	2.34	0.42
1:D:113:PRO:HB3	1:D:213:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:VAL:C	1:E:129:GLN:H	2.27	0.42
1:F:179:ASP:CG	1:F:180:PRO:HD2	2.43	0.42
1:F:455:LEU:HB2	8:F:4304:HOH:O	2.19	0.42
1:H:184:PRO:HG3	1:H:356:LEU:HD21	2.01	0.42
1:E:151:ILE:HD13	1:E:251:SER:HB3	2.01	0.42
1:H:484:LEU:HD21	1:H:543:PRO:HB3	2.00	0.42
1:F:282:ARG:NH1	1:F:286:GLY:O	2.44	0.42
1:D:122:TRP:NE1	1:D:349:LYS:HB2	2.34	0.42
1:E:339:THR:CG2	1:E:340:THR:N	2.83	0.42
1:F:399:GLN:NE2	1:F:441:TRP:CH2	2.88	0.42
1:G:259:ASP:OD2	1:G:262:THR:HG22	2.19	0.42
1:C:483:ARG:NH2	8:C:4123:HOH:O	2.51	0.42
1:E:145:HIS:HB3	8:E:4081:HOH:O	2.20	0.42
1:E:395:HIS:CD2	1:E:444:VAL:HG11	2.55	0.42
1:E:458:PRO:HD2	1:G:558:ASN:ND2	2.34	0.42
1:F:187:THR:HB	8:F:4282:HOH:O	2.19	0.42
1:F:288:ILE:HA	8:F:4083:HOH:O	2.19	0.42
1:H:294:GLY:HA2	2:R:805:AR7:HD1	2.01	0.42
1:H:351:ILE:HB	1:H:364:HIS:HB3	2.01	0.42
1:A:261:LYS:HG2	1:A:521:HIS:O	2.19	0.42
1:E:298:ARG:NH2	1:E:298:ARG:CG	2.78	0.42
1:F:293:SER:HA	1:F:309:THR:HG21	2.02	0.42
1:F:342:SER:HA	1:F:351:ILE:HD11	2.01	0.42
1:G:174:ASP:HB2	1:G:181:ASP:O	2.20	0.42
1:G:346:GLN:HG3	8:G:4315:HOH:O	2.19	0.42
1:G:452:VAL:HG13	1:G:568:LEU:HB3	2.01	0.42
1:G:490:ARG:NH1	8:G:4256:HOH:O	2.52	0.42
1:A:243:ASN:HB3	1:A:246:HIS:HB3	2.01	0.42
1:F:142:PHE:CE1	1:F:384:ALA:HA	2.55	0.42
1:B:560:TYR:CE1	1:C:230:GLU:HG3	2.55	0.42
1:D:233:ASP:CG	1:D:267:ALA:HB3	2.45	0.42
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.88	0.42
1:E:113:PRO:HB3	1:E:213:VAL:HG11	2.02	0.42
1:F:446:PRO:HG2	1:F:448:ARG:NH1	2.34	0.42
1:H:282:ARG:NH1	1:H:286:GLY:O	2.47	0.42
1:C:186:TYR:CE2	1:C:356:LEU:HD22	2.55	0.42
1:H:233:ASP:CG	1:H:267:ALA:HB3	2.45	0.42
3:I:4:MAN:H61	3:I:7:NAG:C8	2.50	0.42
1:B:259:ASP:OD2	1:B:262:THR:HG22	2.20	0.41
1:E:142:PHE:CE1	1:E:384:ALA:HA	2.55	0.41
1:E:172:SER:HB3	1:E:182:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:LYS:O	1:G:120:GLN:HB2	2.20	0.41
1:B:483:ARG:HH21	1:B:483:ARG:HB2	1.84	0.41
1:C:243:ASN:HB3	1:C:246:HIS:HB3	2.03	0.41
1:D:403:PRO:O	1:D:406:LEU:HB2	2.21	0.41
1:H:259:ASP:OD2	1:H:262:THR:CG2	2.68	0.41
1:A:455:LEU:O	8:A:4321:HOH:O	2.22	0.41
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.94	0.41
1:F:123:TYR:O	1:F:131:ASP:HB2	2.20	0.41
1:H:243:ASN:HB3	1:H:246:HIS:HB3	2.01	0.41
1:H:566:PHE:CD1	1:H:566:PHE:C	2.98	0.41
1:C:259:ASP:OD2	1:C:262:THR:HG22	2.20	0.41
1:D:160:HIS:CD2	1:D:358:GLN:HA	2.55	0.41
1:E:243:ASN:HB3	1:E:246:HIS:HB3	2.03	0.41
1:E:403:PRO:HB3	1:E:411:TRP:CH2	2.55	0.41
1:H:391:ARG:HD2	1:H:485:GLU:OE2	2.20	0.41
1:B:455:LEU:HB2	1:B:457:GLU:OE2	2.19	0.41
1:D:232:THR:OG1	1:D:235:VAL:HG23	2.20	0.41
1:E:466:GLU:OE1	1:E:468:ARG:NH2	2.41	0.41
1:H:497:ARG:NH2	1:H:523:TYR:HB3	2.36	0.41
1:B:261:LYS:HG2	1:B:521:HIS:O	2.21	0.41
1:C:134:VAL:HA	1:C:431:ALA:HB3	2.03	0.41
1:E:455:LEU:HD23	1:E:455:LEU:O	2.20	0.41
1:F:278:VAL:HG13	1:F:390:TRP:CE2	2.56	0.41
1:H:406:LEU:HD23	1:H:424:TYR:CG	2.55	0.41
1:H:435:VAL:O	1:H:439:GLN:HG3	2.21	0.41
1:C:174:ASP:HB2	1:C:181:ASP:O	2.21	0.41
1:C:395:HIS:CD2	1:C:444:VAL:HG11	2.56	0.41
1:B:560:TYR:CE1	2:L:801:DKA:H102	2.56	0.41
1:D:172:SER:HB3	1:D:182:PRO:HG3	2.02	0.41
1:H:259:ASP:OD2	1:H:262:THR:HG22	2.20	0.41
2:L:804:LYS:HG3	7:L:4009:SO4:O1	2.20	0.41
1:A:118:PHE:N	1:A:119:PRO:CD	2.83	0.41
1:A:492:THR:HB	1:A:565:LYS:HB3	2.03	0.41
1:E:134:VAL:HG12	1:E:138:TRP:CE2	2.56	0.41
1:E:514:THR:HG21	7:E:4062:SO4:O1	2.21	0.41
1:A:403:PRO:HB3	1:A:411:TRP:CH2	2.56	0.40
1:E:203:ALA:HB3	1:E:221:ILE:HB	2.03	0.40
1:F:113:PRO:HB3	1:F:213:VAL:HG11	2.03	0.40
1:H:118:PHE:N	1:H:119:PRO:CD	2.84	0.40
1:H:278:VAL:HG13	1:H:390:TRP:NE1	2.36	0.40
1:A:396:LEU:HD23	1:A:441:TRP:CZ3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PHE:N	1:E:119:PRO:CD	2.85	0.40
1:E:566:PHE:CD1	1:E:566:PHE:C	2.97	0.40
1:B:315:LEU:N	1:B:315:LEU:HD12	2.36	0.40
1:B:435:VAL:O	1:B:439:GLN:HG3	2.21	0.40
1:F:386:LYS:HE3	1:F:386:LYS:HB3	1.75	0.40
1:H:134:VAL:HA	1:H:431:ALA:HB3	2.03	0.40
1:A:151:ILE:HD13	1:A:251:SER:HB3	2.04	0.40
1:C:172:SER:HB3	1:C:182:PRO:HG3	2.03	0.40
1:C:566:PHE:C	1:C:566:PHE:CD1	2.98	0.40
1:D:341:TYR:CE1	1:D:428:LEU:HD21	2.56	0.40
1:H:274:PHE:HB3	1:H:313:TYR:CD1	2.56	0.40
1:C:134:VAL:HG23	1:C:135:LYS:N	2.37	0.40
1:C:233:ASP:CG	1:C:267:ALA:HB3	2.47	0.40
1:D:278:VAL:HG13	1:D:390:TRP:CE2	2.57	0.40
1:F:126:GLY:C	1:F:128:THR:H	2.28	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	468/471 (99%)	450 (96%)	16 (3%)	2 (0%)	30	51
1	B	466/471 (99%)	441 (95%)	22 (5%)	3 (1%)	21	42
1	C	465/471 (99%)	445 (96%)	19 (4%)	1 (0%)	43	66
1	D	465/471 (99%)	448 (96%)	16 (3%)	1 (0%)	43	66
1	E	465/471 (99%)	447 (96%)	17 (4%)	1 (0%)	43	66
1	F	466/471 (99%)	445 (96%)	20 (4%)	1 (0%)	43	66
1	G	465/471 (99%)	452 (97%)	12 (3%)	1 (0%)	43	66
1	H	464/471 (98%)	443 (96%)	19 (4%)	2 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
2	L	2/6 (33%)	2 (100%)	0	0	100	100
2	M	2/6 (33%)	2 (100%)	0	0	100	100
2	N	2/6 (33%)	2 (100%)	0	0	100	100
2	P	2/6 (33%)	2 (100%)	0	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	0	100	100
2	R	2/6 (33%)	2 (100%)	0	0	100	100
All	All	3740/3816 (98%)	3587 (96%)	141 (4%)	12 (0%)	36	58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	VAL
1	E	127	VAL
1	B	575	PRO
1	F	109	VAL
1	C	153	ASP
1	G	153	ASP
1	A	153	ASP
1	A	575	PRO
1	H	153	ASP
1	B	458	PRO
1	D	127	VAL
1	H	127	VAL

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	379/380 (100%)	360 (95%)	19 (5%)	22	46
1	B	378/380 (100%)	360 (95%)	18 (5%)	23	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	377/380 (99%)	365 (97%)	12 (3%)	34	62
1	D	377/380 (99%)	363 (96%)	14 (4%)	30	57
1	E	377/380 (99%)	362 (96%)	15 (4%)	28	55
1	F	378/380 (100%)	365 (97%)	13 (3%)	32	60
1	G	377/380 (99%)	368 (98%)	9 (2%)	43	70
1	H	376/380 (99%)	362 (96%)	14 (4%)	30	57
2	J	3/3 (100%)	3 (100%)	0	100	100
2	K	3/3 (100%)	3 (100%)	0	100	100
2	L	3/3 (100%)	3 (100%)	0	100	100
2	M	3/3 (100%)	3 (100%)	0	100	100
2	N	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	3 (100%)	0	100	100
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
All	All	3043/3064 (99%)	2929 (96%)	114 (4%)	30	57

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	129	GLN
1	A	178	GLN
1	A	262	THR
1	A	268	ARG
1	A	278	VAL
1	A	291	TRP
1	A	303	CYS
1	A	340	THR
1	A	406	LEU
1	A	420	VAL
1	A	435	VAL
1	A	452	VAL
1	A	455	LEU
1	A	459	LYS
1	A	483	ARG
1	A	509	MET
1	A	558	ASN

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Mol	Chain	Res	Type
1	A	578	LEU
1	B	120	GLN
1	B	130	ARG
1	B	178	GLN
1	B	240	LEU
1	B	262	THR
1	B	278	VAL
1	B	291	TRP
1	B	303	CYS
1	B	386	LYS
1	B	406	LEU
1	B	420	VAL
1	B	435	VAL
1	B	452	VAL
1	B	456	VAL
1	B	457	GLU
1	B	483	ARG
1	B	497	ARG
1	B	556	GLU
1	C	262	THR
1	C	268	ARG
1	C	278	VAL
1	C	291	TRP
1	C	303	CYS
1	C	362	GLU
1	C	406	LEU
1	C	420	VAL
1	C	435	VAL
1	C	452	VAL
1	C	455	LEU
1	C	558	ASN
1	D	129	GLN
1	D	135	LYS
1	D	178	GLN
1	D	261	LYS
1	D	262	THR
1	D	278	VAL
1	D	291	TRP
1	D	303	CYS
1	D	406	LEU
1	D	435	VAL
1	D	452	VAL

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Mol	Chain	Res	Type
1	D	465	LEU
1	D	469	LYS
1	D	497	ARG
1	E	120	GLN
1	E	135	LYS
1	E	240	LEU
1	E	262	THR
1	E	278	VAL
1	E	291	TRP
1	E	298	ARG
1	E	303	CYS
1	E	340	THR
1	E	346	GLN
1	E	406	LEU
1	E	435	VAL
1	E	452	VAL
1	E	455	LEU
1	E	497	ARG
1	F	112	GLU
1	F	120	GLN
1	F	178	GLN
1	F	262	THR
1	F	268	ARG
1	F	278	VAL
1	F	291	TRP
1	F	303	CYS
1	F	315	LEU
1	F	406	LEU
1	F	435	VAL
1	F	452	VAL
1	F	456	VAL
1	G	127	VAL
1	G	262	THR
1	G	278	VAL
1	G	291	TRP
1	G	303	CYS
1	G	406	LEU
1	G	435	VAL
1	G	452	VAL
1	G	455	LEU
1	H	111	GLN
1	H	120	GLN

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Mol	Chain	Res	Type
1	H	178	GLN
1	H	240	LEU
1	H	262	THR
1	H	278	VAL
1	H	291	TRP
1	H	303	CYS
1	H	414	ASN
1	H	420	VAL
1	H	435	VAL
1	H	452	VAL
1	H	469	LYS
1	H	565	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	145	HIS
1	A	325	ASN
1	A	399	GLN
1	A	407	ASN
1	A	488	GLN
1	A	529	ASN
1	A	558	ASN
1	B	111	GLN
1	B	358	GLN
1	B	480	HIS
1	B	488	GLN
1	C	120	GLN
1	C	140	GLN
1	C	145	HIS
1	C	190	ASN
1	C	243	ASN
1	C	358	GLN
1	C	440	ASN
1	C	488	GLN
1	D	140	GLN
1	D	178	GLN
1	D	218	ASN
1	D	243	ASN
1	D	325	ASN
1	D	358	GLN

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Mol	Chain	Res	Type
1	D	405	HIS
1	D	488	GLN
1	E	120	GLN
1	E	243	ASN
1	E	325	ASN
1	E	358	GLN
1	E	480	HIS
1	E	488	GLN
1	E	521	HIS
1	F	176	ASN
1	F	243	ASN
1	F	325	ASN
1	F	405	HIS
1	F	407	ASN
1	F	488	GLN
1	F	558	ASN
1	G	133	ASN
1	G	140	GLN
1	G	178	GLN
1	G	245	ASN
1	G	358	GLN
1	G	488	GLN
1	G	521	HIS
1	G	529	ASN
1	G	558	ASN
1	H	178	GLN
1	H	243	ASN
1	H	358	GLN
1	H	414	ASN
1	H	480	HIS
1	H	488	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	AR7	Q	805	2	10,10,11	0.50	0	9,11,13	0.62	0
2	AR7	K	805	2	10,10,11	0.35	0	9,11,13	0.65	0
2	AR7	J	805	2	10,10,11	0.39	0	9,11,13	0.71	0
2	AR7	P	805	2	10,10,11	0.44	0	9,11,13	0.66	0
2	AR7	M	805	2	10,10,11	0.52	0	9,11,13	0.65	0
2	AR7	R	805	2	10,10,11	0.62	0	9,11,13	0.66	0
2	AR7	L	805	2	10,10,11	0.45	0	9,11,13	0.61	0
2	AR7	N	805	2	10,10,11	0.46	0	9,11,13	0.68	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
2	AR7	Q	805	2	-	1/9/9/11	-
2	AR7	K	805	2	-	1/9/9/11	-
2	AR7	J	805	2	-	1/9/9/11	-
2	AR7	P	805	2	-	2/9/9/11	-
2	AR7	M	805	2	-	1/9/9/11	-
2	AR7	R	805	2	-	1/9/9/11	-
2	AR7	L	805	2	-	1/9/9/11	-
2	AR7	N	805	2	-	1/9/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	805	AR7	O-C-CA-N
2	K	805	AR7	O-C-CA-N
2	L	805	AR7	O-C-CA-N
2	M	805	AR7	O-C-CA-N
2	N	805	AR7	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	P	805	AR7	O-C-CA-N
2	Q	805	AR7	O-C-CA-N
2	R	805	AR7	O-C-CA-N
2	P	805	AR7	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	805	AR7	1	0
2	R	805	AR7	1	0

5.5 Carbohydrates

15 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	I	1	1,3	14,14,15	0.57	0	17,19,21	0.89	1 (5%)
3	NAG	I	10	3	14,14,15	0.78	1 (7%)	17,19,21	0.54	0
3	FUL	I	11	3	10,10,11	0.48	0	14,14,16	0.85	0
3	NAG	I	2	3	14,14,15	0.41	0	17,19,21	0.68	1 (5%)
3	BMA	I	3	3	11,11,12	0.37	0	15,15,17	1.27	2 (13%)
3	MAN	I	4	3	11,11,12	0.67	0	15,15,17	0.45	0
3	NAG	I	5	3	14,14,15	0.64	0	17,19,21	0.55	0
3	GAL	I	6	3	11,11,12	0.58	0	15,15,17	0.35	0
3	NAG	I	7	3	14,14,15	0.60	0	17,19,21	0.68	0
3	GAL	I	8	3	11,11,12	0.50	0	15,15,17	0.45	0
3	MAN	I	9	3	11,11,12	0.77	0	15,15,17	0.54	0
4	NAG	O	1	4,1	14,14,15	0.77	0	17,19,21	0.89	1 (5%)
4	NAG	O	2	4	14,14,15	0.76	0	17,19,21	0.88	1 (5%)
4	BMA	O	3	4	11,11,12	0.83	0	15,15,17	0.70	0
4	FUC	O	4	4	10,10,11	0.58	0	14,14,16	0.98	1 (7%)

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	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	10	3	-	5/6/23/26	0/1/1/1
3	FUL	I	11	3	-	-	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	MAN	I	4	3	-	2/2/19/22	0/1/1/1
3	NAG	I	5	3	-	4/6/23/26	0/1/1/1
3	GAL	I	6	3	-	2/2/19/22	0/1/1/1
3	NAG	I	7	3	-	1/6/23/26	0/1/1/1
3	GAL	I	8	3	-	2/2/19/22	0/1/1/1
3	MAN	I	9	3	-	0/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	FUC	O	4	4	1/1/4/5	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	10	NAG	C1-C2	2.18	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	4	FUC	C1-C2-C3	-3.26	104.90	109.64
3	I	3	BMA	C3-C4-C5	3.03	115.72	110.23
3	I	1	NAG	C2-N2-C7	-2.84	119.09	122.90
3	I	3	BMA	C6-C5-C4	-2.82	106.09	113.02
4	O	1	NAG	C4-C3-C2	2.14	114.16	111.02
3	I	2	NAG	C2-N2-C7	-2.09	120.10	122.90
4	O	2	NAG	C2-N2-C7	-2.00	120.21	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	O	4	FUC	C1

All (30) torsion outliers are listed below:

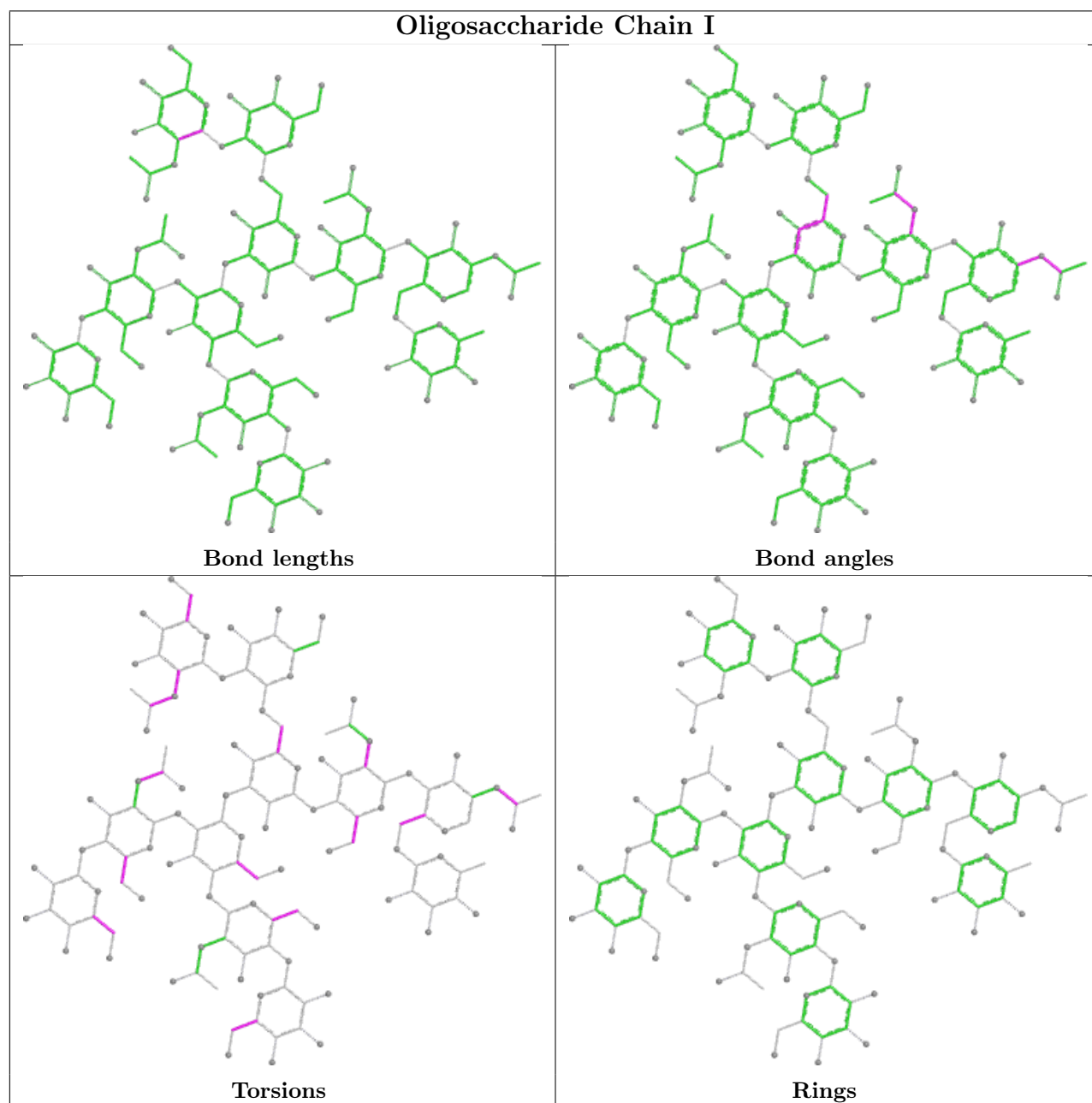
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	10	NAG	C1-C2-N2-C7
3	I	10	NAG	C8-C7-N2-C2
3	I	10	NAG	O7-C7-N2-C2
4	O	3	BMA	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	4	MAN	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
3	I	6	GAL	O5-C5-C6-O6
3	I	8	GAL	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
3	I	6	GAL	C4-C5-C6-O6
3	I	8	GAL	C4-C5-C6-O6
3	I	4	MAN	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	10	NAG	C4-C5-C6-O6
3	I	5	NAG	C8-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
3	I	10	NAG	O5-C5-C6-O6
3	I	5	NAG	O7-C7-N2-C2
3	I	5	NAG	C4-C5-C6-O6
3	I	5	NAG	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
3	I	7	NAG	C4-C5-C6-O6

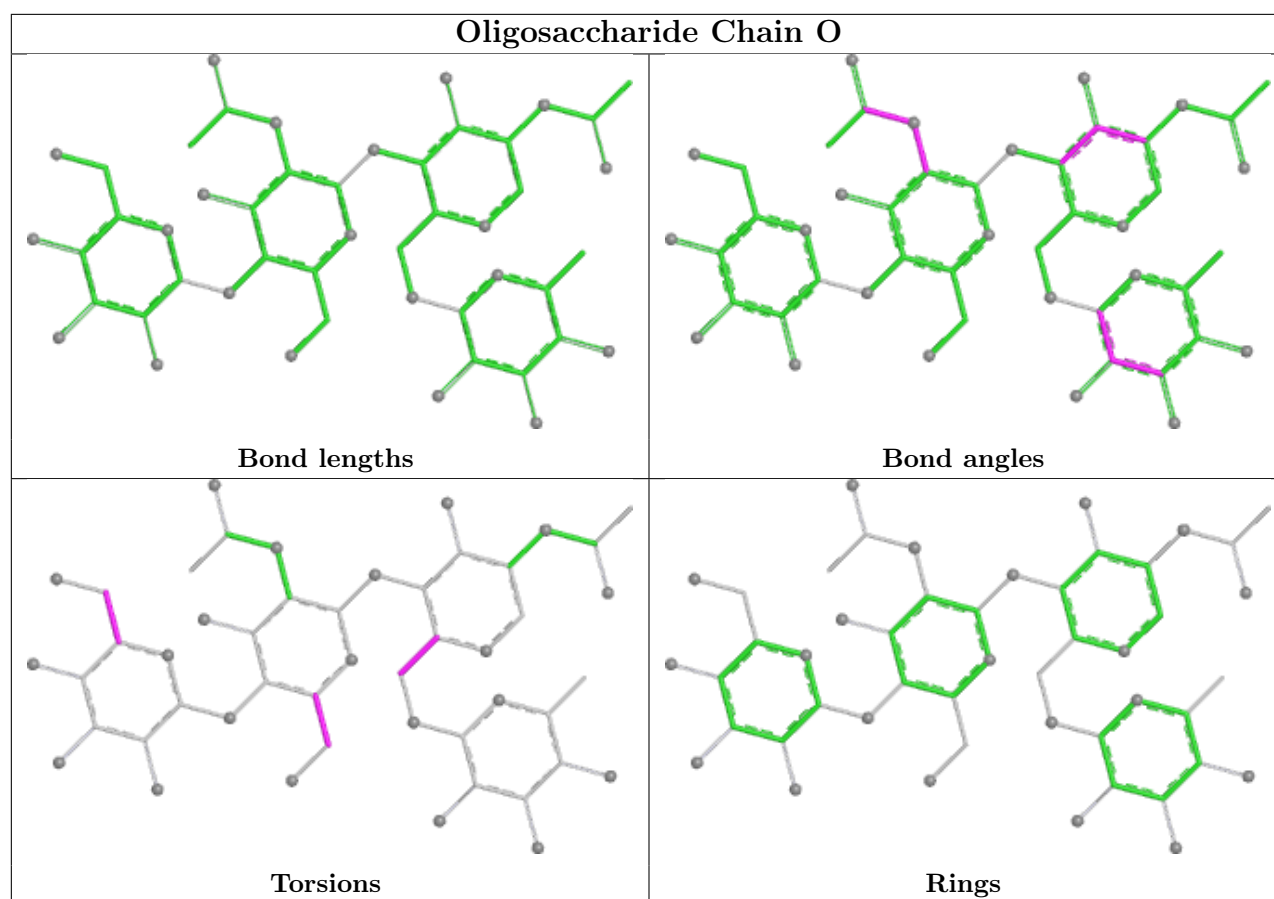
There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	4	MAN	2	0
3	I	2	NAG	1	0
4	O	3	BMA	3	0
3	I	7	NAG	2	0
4	O	2	NAG	3	0
3	I	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](#)

Of 92 ligands modelled in this entry, 16 are monoatomic - leaving 76 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	$\# Z > 2$
7	SO4	F	4036	-	4,4,4	0.39	0	6,6,6	0.09	0
7	SO4	B	4050	-	4,4,4	0.36	0	6,6,6	0.08	0
7	SO4	G	4032	-	4,4,4	0.42	0	6,6,6	0.11	0
7	SO4	B	4026	-	4,4,4	0.36	0	6,6,6	0.20	0
7	SO4	A	4054	-	4,4,4	0.39	0	6,6,6	0.12	0
7	SO4	H	4048	-	4,4,4	0.38	0	6,6,6	0.13	0
7	SO4	A	4064	-	4,4,4	0.38	0	6,6,6	0.13	0
7	SO4	C	4008	-	4,4,4	0.37	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	C	4013	-	4,4,4	0.44	0	6,6,6	0.16	0
7	SO4	A	4014	-	4,4,4	0.40	0	6,6,6	0.17	0
7	SO4	C	4059	-	4,4,4	0.43	0	6,6,6	0.17	0
7	SO4	D	4065	-	4,4,4	0.40	0	6,6,6	0.10	0
7	SO4	E	4040	-	4,4,4	0.40	0	6,6,6	0.15	0
7	SO4	E	4046	-	4,4,4	0.38	0	6,6,6	0.15	0
7	SO4	F	4003	-	4,4,4	0.42	0	6,6,6	0.24	0
7	SO4	A	4066	-	4,4,4	0.40	0	6,6,6	0.11	0
7	SO4	E	4037	-	4,4,4	0.40	0	6,6,6	0.07	0
7	SO4	F	4002	-	4,4,4	0.39	0	6,6,6	0.13	0
5	NAG	F	951	1	14,14,15	0.67	0	17,19,21	0.77	0
7	SO4	A	4025	-	4,4,4	0.36	0	6,6,6	0.11	0
7	SO4	Q	4033	-	4,4,4	0.35	0	6,6,6	0.17	0
5	NAG	E	901	1	14,14,15	0.69	0	17,19,21	0.82	1 (5%)
7	SO4	R	4053	-	4,4,4	0.40	0	6,6,6	0.06	0
7	SO4	B	4023	-	4,4,4	0.39	0	6,6,6	0.19	0
7	SO4	D	4011	-	4,4,4	0.42	0	6,6,6	0.06	0
7	SO4	C	4007	-	4,4,4	0.37	0	6,6,6	0.05	0
7	SO4	F	4068	-	4,4,4	0.37	0	6,6,6	0.11	0
7	SO4	B	4021	-	4,4,4	0.39	0	6,6,6	0.12	0
7	SO4	D	4018	-	4,4,4	0.37	0	6,6,6	0.21	0
7	SO4	G	4035	-	4,4,4	0.41	0	6,6,6	0.21	0
7	SO4	A	4061	-	4,4,4	0.38	0	6,6,6	0.18	0
7	SO4	B	4027	-	4,4,4	0.41	0	6,6,6	0.33	0
7	SO4	A	4069	-	4,4,4	0.41	0	6,6,6	0.34	0
7	SO4	A	4004	-	4,4,4	0.36	0	6,6,6	0.16	0
7	SO4	D	4016	-	4,4,4	0.45	0	6,6,6	0.13	0
7	SO4	F	4067	-	4,4,4	0.41	0	6,6,6	0.07	0
7	SO4	A	4005	-	4,4,4	0.41	0	6,6,6	0.07	0
7	SO4	F	4070	-	4,4,4	0.44	0	6,6,6	0.34	0
7	SO4	H	4047	-	4,4,4	0.39	0	6,6,6	0.08	0
7	SO4	E	4041	-	4,4,4	0.42	0	6,6,6	0.12	0
7	SO4	E	4060	-	4,4,4	0.38	0	6,6,6	0.18	0
7	SO4	J	4001	-	4,4,4	0.38	0	6,6,6	0.13	0
7	SO4	L	4009	-	4,4,4	0.40	0	6,6,6	0.16	0
5	NAG	A	901	1	14,14,15	0.75	0	17,19,21	0.71	1 (5%)
7	SO4	M	4017	-	4,4,4	0.41	0	6,6,6	0.12	0
7	SO4	C	4058	-	4,4,4	0.40	0	6,6,6	0.12	0
7	SO4	E	4038	-	4,4,4	0.35	0	6,6,6	0.08	0
7	SO4	H	4044	-	4,4,4	0.40	0	6,6,6	0.08	0
7	SO4	K	4024	-	4,4,4	0.41	0	6,6,6	0.13	0
7	SO4	F	4051	-	4,4,4	0.37	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	N	4006	-	4,4,4	0.39	0	6,6,6	0.18	0
7	SO4	E	4062	-	4,4,4	0.42	0	6,6,6	0.10	0
7	SO4	F	4056	-	4,4,4	0.39	0	6,6,6	0.09	0
5	NAG	H	901	1	14,14,15	0.68	0	17,19,21	0.96	1 (5%)
7	SO4	E	4039	-	4,4,4	0.41	0	6,6,6	0.06	0
7	SO4	A	4028	-	4,4,4	0.39	0	6,6,6	0.08	0
7	SO4	E	4049	-	4,4,4	0.40	0	6,6,6	0.06	0
7	SO4	F	4057	-	4,4,4	0.40	0	6,6,6	0.13	0
7	SO4	D	4012	-	4,4,4	0.40	0	6,6,6	0.24	0
7	SO4	B	4022	-	4,4,4	0.37	0	6,6,6	0.24	0
7	SO4	D	4015	-	4,4,4	0.40	0	6,6,6	0.10	0
7	SO4	H	4045	-	4,4,4	0.39	0	6,6,6	0.17	0
7	SO4	D	4019	-	4,4,4	0.42	0	6,6,6	0.12	0
7	SO4	G	4030	-	4,4,4	0.37	0	6,6,6	0.16	0
7	SO4	G	4034	-	4,4,4	0.43	0	6,6,6	0.09	0
5	NAG	F	901	1	14,14,15	0.61	0	17,19,21	0.70	1 (5%)
7	SO4	H	4042	-	4,4,4	0.41	0	6,6,6	0.07	0
7	SO4	C	4010	-	4,4,4	0.42	0	6,6,6	0.08	0
7	SO4	D	4020	-	4,4,4	0.41	0	6,6,6	0.12	0
5	NAG	B	901	1	14,14,15	0.67	0	17,19,21	0.73	1 (5%)
7	SO4	A	4055	-	4,4,4	0.43	0	6,6,6	0.06	0
7	SO4	G	4031	-	4,4,4	0.41	0	6,6,6	0.10	0
7	SO4	D	4063	-	4,4,4	0.39	0	6,6,6	0.11	0
7	SO4	G	4029	-	4,4,4	0.37	0	6,6,6	0.24	0
7	SO4	P	4052	-	4,4,4	0.40	0	6,6,6	0.09	0
7	SO4	H	4043	-	4,4,4	0.39	0	6,6,6	0.09	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	F	901	1	-	4/6/23/26	0/1/1/1
5	NAG	H	901	1	-	2/6/23/26	0/1/1/1
5	NAG	B	901	1	-	1/6/23/26	0/1/1/1
5	NAG	A	901	1	-	4/6/23/26	0/1/1/1
5	NAG	F	951	1	-	4/6/23/26	0/1/1/1
5	NAG	E	901	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	901	NAG	C2-N2-C7	-2.65	119.35	122.90
5	A	901	NAG	C2-N2-C7	-2.26	119.87	122.90
5	B	901	NAG	C2-N2-C7	-2.20	119.95	122.90
5	E	901	NAG	C2-N2-C7	-2.14	120.03	122.90
5	F	901	NAG	C2-N2-C7	-2.05	120.16	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	901	NAG	C8-C7-N2-C2
5	E	901	NAG	O7-C7-N2-C2
5	F	901	NAG	C8-C7-N2-C2
5	F	901	NAG	O7-C7-N2-C2
5	F	951	NAG	C8-C7-N2-C2
5	F	951	NAG	O7-C7-N2-C2
5	F	901	NAG	C4-C5-C6-O6
5	H	901	NAG	C4-C5-C6-O6
5	F	901	NAG	O5-C5-C6-O6
5	F	951	NAG	C4-C5-C6-O6
5	F	951	NAG	O5-C5-C6-O6
5	H	901	NAG	O5-C5-C6-O6
5	A	901	NAG	C4-C5-C6-O6
5	A	901	NAG	O5-C5-C6-O6
5	A	901	NAG	C8-C7-N2-C2
5	A	901	NAG	O7-C7-N2-C2
5	B	901	NAG	C1-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	951	NAG	1	0
7	B	4027	SO4	1	0
7	A	4069	SO4	1	0
7	F	4070	SO4	1	0
7	E	4060	SO4	1	0
7	L	4009	SO4	1	0
7	E	4062	SO4	1	0
7	D	4012	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	NAG	1	0
7	G	4029	SO4	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	470/471 (99%)	-0.45	2 (0%) 88 86	8, 18, 29, 52	17 (3%)
1	B	468/471 (99%)	-0.42	6 (1%) 75 71	8, 18, 32, 47	13 (2%)
1	C	467/471 (99%)	-0.46	1 (0%) 91 90	8, 18, 31, 49	22 (4%)
1	D	467/471 (99%)	-0.27	4 (0%) 81 78	9, 21, 36, 56	20 (4%)
1	E	467/471 (99%)	-0.44	5 (1%) 78 74	7, 19, 32, 52	18 (3%)
1	F	468/471 (99%)	-0.47	2 (0%) 88 86	7, 18, 30, 44	15 (3%)
1	G	467/471 (99%)	-0.50	0 100 100	8, 17, 27, 42	17 (3%)
1	H	466/471 (98%)	-0.35	2 (0%) 88 86	6, 20, 35, 54	19 (4%)
2	J	3/6 (50%)	-0.79	0 100 100	11, 11, 15, 17	0
2	K	3/6 (50%)	-0.65	0 100 100	14, 14, 18, 18	0
2	L	3/6 (50%)	-1.00	0 100 100	12, 12, 16, 17	0
2	M	3/6 (50%)	-0.43	0 100 100	15, 15, 19, 20	0
2	N	3/6 (50%)	-1.24	0 100 100	11, 11, 14, 16	0
2	P	3/6 (50%)	-0.82	0 100 100	11, 11, 16, 19	0
2	Q	3/6 (50%)	-0.91	0 100 100	11, 11, 18, 18	0
2	R	3/6 (50%)	-0.55	0 100 100	14, 14, 19, 20	0
All	All	3764/3816 (98%)	-0.42	22 (0%) 85 83	6, 18, 32, 56	141 (3%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	VAL	4.4
1	H	575	PRO	3.4
1	B	109	VAL	3.3
1	E	128	THR	3.2
1	D	127	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	575	PRO	3.0
1	D	129	GLN	3.0
1	E	575	PRO	2.8
1	B	576	GLU	2.7
1	B	456	VAL	2.7
1	A	576	GLU	2.6
1	F	108	ASP	2.5
1	E	109	VAL	2.4
1	E	456	VAL	2.3
1	B	575	PRO	2.2
1	C	127	VAL	2.2
1	B	128	THR	2.2
1	D	128	THR	2.2
1	H	128	THR	2.1
1	D	575	PRO	2.1
1	F	230	GLU	2.1
1	E	126	GLY	2.1

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

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	AR7	M	805	11/12	0.95	0.08	15,16,17,18	0
2	AR7	K	805	11/12	0.96	0.08	9,12,16,16	0
2	AR7	P	805	11/12	0.96	0.07	11,14,16,17	0
2	AR7	R	805	11/12	0.96	0.08	15,15,17,18	0
2	AR7	N	805	11/12	0.97	0.06	9,11,15,16	0
2	AR7	J	805	11/12	0.98	0.06	13,14,15,16	0
2	AR7	Q	805	11/12	0.98	0.06	13,13,15,15	0
2	AR7	L	805	11/12	0.98	0.06	13,14,15,15	0

6.3 Carbohydrates ⓘ

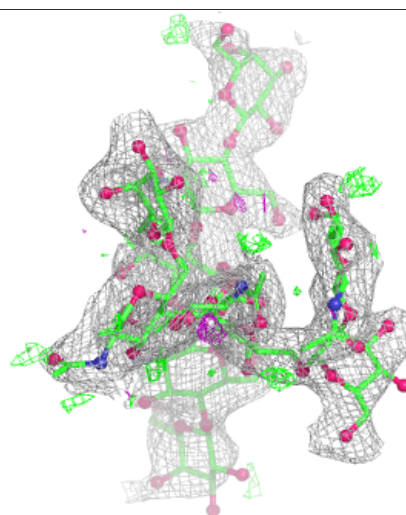
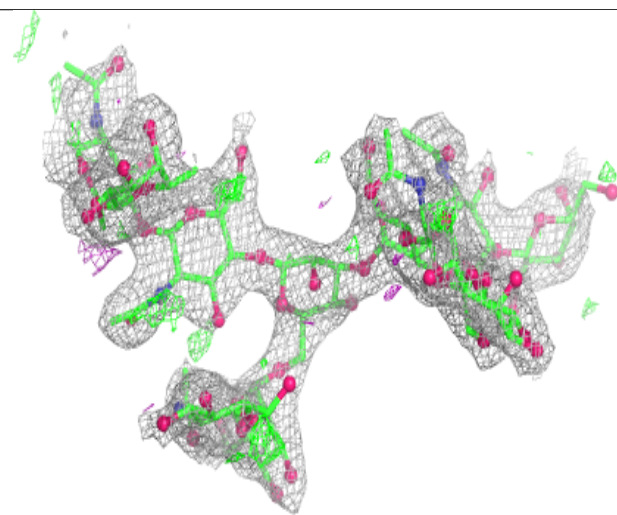
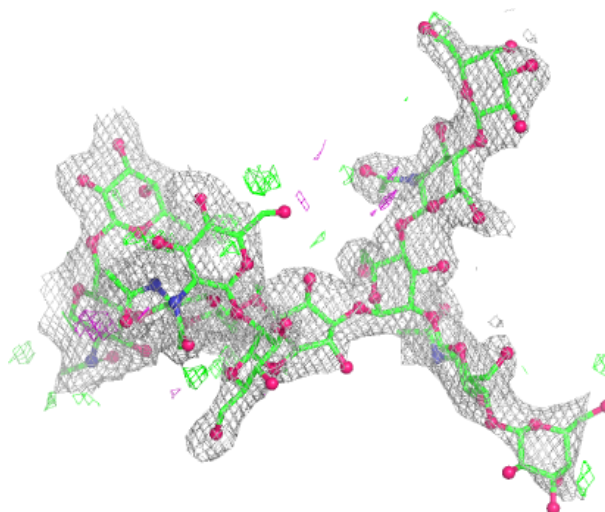
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

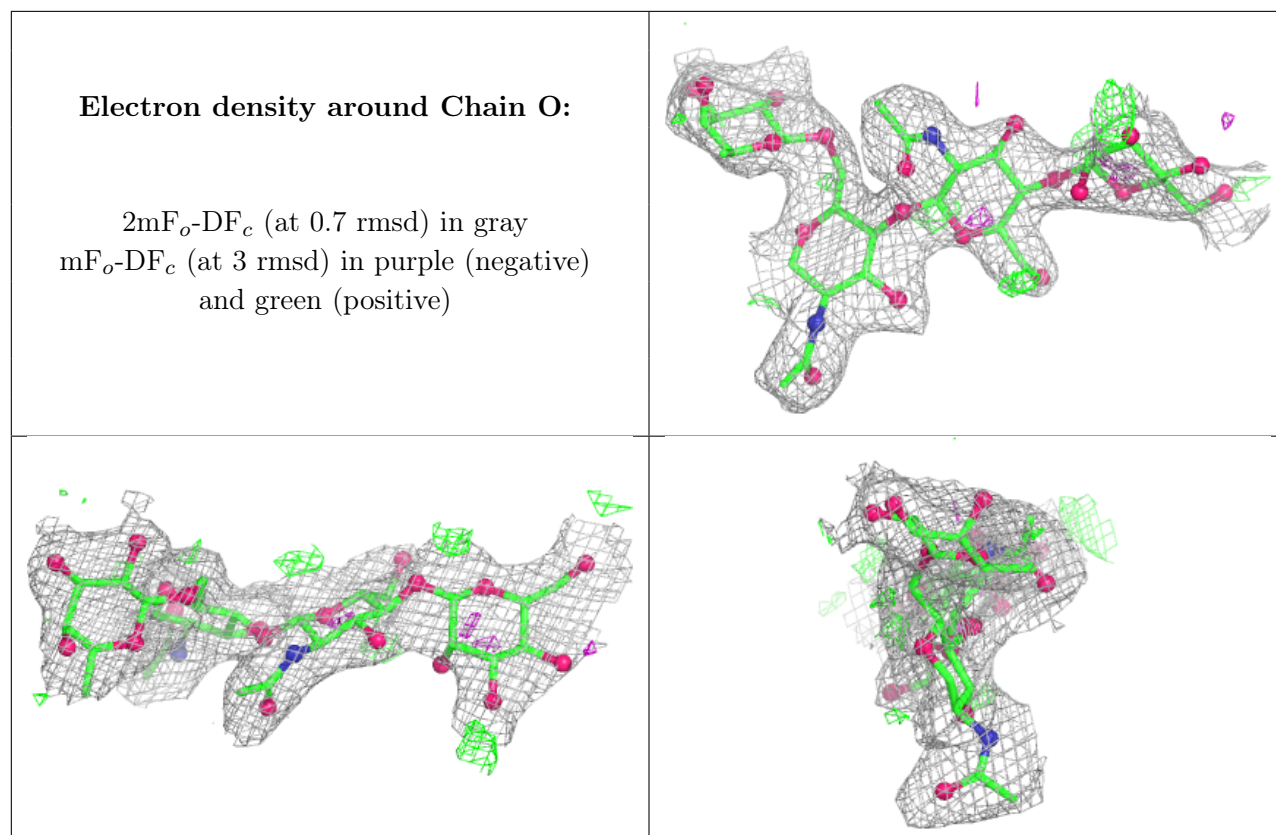
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	I	1	14/15	-	-	33,35,44,44	0
3	NAG	I	2	14/15	-	-	41,43,46,49	0
3	BMA	I	3	11/12	-	-	51,53,57,58	0
3	MAN	I	4	11/12	-	-	51,52,54,56	0
3	NAG	I	5	14/15	-	-	57,59,61,63	0
3	GAL	I	6	11/12	-	-	64,64,65,65	3
3	NAG	I	7	14/15	-	-	44,51,53,56	0
3	GAL	I	8	11/12	-	-	59,60,61,62	0
3	MAN	I	9	11/12	-	-	59,62,63,63	0
3	NAG	I	10	14/15	-	-	62,64,64,65	1
3	FUL	I	11	10/11	-	-	25,28,29,30	0
4	NAG	O	1	14/15	-	-	30,32,37,39	0
4	NAG	O	2	14/15	-	-	39,46,48,51	0
4	BMA	O	3	11/12	-	-	54,56,57,57	0
4	FUC	O	4	10/11	-	-	38,39,40,41	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($\text{\AA}^2$)	Q<0.9
5	NAG	E	901	14/15	0.47	0.16	52,55,58,59	3
5	NAG	H	901	14/15	0.48	0.17	58,64,66,66	0
5	NAG	F	901	14/15	0.56	0.18	54,59,61,62	0
5	NAG	B	901	14/15	0.59	0.16	53,58,60,60	0
7	SO4	D	4016	5/5	0.63	0.19	90,90,90,91	0
5	NAG	F	951	14/15	0.65	0.14	55,58,59,59	0
5	NAG	A	901	14/15	0.70	0.14	45,50,52,52	0
7	SO4	F	4056	5/5	0.70	0.16	100,100,100,100	0
7	SO4	D	4065	5/5	0.72	0.19	86,86,87,87	0
7	SO4	E	4062	5/5	0.74	0.24	89,90,90,90	0
7	SO4	D	4020	5/5	0.74	0.17	82,82,83,83	0
7	SO4	F	4057	5/5	0.76	0.23	89,90,90,91	0
7	SO4	A	4064	5/5	0.79	0.14	91,91,91,92	0
7	SO4	A	4054	5/5	0.80	0.17	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	C	4010	5/5	0.80	0.23	89,89,90,90	0
7	SO4	B	4027	5/5	0.81	0.23	62,63,64,65	0
7	SO4	D	4019	5/5	0.81	0.11	76,77,78,78	0
7	SO4	E	4060	5/5	0.81	0.23	72,72,74,74	0
7	SO4	F	4070	5/5	0.81	0.22	61,61,63,63	0
7	SO4	C	4013	5/5	0.82	0.22	63,63,65,66	0
7	SO4	F	4067	5/5	0.83	0.18	95,95,96,96	0
7	SO4	A	4066	5/5	0.84	0.19	94,94,95,95	0
7	SO4	E	4040	5/5	0.84	0.15	85,85,86,86	0
7	SO4	A	4055	5/5	0.84	0.18	72,72,73,73	0
7	SO4	D	4012	5/5	0.84	0.21	73,74,75,75	0
7	SO4	G	4034	5/5	0.84	0.14	77,77,78,78	0
7	SO4	B	4021	5/5	0.85	0.12	85,85,86,86	0
7	SO4	A	4005	5/5	0.85	0.13	84,84,85,85	0
7	SO4	D	4063	5/5	0.85	0.19	91,91,91,91	0
7	SO4	H	4047	5/5	0.85	0.17	87,87,88,88	0
7	SO4	E	4049	5/5	0.86	0.15	77,78,78,78	0
7	SO4	A	4069	5/5	0.86	0.20	65,65,67,67	0
7	SO4	A	4061	5/5	0.86	0.15	64,65,65,65	0
7	SO4	H	4048	5/5	0.86	0.14	90,90,90,90	0
7	SO4	B	4050	5/5	0.87	0.17	71,71,72,72	0
7	SO4	C	4059	5/5	0.87	0.14	64,64,65,66	0
7	SO4	G	4031	5/5	0.87	0.12	74,74,75,75	0
7	SO4	E	4039	5/5	0.88	0.15	83,83,84,84	0
7	SO4	B	4023	5/5	0.88	0.12	63,64,64,64	0
7	SO4	G	4035	5/5	0.88	0.15	58,58,59,59	0
7	SO4	A	4028	5/5	0.88	0.15	66,66,67,67	0
7	SO4	G	4030	5/5	0.88	0.15	53,54,55,56	0
7	SO4	M	4017	5/5	0.88	0.14	82,82,83,83	0
7	SO4	R	4053	5/5	0.88	0.16	81,81,81,82	0
7	SO4	C	4007	5/5	0.89	0.10	72,72,73,73	0
7	SO4	H	4045	5/5	0.89	0.13	71,71,72,72	0
7	SO4	E	4041	5/5	0.89	0.15	63,63,64,64	0
7	SO4	F	4002	5/5	0.90	0.12	61,62,62,63	0
7	SO4	F	4068	5/5	0.90	0.17	75,76,77,77	0
7	SO4	C	4058	5/5	0.90	0.13	80,80,81,81	0
7	SO4	C	4008	5/5	0.90	0.13	58,58,58,59	0
7	SO4	H	4044	5/5	0.91	0.12	71,72,72,72	0
7	SO4	P	4052	5/5	0.91	0.12	66,66,66,66	0
7	SO4	H	4042	5/5	0.91	0.14	58,59,60,60	0
7	SO4	F	4051	5/5	0.92	0.12	76,76,77,77	0
7	SO4	D	4011	5/5	0.92	0.15	67,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	E	4046	5/5	0.92	0.12	63,63,64,64	0
7	SO4	G	4029	5/5	0.92	0.14	67,68,68,68	0
7	SO4	B	4026	5/5	0.93	0.10	52,52,53,54	0
7	SO4	E	4037	5/5	0.93	0.09	58,59,60,60	0
7	SO4	K	4024	5/5	0.93	0.12	61,61,62,62	0
7	SO4	A	4014	5/5	0.94	0.18	82,82,82,82	0
7	SO4	G	4032	5/5	0.95	0.12	48,48,50,50	0
7	SO4	Q	4033	5/5	0.95	0.11	46,47,47,48	0
7	SO4	F	4003	5/5	0.95	0.08	40,41,42,42	0
7	SO4	B	4022	5/5	0.96	0.08	45,47,48,48	0
7	SO4	A	4004	5/5	0.96	0.11	49,49,49,49	0
7	SO4	D	4018	5/5	0.96	0.10	61,61,62,62	0
7	SO4	J	4001	5/5	0.97	0.11	41,42,43,44	0
7	SO4	H	4043	5/5	0.97	0.08	55,55,56,56	0
6	CA	D	3007	1/1	0.97	0.06	29,29,29,29	0
7	SO4	E	4038	5/5	0.97	0.08	51,51,52,52	0
7	SO4	F	4036	5/5	0.97	0.07	47,47,47,47	0
7	SO4	D	4015	5/5	0.97	0.07	41,42,43,43	0
7	SO4	A	4025	5/5	0.98	0.07	41,41,42,43	0
7	SO4	L	4009	5/5	0.98	0.06	33,33,34,34	0
6	CA	H	3016	1/1	0.98	0.04	16,16,16,16	0
7	SO4	N	4006	5/5	0.98	0.06	36,36,38,38	0
6	CA	B	3003	1/1	0.98	0.02	18,18,18,18	0
6	CA	D	3008	1/1	0.98	0.03	16,16,16,16	0
6	CA	G	3014	1/1	0.98	0.03	16,16,16,16	0
6	CA	A	3001	1/1	0.99	0.03	17,17,17,17	0
6	CA	B	3004	1/1	0.99	0.05	11,11,11,11	0
6	CA	E	3009	1/1	0.99	0.01	21,21,21,21	0
6	CA	E	3010	1/1	0.99	0.01	9,9,9,9	0
6	CA	F	3011	1/1	0.99	0.03	19,19,19,19	0
6	CA	F	3012	1/1	0.99	0.04	12,12,12,12	0
6	CA	G	3013	1/1	0.99	0.02	19,19,19,19	0
6	CA	C	3005	1/1	0.99	0.01	21,21,21,21	0
6	CA	H	3015	1/1	0.99	0.03	35,35,35,35	0
6	CA	C	3006	1/1	0.99	0.03	10,10,10,10	0
6	CA	A	3002	1/1	1.00	0.05	7,7,7,7	0

6.5 Other polymers

There are no such residues in this entry.