



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:00 AM UTC

PDB ID : 5EJB / pdb_00005ejb
Title : Crystal structure of prefusion Hendra virus F protein
Authors : Wong, J.W.; Jardetzky, T.S.; Paterson, R.G.; Lamb, R.A.
Deposited on : 2015-11-01
Resolution : 3.20 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

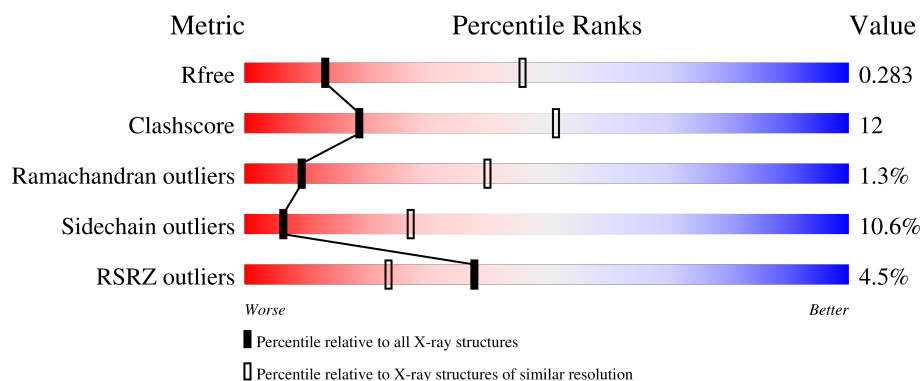
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



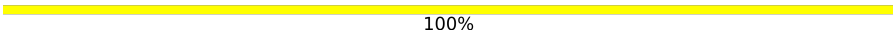
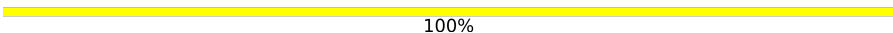
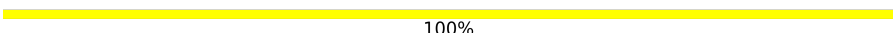
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	501	4% 60% 25% 12%
1	B	501	3% 60% 25% 11%
1	C	501	4% 62% 25% 9%
1	D	501	3% 62% 25% 8%
1	E	501	4% 60% 24% 13%

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Mol	Chain	Length	Quality of chain
1	F	501	 5% 58% 26% 13%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20415 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	447	Total	C	N	O	S	0	0	0
			3376	2135	553	670	18			
1	C	454	Total	C	N	O	S	0	0	0
			3390	2142	558	672	18			
1	D	460	Total	C	N	O	S	0	0	0
			3441	2174	566	683	18			
1	F	436	Total	C	N	O	S	0	0	0
			3298	2086	540	654	18			
1	E	436	Total	C	N	O	S	0	0	0
			3298	2086	540	654	18			
1	A	440	Total	C	N	O	S	0	0	0
			3330	2107	545	660	18			

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

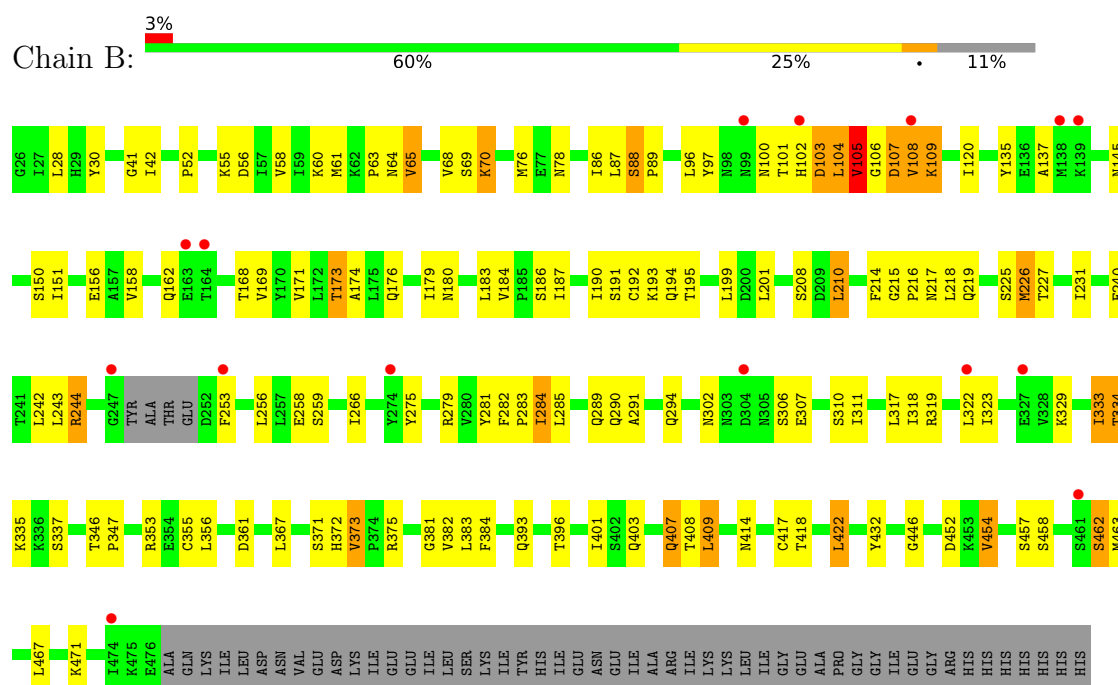


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1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

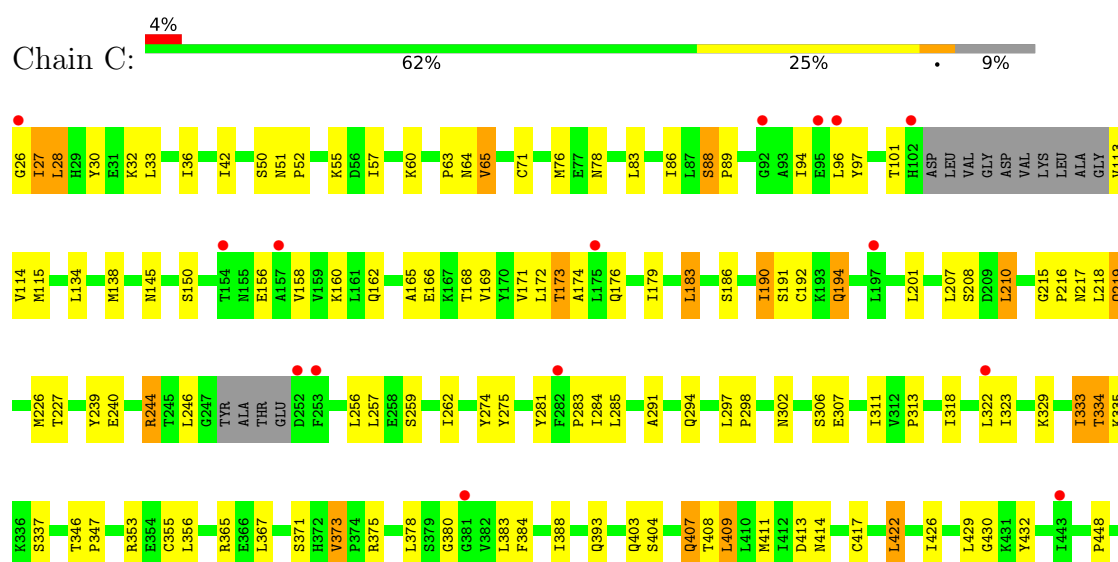
3 Residue-property plots [i](#)

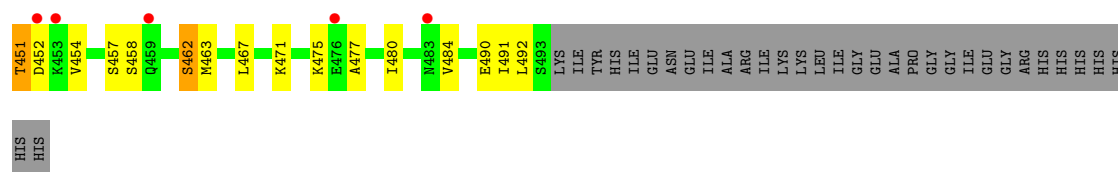
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Fusion glycoprotein F0

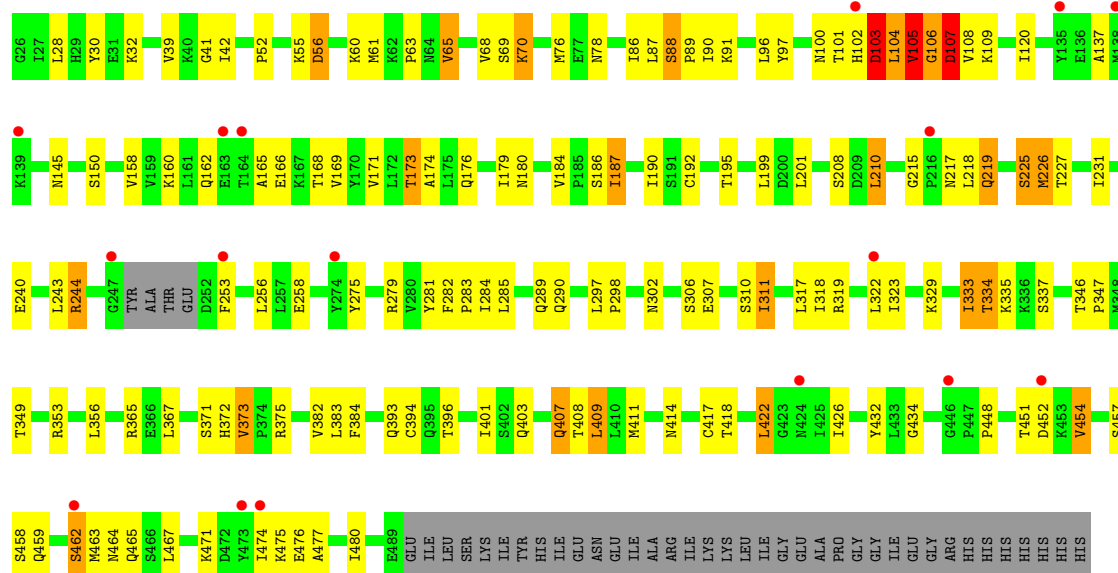


• Molecule 1: Fusion glycoprotein F0

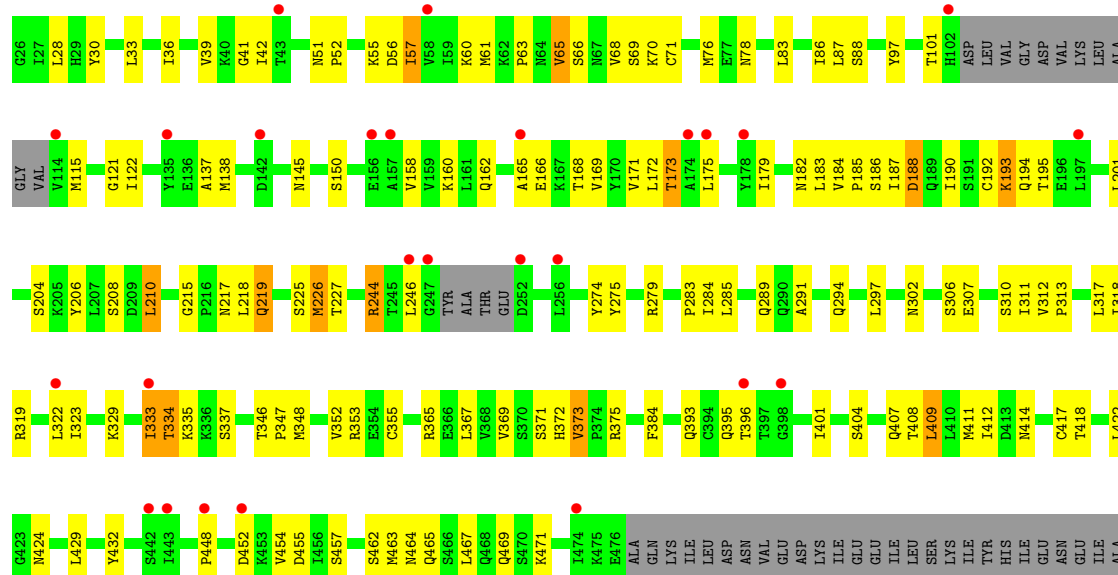


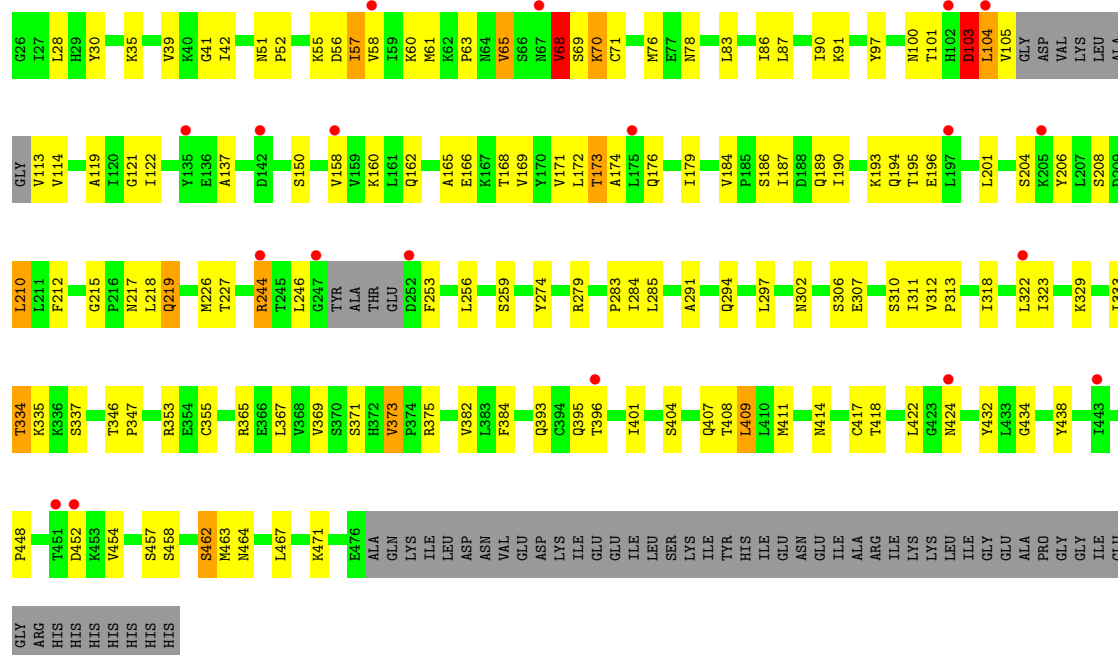


• Molecule 1: Fusion glycoprotein F0



• Molecule 1: Fusion glycoprotein F0





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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

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

Chain I:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.61Å 163.50Å 147.94Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	49.62 – 3.20 49.62 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.62-3.20) 99.6 (49.62-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.253 , 0.283 0.253 , 0.283	Depositor DCC
R_{free} test set	4233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 93.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20415	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	0/3375	1.07	9/4593 (0.2%)
1	B	0.82	0/3422	1.12	13/4657 (0.3%)
1	C	0.74	0/3435	1.07	10/4677 (0.2%)
1	D	0.81	1/3487 (0.0%)	1.13	13/4748 (0.3%)
1	E	0.72	0/3343	1.05	5/4548 (0.1%)
1	F	0.74	0/3343	1.05	7/4548 (0.2%)
All	All	0.77	1/20405 (0.0%)	1.08	57/27771 (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
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	225	SER	CA-C	-5.12	1.47	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ASP	N-CA-C	7.53	119.41	108.34
1	D	41	GLY	N-CA-C	-7.15	102.38	112.60
1	D	373	VAL	CA-C-N	6.78	126.77	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	373	VAL	C-N-CA	6.78	126.77	119.78
1	B	373	VAL	CA-C-N	6.66	126.64	119.78
1	B	373	VAL	C-N-CA	6.66	126.64	119.78
1	A	373	VAL	CA-C-N	6.39	126.37	119.78
1	A	373	VAL	C-N-CA	6.39	126.37	119.78
1	C	388	ILE	N-CA-C	-6.17	105.71	111.45
1	F	373	VAL	CA-C-N	6.07	126.03	119.78
1	F	373	VAL	C-N-CA	6.07	126.03	119.78
1	F	393	GLN	N-CA-C	5.95	118.22	109.24
1	D	70	LYS	N-CA-C	-5.92	104.81	112.68
1	D	107	ASP	N-CA-C	5.90	123.36	110.80
1	B	381	GLY	N-CA-C	-5.89	107.19	115.32
1	D	103	ASP	N-CA-CB	-5.84	106.16	111.59
1	F	373	VAL	N-CA-CB	5.80	116.61	110.17
1	C	259	SER	N-CA-C	-5.75	105.60	113.30
1	C	64	ASN	N-CA-C	5.74	117.40	111.03
1	C	114	VAL	N-CA-C	5.66	116.89	108.23
1	B	108	VAL	N-CA-C	5.64	117.30	109.80
1	B	373	VAL	N-CA-C	-5.61	102.79	108.96
1	D	282	PHE	CB-CA-C	5.61	115.49	110.44
1	A	393	GLN	N-CA-C	5.60	117.69	109.24
1	F	138	MET	N-CA-C	5.51	117.72	111.11
1	D	56	ASP	N-CA-C	5.49	118.44	109.59
1	E	388	ILE	N-CA-C	-5.48	106.35	111.45
1	B	56	ASP	N-CA-C	5.43	118.33	109.59
1	C	138	MET	N-CA-C	5.42	117.62	111.11
1	C	451	THR	CA-C-N	5.41	128.52	120.95
1	C	451	THR	C-N-CA	5.41	128.52	120.95
1	A	253	PHE	N-CA-CB	-5.41	101.25	110.33
1	D	373	VAL	N-CA-C	-5.37	103.05	108.96
1	B	107	ASP	N-CA-C	5.33	122.16	110.80
1	B	183	LEU	N-CA-C	5.29	116.90	111.03
1	A	373	VAL	N-CA-CB	5.27	116.02	110.17
1	B	259	SER	N-CA-C	-5.26	106.10	112.88
1	C	393	GLN	N-CA-C	5.25	117.18	109.24
1	A	253	PHE	N-CA-C	-5.20	105.76	112.68
1	A	259	SER	N-CA-C	-5.20	106.34	113.30
1	C	373	VAL	CA-C-N	5.19	125.13	119.78
1	C	373	VAL	C-N-CA	5.19	125.13	119.78
1	E	393	GLN	N-CA-C	5.18	117.06	109.24
1	A	57	ILE	N-CA-C	5.16	115.80	108.42
1	B	41	GLY	N-CA-C	-5.15	105.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	57	ILE	N-CA-C	5.09	115.70	108.42
1	E	138	MET	N-CA-C	5.09	117.22	111.11
1	E	259	SER	N-CA-C	-5.09	106.48	113.30
1	E	373	VAL	N-CA-CB	5.08	115.81	110.17
1	D	393	GLN	N-CA-C	5.08	116.91	109.24
1	B	282	PHE	CB-CA-C	5.08	115.01	110.44
1	B	216	PRO	CA-C-N	5.07	127.04	120.44
1	B	216	PRO	C-N-CA	5.07	127.04	120.44
1	D	451	THR	CA-C-N	5.07	128.07	120.87
1	D	451	THR	C-N-CA	5.07	128.07	120.87
1	A	41	GLY	N-CA-C	-5.04	105.39	112.60
1	F	41	GLY	N-CA-C	-5.01	105.43	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Peptide
1	B	102	HIS	Peptide
1	D	102	HIS	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	3330	0	3324	94	0
1	B	3376	0	3377	94	1
1	C	3390	0	3336	80	0
1	D	3441	0	3403	95	0
1	E	3298	0	3288	81	0
1	F	3298	0	3290	88	1
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	28	0	26	0	0
4	C	14	0	13	0	0
4	D	42	0	39	2	0
4	E	56	0	52	1	0
4	F	28	0	26	2	0
All	All	20415	0	20249	481	1

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 (481) 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:F:318:ILE:HG12	1:F:323:ILE:HG22	1.49	0.92
1:E:318:ILE:HG12	1:E:323:ILE:HG22	1.52	0.91
1:C:65:VAL:HG21	1:C:76:MET:CE	2.00	0.91
1:D:307:GLU:HG3	1:D:375:ARG:HH21	1.36	0.91
1:E:65:VAL:HG21	1:E:76:MET:CE	2.01	0.91
1:F:184:VAL:O	1:F:187:ILE:HG12	1.70	0.91
1:B:318:ILE:HG12	1:B:323:ILE:HG22	1.53	0.91
1:C:318:ILE:HG12	1:C:323:ILE:HG22	1.50	0.91
1:B:307:GLU:HG3	1:B:375:ARG:HH21	1.35	0.90
1:D:318:ILE:HG12	1:D:323:ILE:HG22	1.54	0.90
1:A:318:ILE:HG12	1:A:323:ILE:HG22	1.55	0.87
1:B:65:VAL:HG21	1:B:76:MET:CE	2.04	0.87
1:C:307:GLU:HG3	1:C:375:ARG:HH21	1.41	0.86
1:F:307:GLU:HG3	1:F:375:ARG:HH21	1.41	0.85
1:F:414:ASN:HA	1:F:417:CYS:O	1.78	0.83
1:D:105:VAL:CG1	1:F:395:GLN:HE22	1.91	0.83
1:A:307:GLU:HG3	1:A:375:ARG:HH21	1.43	0.82
1:E:307:GLU:HG3	1:E:375:ARG:HH21	1.44	0.80
1:F:65:VAL:HG21	1:F:76:MET:CE	2.13	0.79
1:B:307:GLU:HG3	1:B:375:ARG:NH2	2.00	0.77
1:D:459:GLN:HG2	4:F:602:NAG:H83	1.67	0.76
1:A:414:ASN:HA	1:A:417:CYS:O	1.84	0.75
1:B:103:ASP:C	1:B:105:VAL:H	1.95	0.75
1:E:334:THR:HG22	1:E:337:SER:H	1.51	0.75
1:B:414:ASN:HA	1:B:417:CYS:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:THR:HG22	1:C:337:SER:H	1.51	0.73
1:D:307:GLU:HG3	1:D:375:ARG:NH2	2.03	0.73
1:A:334:THR:HG22	1:A:337:SER:H	1.54	0.73
1:B:28:LEU:HD22	1:B:356:LEU:HB3	1.70	0.72
1:C:65:VAL:HG21	1:C:76:MET:HE3	1.72	0.72
1:D:28:LEU:HB2	1:D:30:TYR:CE1	2.24	0.72
1:D:372:HIS:HB2	3:D:606:SO4:O4	1.89	0.71
1:B:103:ASP:O	1:B:105:VAL:N	2.23	0.71
1:A:105:VAL:HG23	1:A:113:VAL:N	2.06	0.71
1:A:65:VAL:HG22	1:A:179:ILE:HD13	1.72	0.71
1:C:323:ILE:HD11	1:C:353:ARG:HG3	1.73	0.71
1:B:396:THR:HG21	1:B:418:THR:OG1	1.91	0.70
1:F:334:THR:HG22	1:F:337:SER:H	1.57	0.70
4:D:605:NAG:H83	1:E:459:GLN:HE21	1.56	0.69
1:B:60:LYS:HB3	1:B:173:THR:HB	1.73	0.69
1:B:104:LEU:HG	1:B:135:TYR:OH	1.92	0.69
1:D:105:VAL:HG11	1:F:395:GLN:HE22	1.58	0.69
1:F:218:LEU:O	1:F:218:LEU:HG	1.92	0.69
1:D:323:ILE:HD11	1:D:353:ARG:HG3	1.75	0.69
1:A:190:ILE:HG23	1:A:194:GLN:HB3	1.74	0.69
1:B:323:ILE:HD11	1:B:353:ARG:HG3	1.75	0.68
1:D:186:SER:HB2	1:D:190:ILE:HD12	1.75	0.68
1:D:100:ASN:HD22	1:D:120:ILE:HD13	1.59	0.68
1:F:68:VAL:HG12	1:F:68:VAL:O	1.93	0.68
1:B:289:GLN:HB3	1:F:424:ASN:OD1	1.92	0.68
1:B:184:VAL:HA	1:B:187:ILE:HD12	1.76	0.67
1:A:218:LEU:O	1:A:218:LEU:HG	1.93	0.67
1:A:323:ILE:HD11	1:A:353:ARG:HG3	1.75	0.67
1:E:65:VAL:HG21	1:E:76:MET:HE3	1.75	0.67
1:E:323:ILE:HD11	1:E:353:ARG:HG3	1.76	0.67
1:F:186:SER:HB2	1:F:190:ILE:HD12	1.77	0.67
1:D:334:THR:HG22	1:D:337:SER:H	1.61	0.66
1:F:323:ILE:HD11	1:F:353:ARG:HG3	1.75	0.66
1:D:60:LYS:HB3	1:D:173:THR:HB	1.78	0.66
1:E:60:LYS:HB3	1:E:173:THR:HB	1.78	0.65
1:B:28:LEU:HB2	1:B:30:TYR:CE1	2.31	0.65
1:B:103:ASP:C	1:B:105:VAL:N	2.51	0.65
1:D:289:GLN:OE1	1:A:424:ASN:ND2	2.30	0.65
1:C:307:GLU:HG3	1:C:375:ARG:NH2	2.11	0.65
1:A:346:THR:CG2	1:A:347:PRO:HD2	2.26	0.64
1:D:289:GLN:HB3	1:A:424:ASN:OD1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:O	1:A:104:LEU:HB2	1.97	0.63
1:B:63:PRO:HB2	1:B:179:ILE:HD12	1.81	0.63
1:D:68:VAL:HG22	1:D:184:VAL:HG22	1.80	0.63
1:B:334:THR:HG22	1:B:337:SER:H	1.62	0.63
1:F:346:THR:CG2	1:F:347:PRO:HD2	2.29	0.63
1:A:103:ASP:CB	1:A:114:VAL:H	2.11	0.63
1:B:192:CYS:C	1:B:194:GLN:H	2.06	0.63
1:B:218:LEU:HG	1:B:218:LEU:O	1.99	0.63
1:A:307:GLU:HG3	1:A:375:ARG:NH2	2.14	0.63
1:F:182:ASN:O	1:F:186:SER:OG	2.15	0.63
1:A:103:ASP:HB3	1:A:114:VAL:H	1.64	0.63
1:D:218:LEU:O	1:D:218:LEU:HG	1.97	0.62
1:A:190:ILE:HG22	1:A:195:THR:HG23	1.81	0.62
1:F:372:HIS:HB2	3:F:603:SO4:O2	1.99	0.62
1:B:104:LEU:HD22	1:B:109:LYS:HA	1.82	0.62
1:B:289:GLN:OE1	1:F:424:ASN:ND2	2.32	0.62
1:B:105:VAL:CG1	1:A:395:GLN:HE22	2.13	0.61
1:D:396:THR:HG21	1:D:418:THR:OG1	1.99	0.61
1:A:346:THR:HG22	1:A:347:PRO:HD2	1.80	0.61
1:B:97:TYR:O	1:B:101:THR:HG23	2.00	0.61
1:D:106:GLY:O	1:D:108:VAL:N	2.31	0.61
1:F:307:GLU:HG3	1:F:375:ARG:NH2	2.13	0.61
1:B:65:VAL:HG21	1:B:76:MET:HE3	1.80	0.61
1:C:60:LYS:HB3	1:C:173:THR:HB	1.82	0.61
1:D:474:ILE:HD13	1:E:473:TYR:HD2	1.64	0.61
1:E:97:TYR:O	1:E:101:THR:HG23	2.00	0.61
1:F:60:LYS:HB3	1:F:173:THR:HB	1.83	0.61
1:E:307:GLU:HG3	1:E:375:ARG:NH2	2.13	0.61
1:E:72:THR:O	1:E:75:VAL:HG22	2.01	0.60
1:D:76:MET:HE2	1:D:199:LEU:HD21	1.82	0.60
1:F:463:MET:HE1	1:E:463:MET:HB3	1.82	0.60
4:D:605:NAG:C8	1:E:459:GLN:HE21	2.15	0.60
1:C:83:LEU:HD23	1:C:274:TYR:CD1	2.36	0.60
1:D:414:ASN:HA	1:D:417:CYS:O	2.02	0.59
1:E:179:ILE:O	1:E:184:VAL:HG23	2.02	0.59
1:B:68:VAL:O	1:B:70:LYS:N	2.35	0.59
1:F:65:VAL:HG21	1:F:76:MET:HE1	1.84	0.59
1:C:218:LEU:O	1:C:218:LEU:HG	2.01	0.59
1:D:215:GLY:C	1:D:217:ASN:H	2.09	0.59
1:D:78:ASN:HB3	1:F:244:ARG:HH21	1.67	0.59
1:F:57:ILE:HD11	1:F:172:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:LEU:HG	1:E:218:LEU:O	2.02	0.59
1:E:63:PRO:HB2	1:E:179:ILE:HD12	1.84	0.58
1:A:103:ASP:OD1	1:A:103:ASP:N	2.36	0.58
1:C:26:GLY:O	1:C:28:LEU:N	2.36	0.58
1:D:63:PRO:HB2	1:D:179:ILE:HD12	1.85	0.58
1:E:68:VAL:HG12	1:E:68:VAL:O	2.03	0.58
1:D:68:VAL:O	1:D:70:LYS:N	2.33	0.58
1:E:28:LEU:HB2	1:E:30:TYR:CE1	2.38	0.57
1:B:78:ASN:HB3	1:A:244:ARG:HH21	1.69	0.57
1:C:63:PRO:HB2	1:C:179:ILE:HD12	1.85	0.57
1:E:83:LEU:HD23	1:E:274:TYR:CD1	2.40	0.57
1:C:97:TYR:O	1:C:101:THR:HG23	2.05	0.57
1:F:346:THR:HG22	1:F:347:PRO:HD2	1.86	0.57
1:B:100:ASN:HD22	1:B:120:ILE:HD13	1.70	0.57
1:B:372:HIS:HB2	3:B:603:SO4:O2	2.05	0.57
1:A:65:VAL:HG21	1:A:76:MET:CE	2.35	0.57
1:C:215:GLY:C	1:C:217:ASN:H	2.11	0.57
1:D:475:LYS:C	1:D:477:ALA:H	2.13	0.57
1:A:162:GLN:HE22	1:A:168:THR:HG22	1.70	0.56
1:C:210:LEU:C	1:C:210:LEU:HD12	2.30	0.56
1:D:333:ILE:HD12	1:E:219:GLN:OE1	2.05	0.56
1:A:105:VAL:CG2	1:A:113:VAL:N	2.69	0.56
1:D:103:ASP:C	1:D:105:VAL:H	2.13	0.56
1:A:60:LYS:HB3	1:A:173:THR:HB	1.88	0.56
1:E:215:GLY:C	1:E:217:ASN:H	2.12	0.55
1:F:463:MET:HE1	1:E:463:MET:CB	2.36	0.55
1:A:63:PRO:HB2	1:A:179:ILE:HD12	1.89	0.55
1:B:210:LEU:HD12	1:B:210:LEU:C	2.32	0.55
1:D:346:THR:CG2	1:D:347:PRO:HD2	2.37	0.55
1:E:162:GLN:HE22	1:E:168:THR:HG22	1.72	0.55
1:E:257:LEU:HD13	1:E:262:ILE:HD12	1.88	0.55
1:E:467:LEU:O	1:E:471:LYS:HB2	2.07	0.54
1:A:39:VAL:CG2	1:A:297:LEU:HB2	2.37	0.54
1:D:459:GLN:HG2	4:F:602:NAG:C8	2.35	0.54
1:F:39:VAL:CG2	1:F:297:LEU:HB2	2.37	0.54
1:A:30:TYR:OH	1:A:294:GLN:HG2	2.08	0.54
1:D:137:ALA:HB2	1:D:279:ARG:HD2	1.90	0.54
1:D:384:PHE:HB3	1:D:409:LEU:HD21	1.89	0.53
1:F:215:GLY:C	1:F:217:ASN:H	2.14	0.53
1:A:215:GLY:C	1:A:217:ASN:H	2.15	0.53
1:B:64:ASN:HB2	1:B:176:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:THR:HG22	1:F:455:ASP:OD2	2.08	0.53
1:D:467:LEU:O	1:D:471:LYS:HB2	2.09	0.53
1:F:190:ILE:HG22	1:F:195:THR:HG23	1.90	0.53
1:C:333:ILE:HD12	1:A:219:GLN:OE1	2.08	0.53
1:B:106:GLY:O	1:B:108:VAL:N	2.33	0.53
1:D:61:MET:CE	1:D:87:LEU:HD21	2.39	0.53
1:A:186:SER:O	1:A:190:ILE:HD12	2.08	0.53
1:F:51:ASN:N	1:F:52:PRO:HD3	2.23	0.53
1:D:210:LEU:HD12	1:D:210:LEU:C	2.35	0.52
1:D:349:THR:HG22	1:F:455:ASP:CG	2.34	0.52
1:B:162:GLN:HE22	1:B:168:THR:HG22	1.74	0.52
1:B:401:ILE:HD11	1:B:417:CYS:SG	2.49	0.52
1:B:65:VAL:HG12	1:B:65:VAL:O	2.09	0.52
1:B:467:LEU:O	1:B:471:LYS:HB2	2.10	0.52
1:D:162:GLN:HE22	1:D:168:THR:HG22	1.75	0.52
1:A:467:LEU:O	1:A:471:LYS:HB2	2.10	0.52
1:C:257:LEU:HD13	1:C:262:ILE:HD12	1.92	0.52
1:D:103:ASP:C	1:D:105:VAL:N	2.68	0.52
1:D:145:ASN:ND2	1:D:275:TYR:OH	2.42	0.52
1:D:104:LEU:HD22	1:D:109:LYS:HA	1.90	0.52
1:F:56:ASP:OD1	1:F:279:ARG:HA	2.10	0.52
1:E:458:SER:O	1:E:462:SER:HB2	2.09	0.52
1:A:396:THR:HG21	1:A:418:THR:OG1	2.10	0.52
1:F:467:LEU:O	1:F:471:LYS:HB2	2.09	0.52
1:D:290:GLN:HE22	1:A:424:ASN:HA	1.74	0.52
1:E:384:PHE:HB3	1:E:409:LEU:HD21	1.92	0.51
1:B:467:LEU:CD1	1:C:467:LEU:HB2	2.41	0.51
1:B:52:PRO:HA	1:B:283:PRO:HA	1.91	0.51
1:F:122:ILE:HA	1:E:378:LEU:O	2.11	0.51
1:B:186:SER:O	1:B:190:ILE:HG12	2.10	0.51
1:D:65:VAL:HG22	1:D:68:VAL:HB	1.92	0.51
1:D:97:TYR:O	1:D:101:THR:HG23	2.11	0.51
1:A:97:TYR:O	1:A:101:THR:HG23	2.10	0.51
1:A:184:VAL:O	1:A:187:ILE:HG13	2.11	0.51
1:B:384:PHE:HB3	1:B:409:LEU:HD21	1.92	0.51
1:E:210:LEU:C	1:E:210:LEU:HD12	2.35	0.51
1:A:52:PRO:HA	1:A:283:PRO:HA	1.93	0.51
1:B:156:GLU:OE1	1:C:194:GLN:HG2	2.11	0.51
1:D:187:ILE:HD12	1:D:195:THR:HG21	1.93	0.51
1:E:281:TYR:O	1:E:283:PRO:HD3	2.11	0.51
1:B:28:LEU:CD2	1:B:356:LEU:HB3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:VAL:HG21	1:F:76:MET:HE3	1.92	0.51
1:E:75:VAL:HG21	1:E:199:LEU:HD23	1.93	0.51
1:D:190:ILE:HD11	1:F:185:PRO:HG3	1.92	0.50
1:D:334:THR:O	1:D:335:LYS:C	2.54	0.50
1:D:225:SER:O	1:D:226:MET:C	2.54	0.50
1:D:382:VAL:HG21	1:D:432:TYR:CA	2.42	0.50
1:B:463:MET:HE1	1:A:463:MET:HB3	1.92	0.50
1:C:463:MET:HB3	1:A:463:MET:HE1	1.94	0.50
1:C:467:LEU:O	1:C:471:LYS:HB2	2.11	0.50
1:D:103:ASP:O	1:D:105:VAL:N	2.44	0.50
1:F:63:PRO:HB2	1:F:179:ILE:HD12	1.92	0.50
1:A:190:ILE:HG23	1:A:194:GLN:CB	2.40	0.50
1:E:383:LEU:HD21	1:E:422:LEU:CD2	2.42	0.50
1:C:162:GLN:HE22	1:C:168:THR:HG22	1.76	0.50
1:A:334:THR:O	1:A:335:LYS:C	2.55	0.50
1:B:346:THR:CG2	1:B:347:PRO:HD2	2.41	0.50
1:C:186:SER:OG	1:C:190:ILE:HD11	2.12	0.50
1:F:83:LEU:HD23	1:F:274:TYR:CD1	2.47	0.50
1:A:365:ARG:O	1:A:448:PRO:HA	2.11	0.50
1:A:51:ASN:N	1:A:52:PRO:HD3	2.27	0.50
1:B:215:GLY:C	1:B:217:ASN:H	2.20	0.49
1:D:401:ILE:HD11	1:D:417:CYS:SG	2.52	0.49
1:F:162:GLN:HE22	1:F:168:THR:HG22	1.77	0.49
1:C:156:GLU:OE1	1:A:194:GLN:HG2	2.12	0.49
1:C:186:SER:O	1:C:190:ILE:HG13	2.12	0.49
1:D:215:GLY:C	1:D:217:ASN:N	2.70	0.49
1:F:78:ASN:HB3	1:E:244:ARG:HH21	1.78	0.49
1:B:226:MET:HE2	1:B:231:ILE:HG12	1.95	0.49
1:C:378:LEU:O	1:A:122:ILE:HA	2.12	0.49
1:F:137:ALA:HB2	1:F:279:ARG:HD2	1.95	0.49
1:A:57:ILE:HD11	1:A:172:LEU:HD13	1.93	0.49
1:B:61:MET:HE3	1:B:87:LEU:HD11	1.94	0.49
1:C:281:TYR:O	1:C:283:PRO:HD3	2.11	0.49
1:E:65:VAL:HG21	1:E:76:MET:HE1	1.87	0.49
1:C:57:ILE:HD11	1:C:172:LEU:HD13	1.95	0.49
1:F:52:PRO:HA	1:F:283:PRO:HA	1.95	0.49
1:F:334:THR:O	1:F:335:LYS:C	2.54	0.49
1:A:401:ILE:HD11	1:A:417:CYS:SG	2.53	0.49
1:E:28:LEU:CD2	1:E:356:LEU:HB3	2.43	0.49
1:C:240:GLU:HB3	1:A:204:SER:HB2	1.94	0.48
1:B:382:VAL:HG21	1:B:432:TYR:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:CE	1:A:87:LEU:HD21	2.43	0.48
1:B:463:MET:HE1	1:A:463:MET:CB	2.43	0.48
1:C:346:THR:CG2	1:C:347:PRO:HD2	2.43	0.48
1:F:210:LEU:C	1:F:210:LEU:HD12	2.38	0.48
1:B:383:LEU:HD21	1:B:422:LEU:HD22	1.96	0.48
1:C:26:GLY:O	1:C:27:ILE:C	2.55	0.48
1:C:411:MET:HE2	1:C:432:TYR:CD2	2.48	0.48
1:B:334:THR:O	1:B:335:LYS:C	2.55	0.48
1:B:61:MET:CE	1:B:87:LEU:HD21	2.44	0.48
1:A:83:LEU:HD23	1:A:274:TYR:CD1	2.49	0.48
1:B:226:MET:HE2	1:B:226:MET:HB3	1.68	0.48
1:D:226:MET:HE2	1:D:231:ILE:HG12	1.95	0.48
1:E:64:ASN:HB2	1:E:176:GLN:OE1	2.14	0.47
1:E:463:MET:O	1:E:464:ASN:C	2.57	0.47
1:C:380:GLY:N	1:A:121:GLY:O	2.47	0.47
1:A:65:VAL:HG21	1:A:76:MET:HE1	1.96	0.47
1:B:225:SER:O	1:B:226:MET:C	2.55	0.47
1:A:411:MET:HE2	1:A:432:TYR:CD2	2.49	0.47
1:B:333:ILE:HD12	1:C:219:GLN:OE1	2.15	0.47
1:C:190:ILE:HG22	1:C:191:SER:H	1.78	0.47
1:D:454:VAL:HG11	1:E:313:PRO:HD3	1.95	0.47
1:D:464:ASN:O	1:D:465:GLN:C	2.57	0.47
1:E:411:MET:HE2	1:E:432:TYR:CD2	2.49	0.47
1:F:65:VAL:HG22	1:F:179:ILE:HD13	1.97	0.47
1:B:137:ALA:HB2	1:B:279:ARG:HD2	1.96	0.47
1:D:103:ASP:OD1	1:D:103:ASP:N	2.44	0.47
1:F:57:ILE:HD11	1:F:172:LEU:CD1	2.44	0.47
1:E:215:GLY:C	1:E:217:ASN:N	2.73	0.47
1:A:193:LYS:HA	1:A:196:GLU:HG2	1.97	0.47
1:B:454:VAL:HG11	1:C:313:PRO:HD3	1.97	0.47
1:D:61:MET:HE1	1:D:87:LEU:HD21	1.97	0.47
1:B:68:VAL:C	1:B:70:LYS:H	2.23	0.46
1:B:104:LEU:CG	1:B:135:TYR:OH	2.62	0.46
1:F:66:SER:HA	1:F:69:SER:HB3	1.97	0.46
1:F:175:LEU:HD21	1:F:206:TYR:HB2	1.97	0.46
1:C:33:LEU:O	1:C:36:ILE:HG22	2.16	0.46
1:C:215:GLY:C	1:C:217:ASN:N	2.73	0.46
1:D:68:VAL:HG22	1:D:184:VAL:CG2	2.42	0.46
1:F:101:THR:CG2	1:F:115:MET:SD	3.04	0.46
1:B:76:MET:HE2	1:B:199:LEU:HD21	1.95	0.46
1:C:384:PHE:HB3	1:C:409:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ARG:NH2	1:F:369:VAL:O	2.44	0.46
1:E:71:CYS:O	1:E:196:GLU:HB3	2.15	0.46
1:A:68:VAL:C	1:A:70:LYS:H	2.23	0.46
1:A:189:GLN:O	1:A:190:ILE:HG13	2.14	0.46
1:F:30:TYR:OH	1:F:294:GLN:HG2	2.16	0.46
1:E:186:SER:O	1:E:190:ILE:HG13	2.15	0.46
1:A:210:LEU:C	1:A:210:LEU:HD12	2.41	0.46
1:B:103:ASP:OD1	1:B:103:ASP:N	2.49	0.46
1:C:239:TYR:HE1	1:C:257:LEU:HD21	1.80	0.46
1:C:463:MET:CB	1:A:463:MET:HE1	2.45	0.46
1:D:52:PRO:HA	1:D:283:PRO:HA	1.98	0.46
1:D:346:THR:HG22	1:D:347:PRO:HD2	1.98	0.46
1:F:365:ARG:O	1:F:448:PRO:HA	2.15	0.46
1:A:137:ALA:HB2	1:A:279:ARG:HD2	1.98	0.46
1:D:458:SER:O	1:D:462:SER:HB2	2.16	0.46
1:D:290:GLN:O	1:D:319:ARG:HA	2.17	0.45
1:E:51:ASN:N	1:E:52:PRO:HD3	2.31	0.45
1:E:334:THR:O	1:E:335:LYS:C	2.59	0.45
1:E:346:THR:CG2	1:E:347:PRO:HD2	2.46	0.45
1:B:383:LEU:HD21	1:B:422:LEU:CD2	2.46	0.45
1:C:50:SER:O	1:C:51:ASN:C	2.59	0.45
1:F:187:ILE:HG13	1:F:188:ASP:H	1.81	0.45
1:F:215:GLY:C	1:F:217:ASN:N	2.74	0.45
1:A:65:VAL:HG22	1:A:179:ILE:CD1	2.43	0.45
1:B:290:GLN:O	1:B:319:ARG:HA	2.16	0.45
1:A:65:VAL:HG12	1:A:65:VAL:O	2.17	0.45
1:A:100:ASN:CG	1:A:119:ALA:HB1	2.40	0.45
1:C:383:LEU:HD21	1:C:422:LEU:CD2	2.46	0.45
1:F:194:GLN:HG2	1:E:156:GLU:OE1	2.16	0.45
1:E:291:ALA:HA	1:E:318:ILE:O	2.16	0.45
1:A:311:ILE:HD13	1:A:311:ILE:HA	1.71	0.45
1:B:319:ARG:NH2	1:A:369:VAL:O	2.47	0.45
1:F:68:VAL:C	1:F:70:LYS:H	2.25	0.45
1:B:291:ALA:HA	1:B:318:ILE:O	2.17	0.45
1:A:432:TYR:CZ	1:A:434:GLY:HA3	2.51	0.45
1:D:28:LEU:HD22	1:D:356:LEU:HB3	1.98	0.45
1:C:467:LEU:CD1	1:A:467:LEU:HB2	2.46	0.45
1:D:240:GLU:HG3	1:E:207:LEU:HB3	1.97	0.45
1:E:415:THR:HG22	4:E:603:NAG:H82	1.98	0.45
1:B:88:SER:N	1:B:89:PRO:HD2	2.32	0.45
1:C:30:TYR:OH	1:C:294:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:THR:HG21	1:F:418:THR:OG1	2.17	0.45
1:B:151:ILE:HG21	1:B:275:TYR:CD2	2.52	0.44
1:B:242:LEU:HD23	1:B:242:LEU:C	2.42	0.44
1:F:63:PRO:CB	1:F:179:ILE:HD12	2.48	0.44
1:F:204:SER:HB2	1:E:240:GLU:HB3	2.00	0.44
1:D:171:VAL:HG12	1:D:173:THR:HG22	2.00	0.44
1:F:33:LEU:O	1:F:36:ILE:HG22	2.17	0.44
1:E:57:ILE:HD11	1:E:172:LEU:HD13	1.98	0.44
1:B:58:VAL:HG12	1:B:171:VAL:HG13	1.98	0.44
1:D:226:MET:HE2	1:D:226:MET:HB3	1.73	0.44
1:A:162:GLN:NE2	1:A:168:THR:HG22	2.32	0.44
1:F:384:PHE:HB3	1:F:409:LEU:HD21	2.00	0.44
1:B:244:ARG:HH21	1:C:78:ASN:HB3	1.82	0.44
1:C:28:LEU:CD2	1:C:356:LEU:HB3	2.47	0.44
1:C:302:ASN:O	1:C:408:THR:HA	2.18	0.44
1:D:174:ALA:C	1:D:176:GLN:H	2.26	0.44
1:F:145:ASN:ND2	1:F:275:TYR:OH	2.51	0.44
1:A:404:SER:HB3	1:A:407:GLN:OE1	2.18	0.44
1:B:105:VAL:HG11	1:A:395:GLN:HE22	1.83	0.44
1:B:279:ARG:HD3	1:B:281:TYR:OH	2.18	0.44
1:D:382:VAL:HG21	1:D:432:TYR:HA	1.99	0.44
1:B:30:TYR:OH	1:B:294:GLN:HG2	2.18	0.44
1:B:240:GLU:HG3	1:C:207:LEU:HB3	2.00	0.44
1:C:490:GLU:C	1:C:492:LEU:H	2.26	0.44
1:E:174:ALA:C	1:E:176:GLN:H	2.26	0.44
1:A:56:ASP:OD1	1:A:279:ARG:HG3	2.18	0.44
1:B:192:CYS:C	1:B:194:GLN:N	2.74	0.43
1:C:413:ASP:HB2	1:C:430:GLY:O	2.18	0.43
1:D:61:MET:HE3	1:D:87:LEU:HD11	1.99	0.43
1:A:165:ALA:O	1:A:166:GLU:CB	2.66	0.43
1:B:176:GLN:NE2	1:B:180:ASN:OD1	2.51	0.43
1:B:382:VAL:HG21	1:B:432:TYR:HA	2.00	0.43
1:D:88:SER:N	1:D:89:PRO:HD2	2.33	0.43
1:E:58:VAL:HG22	1:E:277:ILE:HG12	2.01	0.43
1:B:284:ILE:HD12	1:B:284:ILE:HA	1.93	0.43
1:C:51:ASN:N	1:C:52:PRO:HD3	2.33	0.43
1:C:414:ASN:HB3	1:C:429:LEU:O	2.18	0.43
1:A:39:VAL:HG22	1:A:297:LEU:HB2	2.00	0.43
1:A:90:ILE:O	1:A:91:LYS:C	2.62	0.43
1:A:382:VAL:HG21	1:A:432:TYR:HA	2.01	0.43
1:E:414:ASN:HB3	1:E:429:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:THR:HG22	1:F:115:MET:SD	2.59	0.43
1:C:291:ALA:HA	1:C:318:ILE:O	2.19	0.43
1:D:244:ARG:HH21	1:E:78:ASN:HB3	1.82	0.43
1:A:56:ASP:OD1	1:A:279:ARG:HA	2.18	0.43
1:B:458:SER:O	1:B:462:SER:HB2	2.19	0.43
1:D:243:LEU:HB3	1:D:253:PHE:HZ	1.83	0.43
1:E:284:ILE:HD12	1:E:284:ILE:HA	1.95	0.43
1:B:145:ASN:ND2	1:B:275:TYR:OH	2.51	0.43
1:C:244:ARG:HH21	1:A:78:ASN:HB3	1.84	0.43
1:F:219:GLN:OE1	1:E:333:ILE:HD12	2.18	0.43
1:F:348:MET:SD	1:F:352:VAL:HG12	2.59	0.43
1:E:162:GLN:NE2	1:E:168:THR:HG22	2.32	0.43
1:A:291:ALA:HA	1:A:318:ILE:O	2.18	0.43
1:B:214:PHE:HE1	1:B:266:ILE:HD11	1.84	0.43
1:C:71:CYS:HB3	1:C:192:CYS:HB3	1.85	0.43
1:C:403:GLN:HG3	1:C:407:GLN:HG3	2.01	0.43
1:C:458:SER:O	1:C:462:SER:HB2	2.18	0.43
1:D:162:GLN:NE2	1:D:168:THR:HG22	2.34	0.43
1:F:165:ALA:O	1:F:166:GLU:CB	2.67	0.43
1:E:58:VAL:HG12	1:E:171:VAL:HG13	2.00	0.43
1:F:193:LYS:H	1:F:193:LYS:HG2	1.33	0.42
1:F:160:LYS:HE2	1:F:168:THR:HG21	2.02	0.42
1:F:412:ILE:O	1:F:429:LEU:HD13	2.19	0.42
1:E:226:MET:HE2	1:E:231:ILE:HG12	2.00	0.42
1:A:171:VAL:HG12	1:A:173:THR:HG22	2.01	0.42
1:C:297:LEU:HA	1:C:298:PRO:HD3	1.89	0.42
1:F:121:GLY:O	1:E:380:GLY:N	2.52	0.42
1:E:98:ASN:C	1:E:100:ASN:H	2.26	0.42
1:E:160:LYS:HE2	1:E:168:THR:HG21	2.02	0.42
1:B:302:ASN:O	1:B:408:THR:HA	2.20	0.42
1:F:97:TYR:O	1:F:101:THR:HG23	2.18	0.42
1:F:226:MET:HB3	1:F:226:MET:HE2	1.74	0.42
1:F:302:ASN:O	1:F:408:THR:HA	2.20	0.42
1:A:212:PHE:CD1	1:A:212:PHE:C	2.98	0.42
1:A:302:ASN:O	1:A:408:THR:HA	2.19	0.42
1:B:162:GLN:NE2	1:B:168:THR:HG22	2.34	0.42
1:B:403:GLN:HG3	1:B:407:GLN:HG3	2.01	0.42
1:C:365:ARG:O	1:C:448:PRO:HA	2.19	0.42
1:D:219:GLN:OE1	1:F:333:ILE:HD12	2.20	0.42
1:D:297:LEU:HA	1:D:298:PRO:HD3	1.93	0.42
1:F:464:ASN:O	1:F:465:GLN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:THR:CG2	1:E:115:MET:SD	3.08	0.42
1:C:404:SER:HB3	1:C:407:GLN:OE1	2.19	0.42
1:D:279:ARG:HD3	1:D:281:TYR:OH	2.19	0.42
1:F:39:VAL:HG22	1:F:297:LEU:HB2	2.02	0.42
1:F:225:SER:O	1:F:226:MET:C	2.62	0.42
1:F:312:VAL:HG13	1:F:313:PRO:HD2	2.02	0.42
1:E:302:ASN:O	1:E:408:THR:HA	2.18	0.42
1:E:403:GLN:HG3	1:E:407:GLN:HG3	2.01	0.42
1:D:463:MET:HB3	1:E:463:MET:HE1	2.01	0.42
1:F:411:MET:HE2	1:F:432:TYR:CD2	2.55	0.42
1:E:33:LEU:O	1:E:36:ILE:HG22	2.20	0.42
1:A:100:ASN:ND2	1:A:119:ALA:HB1	2.35	0.42
1:D:107:ASP:O	1:D:107:ASP:CG	2.62	0.42
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.81	0.42
1:D:302:ASN:O	1:D:408:THR:HA	2.20	0.42
1:E:212:PHE:CD1	1:E:212:PHE:C	2.98	0.42
1:B:215:GLY:C	1:B:217:ASN:N	2.77	0.42
1:C:414:ASN:HA	1:C:417:CYS:O	2.20	0.42
1:E:88:SER:N	1:E:89:PRO:HD2	2.35	0.42
1:E:311:ILE:HD13	1:E:311:ILE:HA	1.77	0.42
1:A:382:VAL:HG21	1:A:432:TYR:CA	2.50	0.42
1:C:165:ALA:O	1:C:166:GLU:CB	2.68	0.42
1:D:403:GLN:HG3	1:D:407:GLN:HG3	2.02	0.42
1:D:432:TYR:CZ	1:D:434:GLY:HA3	2.55	0.42
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.85	0.42
1:B:311:ILE:HD13	1:B:311:ILE:HA	1.77	0.41
1:B:171:VAL:HG12	1:B:173:THR:HG22	2.01	0.41
1:B:243:LEU:HB3	1:B:253:PHE:HZ	1.84	0.41
1:D:56:ASP:OD1	1:D:279:ARG:HA	2.20	0.41
1:D:160:LYS:HE2	1:D:168:THR:HG21	2.03	0.41
1:D:165:ALA:O	1:D:166:GLU:CB	2.68	0.41
1:F:291:ALA:HA	1:F:318:ILE:O	2.20	0.41
1:F:463:MET:CE	1:E:463:MET:HB3	2.49	0.41
1:C:334:THR:O	1:C:335:LYS:C	2.63	0.41
1:E:226:MET:HE2	1:E:226:MET:HB3	1.65	0.41
1:B:361:ASP:HA	1:B:446:GLY:HA2	2.03	0.41
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.41
1:E:225:SER:O	1:E:226:MET:C	2.63	0.41
1:A:160:LYS:HE2	1:A:168:THR:HG21	2.02	0.41
1:D:365:ARG:O	1:D:448:PRO:HA	2.20	0.41
1:E:275:TYR:CD1	1:E:275:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:HG3	1:C:216:PRO:HD2	2.02	0.41
1:C:94:ILE:HG23	1:C:134:LEU:HD21	2.02	0.41
1:C:311:ILE:HG22	1:C:311:ILE:O	2.21	0.41
1:C:475:LYS:C	1:C:477:ALA:H	2.27	0.41
1:E:165:ALA:O	1:E:166:GLU:CB	2.68	0.41
1:C:162:GLN:NE2	1:C:168:THR:HG22	2.35	0.41
1:F:61:MET:CE	1:F:87:LEU:HD21	2.50	0.41
1:F:68:VAL:HG23	1:F:184:VAL:HG22	2.03	0.41
1:D:411:MET:SD	1:D:411:MET:C	3.03	0.41
1:F:171:VAL:HG12	1:F:173:THR:HG22	2.03	0.41
1:F:401:ILE:HD11	1:F:417:CYS:SG	2.60	0.41
1:B:174:ALA:C	1:B:176:GLN:H	2.28	0.41
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.83	0.41
1:C:101:THR:CG2	1:C:115:MET:SD	3.08	0.41
1:D:39:VAL:CG2	1:D:297:LEU:HB2	2.50	0.41
1:D:176:GLN:NE2	1:D:180:ASN:OD1	2.52	0.41
1:F:87:LEU:HD23	1:F:87:LEU:HA	1.94	0.41
1:A:58:VAL:HG12	1:A:171:VAL:HG13	2.03	0.41
1:A:312:VAL:HG13	1:A:313:PRO:HD2	2.02	0.41
1:C:65:VAL:HG21	1:C:76:MET:HE2	1.96	0.41
1:C:174:ALA:C	1:C:176:GLN:H	2.29	0.41
1:C:257:LEU:HD12	1:C:257:LEU:HA	1.84	0.41
1:D:311:ILE:HD13	1:D:311:ILE:HA	1.76	0.41
1:E:101:THR:HG22	1:E:115:MET:SD	2.61	0.41
1:A:384:PHE:HB3	1:A:409:LEU:HD21	2.02	0.41
1:C:145:ASN:ND2	1:C:275:TYR:OH	2.54	0.40
1:D:258:GLU:HG3	1:E:216:PRO:HD2	2.03	0.40
1:A:206:TYR:CZ	1:A:210:LEU:HD23	2.56	0.40
1:A:215:GLY:C	1:A:217:ASN:N	2.74	0.40
1:A:458:SER:O	1:A:462:SER:HB2	2.20	0.40
1:B:346:THR:HG22	1:B:347:PRO:HD2	2.03	0.40
1:C:160:LYS:HE2	1:C:168:THR:HG21	2.02	0.40
1:C:183:LEU:HD12	1:C:183:LEU:HA	1.81	0.40
1:D:90:ILE:O	1:D:91:LYS:C	2.64	0.40
1:D:383:LEU:HD21	1:D:422:LEU:CD2	2.51	0.40
1:F:404:SER:HB3	1:F:407:GLN:OE1	2.20	0.40
1:E:414:ASN:HA	1:E:417:CYS:O	2.21	0.40
1:A:57:ILE:HD11	1:A:172:LEU:CD1	2.51	0.40
1:B:64:ASN:N	1:B:176:GLN:OE1	2.53	0.40
1:C:83:LEU:HD23	1:C:274:TYR:HD1	1.82	0.40
1:C:171:VAL:HG12	1:C:173:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:TYR:OH	1:E:294:GLN:HG2	2.21	0.40
1:A:35:LYS:HG3	1:A:438:TYR:CZ	2.56	0.40
1:A:174:ALA:C	1:A:176:GLN:H	2.29	0.40
1:C:88:SER:N	1:C:89:PRO:HD2	2.37	0.40
1:F:56:ASP:OD1	1:F:279:ARG:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:OE1	1:F:289:GLN:OE1[2_656]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/501 (87%)	393 (91%)	34 (8%)	7 (2%)	7	36
1	B	443/501 (88%)	392 (88%)	43 (10%)	8 (2%)	6	34
1	C	448/501 (89%)	399 (89%)	42 (9%)	7 (2%)	7	36
1	D	456/501 (91%)	406 (89%)	41 (9%)	9 (2%)	6	31
1	E	430/501 (86%)	388 (90%)	40 (9%)	2 (0%)	24	59
1	F	430/501 (86%)	386 (90%)	42 (10%)	2 (0%)	24	59
All	All	2641/3006 (88%)	2364 (90%)	242 (9%)	35 (1%)	9	40

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	69	SER
1	B	104	LEU
1	B	107	ASP

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Mol	Chain	Res	Type
1	B	371	SER
1	C	27	ILE
1	C	371	SER
1	D	69	SER
1	D	104	LEU
1	D	107	ASP
1	D	371	SER
1	F	65	VAL
1	F	371	SER
1	E	371	SER
1	A	65	VAL
1	A	371	SER
1	B	65	VAL
1	B	191	SER
1	C	65	VAL
1	D	192	CYS
1	E	65	VAL
1	A	70	LYS
1	B	193	LYS
1	C	480	ILE
1	A	69	SER
1	B	105	VAL
1	C	28	LEU
1	C	484	VAL
1	D	105	VAL
1	D	480	ILE
1	D	106	GLY
1	D	476	GLU
1	A	103	ASP
1	A	464	ASN
1	C	491	ILE
1	A	68	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	377/443 (85%)	340 (90%)	37 (10%)	7	31
1	B	382/443 (86%)	342 (90%)	40 (10%)	6	28
1	C	374/443 (84%)	333 (89%)	41 (11%)	6	26
1	D	382/443 (86%)	340 (89%)	42 (11%)	6	26
1	E	373/443 (84%)	336 (90%)	37 (10%)	7	31
1	F	373/443 (84%)	330 (88%)	43 (12%)	5	24
All	All	2261/2658 (85%)	2021 (89%)	240 (11%)	6	27

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	ILE
1	B	55	LYS
1	B	70	LYS
1	B	86	ILE
1	B	88	SER
1	B	96	LEU
1	B	103	ASP
1	B	105	VAL
1	B	109	LYS
1	B	150	SER
1	B	158	VAL
1	B	169	VAL
1	B	173	THR
1	B	195	THR
1	B	201	LEU
1	B	208	SER
1	B	210	LEU
1	B	219	GLN
1	B	226	MET
1	B	227	THR
1	B	244	ARG
1	B	284	ILE
1	B	285	LEU
1	B	306	SER
1	B	310	SER
1	B	317	LEU
1	B	322	LEU
1	B	329	LYS
1	B	333	ILE
1	B	334	THR

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Mol	Chain	Res	Type
1	B	355	CYS
1	B	367	LEU
1	B	373	VAL
1	B	407	GLN
1	B	409	LEU
1	B	422	LEU
1	B	452	ASP
1	B	454	VAL
1	B	457	SER
1	B	462	SER
1	C	32	LYS
1	C	42	ILE
1	C	55	LYS
1	C	86	ILE
1	C	88	SER
1	C	96	LEU
1	C	113	VAL
1	C	150	SER
1	C	158	VAL
1	C	169	VAL
1	C	173	THR
1	C	183	LEU
1	C	190	ILE
1	C	194	GLN
1	C	201	LEU
1	C	208	SER
1	C	210	LEU
1	C	219	GLN
1	C	226	MET
1	C	227	THR
1	C	244	ARG
1	C	246	LEU
1	C	284	ILE
1	C	285	LEU
1	C	306	SER
1	C	322	LEU
1	C	329	LYS
1	C	333	ILE
1	C	334	THR
1	C	355	CYS
1	C	367	LEU
1	C	373	VAL

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Mol	Chain	Res	Type
1	C	407	GLN
1	C	409	LEU
1	C	422	LEU
1	C	426	ILE
1	C	451	THR
1	C	452	ASP
1	C	454	VAL
1	C	457	SER
1	C	462	SER
1	D	32	LYS
1	D	42	ILE
1	D	55	LYS
1	D	65	VAL
1	D	86	ILE
1	D	88	SER
1	D	96	LEU
1	D	103	ASP
1	D	105	VAL
1	D	150	SER
1	D	158	VAL
1	D	169	VAL
1	D	173	THR
1	D	187	ILE
1	D	201	LEU
1	D	208	SER
1	D	210	LEU
1	D	219	GLN
1	D	226	MET
1	D	227	THR
1	D	244	ARG
1	D	284	ILE
1	D	285	LEU
1	D	306	SER
1	D	310	SER
1	D	311	ILE
1	D	317	LEU
1	D	322	LEU
1	D	329	LYS
1	D	333	ILE
1	D	334	THR
1	D	367	LEU
1	D	373	VAL

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Mol	Chain	Res	Type
1	D	394	CYS
1	D	407	GLN
1	D	409	LEU
1	D	422	LEU
1	D	426	ILE
1	D	452	ASP
1	D	454	VAL
1	D	457	SER
1	D	462	SER
1	F	28	LEU
1	F	42	ILE
1	F	55	LYS
1	F	71	CYS
1	F	86	ILE
1	F	88	SER
1	F	150	SER
1	F	158	VAL
1	F	169	VAL
1	F	173	THR
1	F	183	LEU
1	F	188	ASP
1	F	192	CYS
1	F	193	LYS
1	F	201	LEU
1	F	208	SER
1	F	210	LEU
1	F	219	GLN
1	F	226	MET
1	F	227	THR
1	F	244	ARG
1	F	246	LEU
1	F	284	ILE
1	F	285	LEU
1	F	306	SER
1	F	310	SER
1	F	311	ILE
1	F	317	LEU
1	F	319	ARG
1	F	322	LEU
1	F	329	LYS
1	F	333	ILE
1	F	334	THR

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Mol	Chain	Res	Type
1	F	355	CYS
1	F	367	LEU
1	F	373	VAL
1	F	409	LEU
1	F	422	LEU
1	F	452	ASP
1	F	454	VAL
1	F	457	SER
1	F	462	SER
1	F	469	GLN
1	E	42	ILE
1	E	55	LYS
1	E	86	ILE
1	E	88	SER
1	E	99	ASN
1	E	150	SER
1	E	158	VAL
1	E	169	VAL
1	E	173	THR
1	E	183	LEU
1	E	184	VAL
1	E	201	LEU
1	E	208	SER
1	E	210	LEU
1	E	219	GLN
1	E	226	MET
1	E	227	THR
1	E	244	ARG
1	E	252	ASP
1	E	284	ILE
1	E	285	LEU
1	E	306	SER
1	E	322	LEU
1	E	329	LYS
1	E	334	THR
1	E	355	CYS
1	E	367	LEU
1	E	373	VAL
1	E	409	LEU
1	E	422	LEU
1	E	426	ILE
1	E	451	THR

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Mol	Chain	Res	Type
1	E	452	ASP
1	E	454	VAL
1	E	457	SER
1	E	462	SER
1	E	469	GLN
1	A	28	LEU
1	A	42	ILE
1	A	55	LYS
1	A	68	VAL
1	A	71	CYS
1	A	86	ILE
1	A	103	ASP
1	A	104	LEU
1	A	150	SER
1	A	158	VAL
1	A	169	VAL
1	A	173	THR
1	A	201	LEU
1	A	208	SER
1	A	210	LEU
1	A	219	GLN
1	A	226	MET
1	A	227	THR
1	A	244	ARG
1	A	246	LEU
1	A	284	ILE
1	A	285	LEU
1	A	306	SER
1	A	310	SER
1	A	322	LEU
1	A	329	LYS
1	A	333	ILE
1	A	334	THR
1	A	355	CYS
1	A	367	LEU
1	A	373	VAL
1	A	409	LEU
1	A	422	LEU
1	A	452	ASP
1	A	454	VAL
1	A	457	SER
1	A	462	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	HIS
1	B	64	ASN
1	B	100	ASN
1	B	127	GLN
1	B	140	ASN
1	B	145	ASN
1	B	162	GLN
1	B	233	GLN
1	B	290	GLN
1	B	314	ASN
1	B	325	ASN
1	C	102	HIS
1	C	145	ASN
1	C	162	GLN
1	C	189	GLN
1	C	233	GLN
1	C	265	GLN
1	C	314	ASN
1	C	325	ASN
1	C	342	GLN
1	C	395	GLN
1	D	100	ASN
1	D	145	ASN
1	D	155	ASN
1	D	162	GLN
1	D	189	GLN
1	D	233	GLN
1	D	290	GLN
1	D	314	ASN
1	D	325	ASN
1	F	145	ASN
1	F	162	GLN
1	F	233	GLN
1	F	265	GLN
1	F	314	ASN
1	F	325	ASN
1	F	395	GLN
1	E	145	ASN
1	E	162	GLN
1	E	182	ASN
1	E	233	GLN

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Mol	Chain	Res	Type
1	E	325	ASN
1	E	342	GLN
1	E	459	GLN
1	A	145	ASN
1	A	162	GLN
1	A	233	GLN
1	A	314	ASN
1	A	325	ASN
1	A	395	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	G	1	1,2	14,14,15	0.61	0	17,19,21	1.60	3 (17%)
2	NAG	G	2	2	14,14,15	0.49	0	17,19,21	1.23	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.86	0	17,19,21	1.63	1 (5%)
2	NAG	H	2	2	14,14,15	0.72	0	17,19,21	1.49	3 (17%)
2	NAG	I	1	1,2	14,14,15	0.85	0	17,19,21	2.34	7 (41%)
2	NAG	I	2	2	14,14,15	0.57	0	17,19,21	1.85	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C2-N2-C7	5.49	130.26	122.90
2	I	1	NAG	C1-O5-C5	4.60	118.35	112.19
2	I	1	NAG	C4-C3-C2	4.26	117.26	111.02
2	I	2	NAG	C1-C2-N2	4.20	117.04	110.43
2	G	1	NAG	C1-O5-C5	4.10	117.68	112.19
2	I	1	NAG	C1-C2-N2	-3.80	104.44	110.43
2	H	2	NAG	C1-O5-C5	3.64	117.07	112.19
2	I	1	NAG	C3-C4-C5	3.63	116.82	110.23
2	I	2	NAG	C1-O5-C5	3.62	117.04	112.19
2	G	1	NAG	C2-N2-C7	-3.60	118.08	122.90
2	H	2	NAG	C4-C3-C2	3.34	115.91	111.02
2	I	1	NAG	O7-C7-N2	3.13	127.51	121.98
2	G	2	NAG	C1-O5-C5	2.74	115.86	112.19
2	I	2	NAG	C3-C4-C5	2.56	114.87	110.23
2	H	2	NAG	C2-N2-C7	2.48	126.23	122.90
2	I	1	NAG	C8-C7-N2	-2.38	112.17	116.12
2	I	2	NAG	O5-C1-C2	-2.29	107.74	111.29
2	G	1	NAG	C4-C3-C2	2.24	114.29	111.02
2	I	1	NAG	O3-C3-C4	-2.16	105.27	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C1-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

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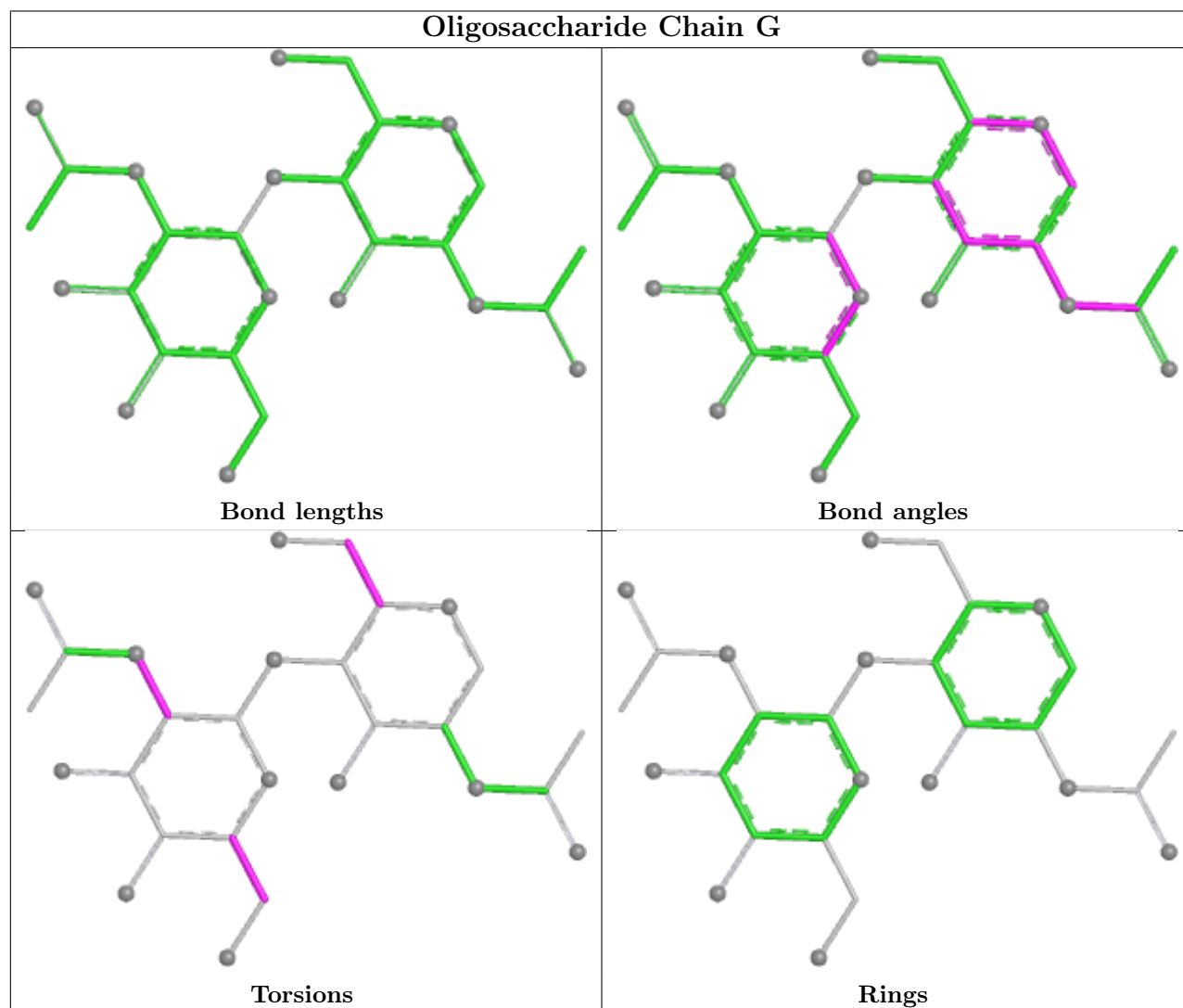
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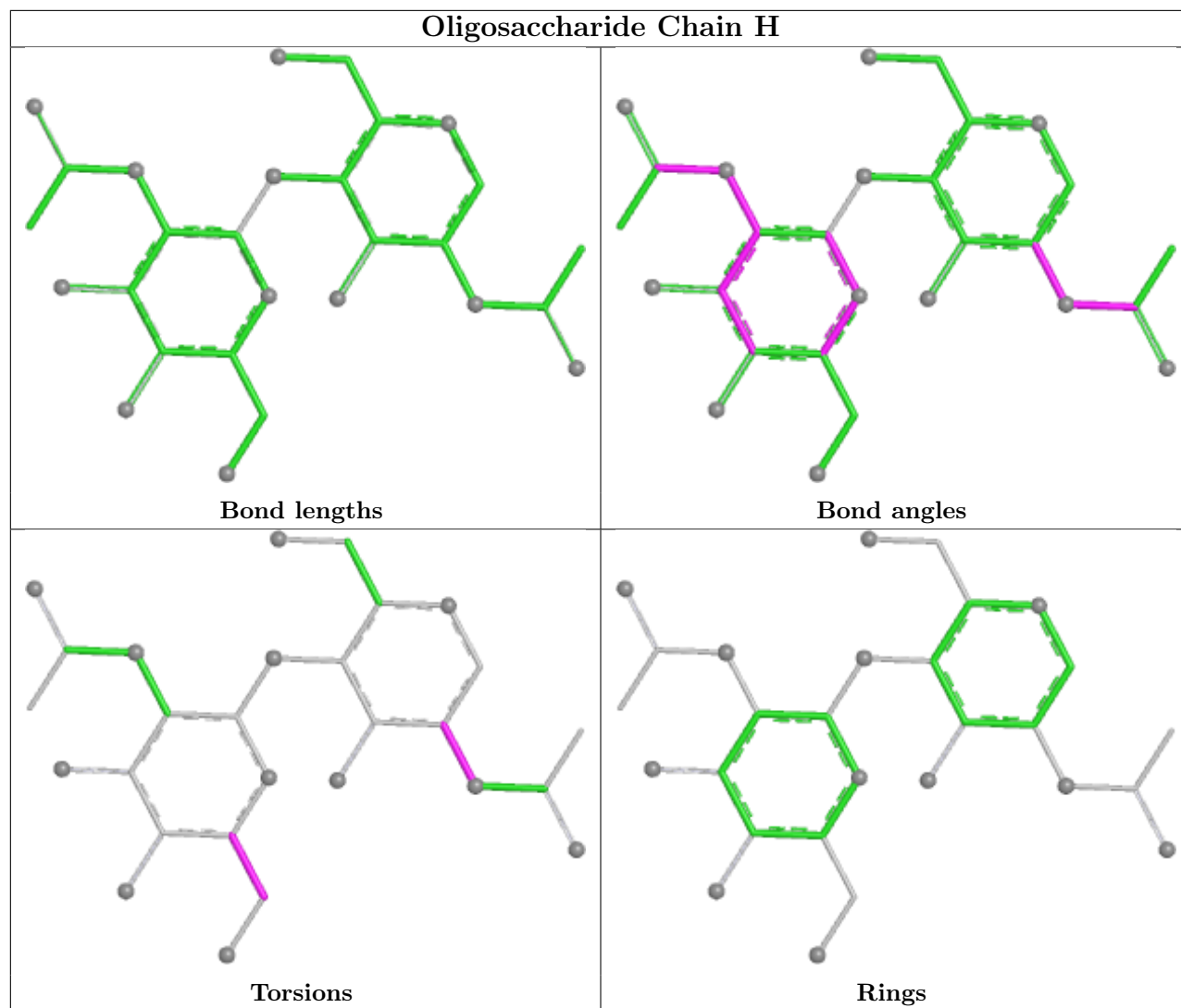
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C4-C5-C6-O6

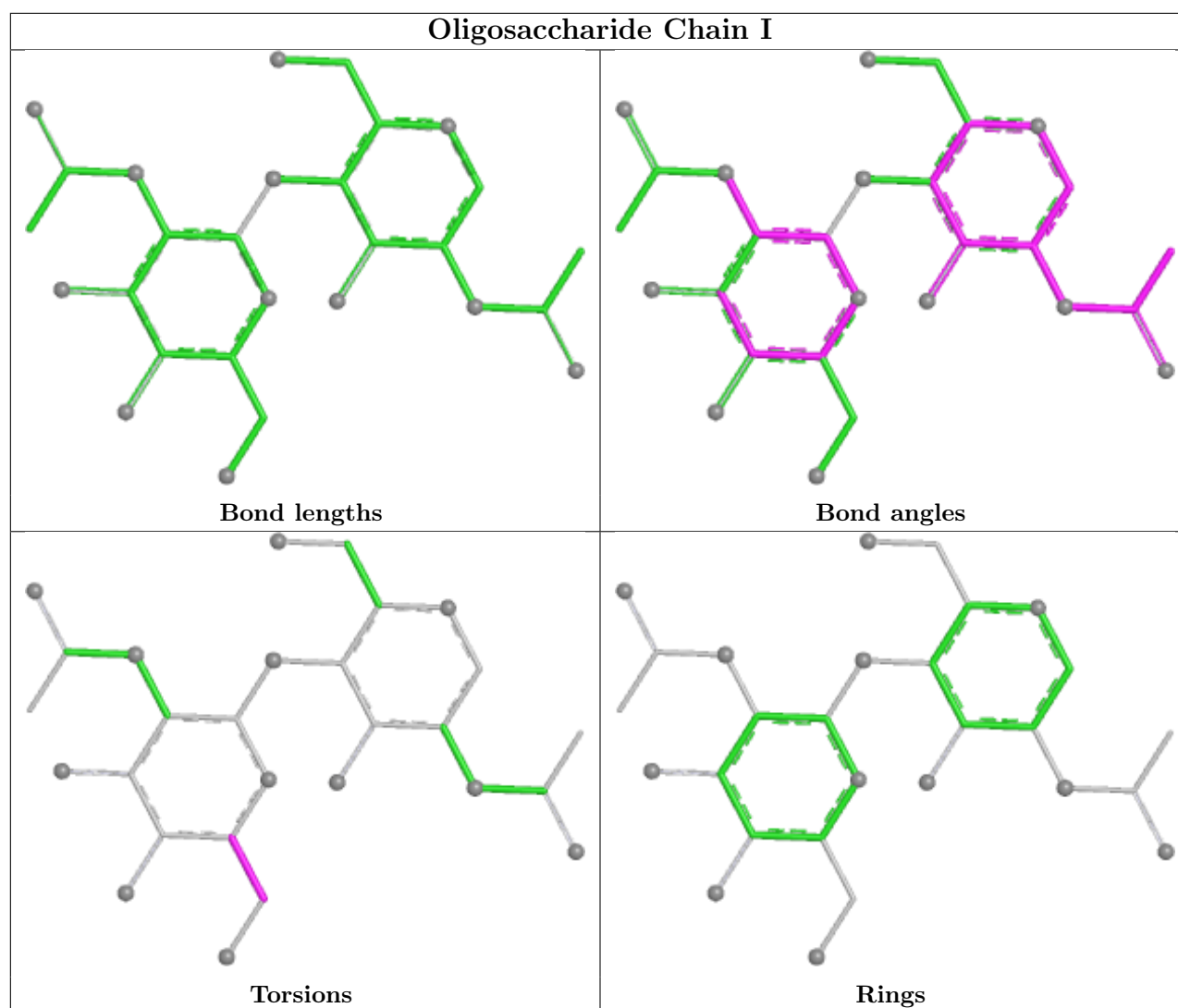
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	C	603	1	14,14,15	0.87	1 (7%)	17,19,21	2.13	3 (17%)
4	NAG	E	604	1	14,14,15	0.62	0	17,19,21	1.37	4 (23%)
3	SO4	D	606	-	4,4,4	0.48	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	603	-	4,4,4	0.59	0	6,6,6	0.86	0
4	NAG	E	603	1	14,14,15	0.55	0	17,19,21	2.15	4 (23%)
4	NAG	F	602	1	14,14,15	0.67	0	17,19,21	1.50	4 (23%)
4	NAG	D	601	1	14,14,15	0.80	0	17,19,21	1.58	3 (17%)
3	SO4	C	604	-	4,4,4	0.91	0	6,6,6	1.78	2 (33%)
4	NAG	D	602	1	14,14,15	0.45	0	17,19,21	1.60	2 (11%)
4	NAG	A	601	1	14,14,15	0.72	1 (7%)	17,19,21	1.75	3 (17%)
3	SO4	E	605	-	4,4,4	0.48	0	6,6,6	1.15	0
4	NAG	A	602	1	14,14,15	0.58	0	17,19,21	2.39	5 (29%)
4	NAG	D	605	1	14,14,15	0.62	0	17,19,21	1.16	2 (11%)
3	SO4	B	603	-	4,4,4	0.44	0	6,6,6	0.22	0
4	NAG	F	601	1	14,14,15	0.66	0	17,19,21	1.63	2 (11%)
4	NAG	E	602	1	14,14,15	0.58	0	17,19,21	1.51	2 (11%)
4	NAG	E	601	1	14,14,15	0.64	0	17,19,21	1.99	4 (23%)
3	SO4	A	603	-	4,4,4	0.69	0	6,6,6	0.81	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	C	603	1	-	1/6/23/26	0/1/1/1
4	NAG	E	604	1	-	2/6/23/26	0/1/1/1
4	NAG	E	603	1	-	1/6/23/26	0/1/1/1
4	NAG	F	602	1	-	2/6/23/26	0/1/1/1
4	NAG	D	601	1	-	0/6/23/26	0/1/1/1
4	NAG	D	602	1	-	2/6/23/26	0/1/1/1
4	NAG	D	605	1	-	1/6/23/26	0/1/1/1
4	NAG	A	602	1	-	1/6/23/26	0/1/1/1
4	NAG	F	601	1	-	1/6/23/26	0/1/1/1
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	E	601	1	-	1/6/23/26	0/1/1/1
4	NAG	E	602	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	NAG	C1-C2	2.33	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	NAG	C1-C2	2.05	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	NAG	C1-O5-C5	6.92	121.46	112.19
4	C	603	NAG	C1-O5-C5	6.89	121.42	112.19
4	E	603	NAG	C1-O5-C5	5.95	120.16	112.19
4	A	601	NAG	C1-O5-C5	4.76	118.56	112.19
4	E	601	NAG	C2-N2-C7	4.62	129.09	122.90
4	D	602	NAG	C1-O5-C5	4.37	118.04	112.19
4	A	602	NAG	O5-C1-C2	-4.31	104.62	111.29
4	E	603	NAG	O5-C1-C2	-4.26	104.70	111.29
4	E	602	NAG	C4-C3-C2	-4.13	104.97	111.02
4	F	601	NAG	C1-O5-C5	4.07	117.64	112.19
4	E	601	NAG	C4-C3-C2	3.87	116.69	111.02
4	D	601	NAG	C4-C3-C2	3.53	116.18	111.02
4	F	602	NAG	C4-C3-C2	3.43	116.04	111.02
4	F	601	NAG	C1-C2-N2	3.38	115.76	110.43
4	E	601	NAG	C1-C2-N2	-3.16	105.45	110.43
4	E	602	NAG	C1-O5-C5	3.15	116.41	112.19
4	A	601	NAG	C1-C2-N2	3.11	115.34	110.43
4	A	602	NAG	O5-C5-C4	3.06	118.26	110.83
4	D	605	NAG	C2-N2-C7	3.01	126.93	122.90
4	D	601	NAG	C3-C4-C5	2.97	115.62	110.23
3	C	604	SO4	O4-S-O2	-2.91	94.37	109.56
4	E	604	NAG	C4-C3-C2	2.78	115.09	111.02
4	E	601	NAG	C3-C4-C5	2.69	115.12	110.23
4	E	604	NAG	C2-N2-C7	2.66	126.47	122.90
4	D	602	NAG	O5-C1-C2	-2.64	107.20	111.29
4	C	603	NAG	O5-C5-C6	2.64	112.79	107.66
4	E	604	NAG	C1-O5-C5	2.62	115.69	112.19
4	E	603	NAG	C1-C2-N2	2.57	114.48	110.43
4	C	603	NAG	C1-C2-N2	2.49	114.36	110.43
4	E	603	NAG	C3-C4-C5	2.49	114.74	110.23
4	A	602	NAG	C3-C4-C5	2.44	114.65	110.23
4	A	602	NAG	C1-C2-N2	2.36	114.15	110.43
4	D	601	NAG	C1-C2-N2	2.27	114.02	110.43
4	F	602	NAG	O7-C7-C8	-2.26	118.03	122.05
4	E	604	NAG	O5-C1-C2	2.24	114.76	111.29
4	F	602	NAG	C2-N2-C7	2.23	125.89	122.90
4	D	605	NAG	O7-C7-N2	2.14	125.76	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	604	SO4	O2-S-O1	2.12	123.96	109.06
4	F	602	NAG	C1-O5-C5	2.01	114.88	112.19
4	A	601	NAG	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	602	NAG	O5-C5-C6-O6
4	E	602	NAG	C4-C5-C6-O6
4	E	602	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	F	602	NAG	C4-C5-C6-O6
4	D	602	NAG	C4-C5-C6-O6
4	E	604	NAG	O5-C5-C6-O6
4	E	604	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	F	602	NAG	O5-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6
4	D	605	NAG	O5-C5-C6-O6
4	E	603	NAG	O5-C5-C6-O6
4	C	603	NAG	O5-C5-C6-O6
4	F	601	NAG	C4-C5-C6-O6
4	E	601	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	606	SO4	1	0
3	F	603	SO4	1	0
4	E	603	NAG	1	0
4	F	602	NAG	2	0
4	D	605	NAG	2	0
3	B	603	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	440/501 (87%)	0.44	19 (4%)	40	24	43, 91, 149, 193	0
1	B	447/501 (89%)	0.44	15 (3%)	48	30	52, 81, 147, 170	0
1	C	454/501 (90%)	0.53	20 (4%)	39	24	51, 94, 151, 183	0
1	D	460/501 (91%)	0.41	17 (3%)	45	28	54, 84, 155, 194	0
1	E	436/501 (87%)	0.48	22 (5%)	34	22	55, 91, 154, 203	0
1	F	436/501 (87%)	0.49	26 (5%)	27	17	48, 90, 149, 184	0
All	All	2673/3006 (88%)	0.47	119 (4%)	38	24	43, 88, 151, 203	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	452	ASP	6.3
1	A	197	LEU	4.7
1	E	452	ASP	4.6
1	F	396	THR	4.2
1	F	102	HIS	4.1
1	E	282	PHE	3.8
1	B	253	PHE	3.7
1	A	452	ASP	3.6
1	B	164	THR	3.4
1	E	102	HIS	3.3
1	B	322	LEU	3.3
1	E	197	LEU	3.3
1	D	164	THR	3.3
1	B	99	ASN	3.3
1	A	102	HIS	3.2
1	F	474	ILE	3.2
1	D	274	TYR	3.2
1	F	452	ASP	3.2
1	E	247	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	102	HIS	3.2
1	F	157	ALA	3.1
1	A	396	THR	3.1
1	F	175	LEU	3.0
1	F	178	TYR	3.0
1	A	104	LEU	3.0
1	C	92	GLY	3.0
1	F	114	VAL	3.0
1	C	282	PHE	3.0
1	F	58	VAL	2.9
1	F	247	GLY	2.9
1	B	163	GLU	2.9
1	D	163	GLU	2.9
1	B	247	GLY	2.9
1	D	446	GLY	2.9
1	C	154	THR	2.9
1	E	304	ASP	2.9
1	E	305	ASN	2.9
1	D	247	GLY	2.8
1	F	333	ILE	2.8
1	F	156	GLU	2.8
1	A	322	LEU	2.8
1	F	135	TYR	2.8
1	C	157	ALA	2.8
1	C	96	LEU	2.8
1	B	304	ASP	2.7
1	D	322	LEU	2.7
1	C	95	GLU	2.7
1	A	67	ASN	2.7
1	B	474	ILE	2.6
1	F	197	LEU	2.6
1	D	424	ASN	2.6
1	E	92	GLY	2.6
1	F	442	SER	2.6
1	D	452	ASP	2.6
1	C	252	ASP	2.6
1	C	459	GLN	2.6
1	A	135	TYR	2.6
1	F	322	LEU	2.6
1	E	310	SER	2.5
1	A	247	GLY	2.5
1	E	95	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	138	MET	2.5
1	B	102	HIS	2.5
1	C	322	LEU	2.5
1	B	461	SER	2.5
1	F	174	ALA	2.5
1	A	158	VAL	2.5
1	F	142	ASP	2.5
1	E	455	ASP	2.5
1	E	468	GLN	2.5
1	B	327	GLU	2.4
1	E	166	GLU	2.4
1	C	253	PHE	2.4
1	B	108	VAL	2.4
1	E	322	LEU	2.4
1	F	165	ALA	2.4
1	C	453	LYS	2.4
1	E	235	PHE	2.4
1	A	252	ASP	2.4
1	D	462	SER	2.3
1	C	443	ILE	2.3
1	F	246	LEU	2.3
1	E	399	ARG	2.3
1	C	26	GLY	2.3
1	C	175	LEU	2.3
1	B	139	LYS	2.3
1	A	443	ILE	2.2
1	A	175	LEU	2.2
1	D	473	TYR	2.2
1	B	274	TYR	2.2
1	C	381	GLY	2.2
1	D	102	HIS	2.2
1	E	154	THR	2.2
1	D	474	ILE	2.2
1	F	443	ILE	2.2
1	F	398	GLY	2.2
1	F	448	PRO	2.2
1	A	142	ASP	2.2
1	B	138	MET	2.1
1	E	381	GLY	2.1
1	A	424	ASN	2.1
1	F	256	LEU	2.1
1	C	483	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	266	ILE	2.1
1	F	43	THR	2.1
1	A	58	VAL	2.1
1	D	139	LYS	2.1
1	E	323	ILE	2.1
1	F	252	ASP	2.1
1	D	135	TYR	2.1
1	D	253	PHE	2.1
1	A	451	THR	2.0
1	D	216	PRO	2.0
1	C	476	GLU	2.0
1	E	327	GLU	2.0
1	A	205	LYS	2.0
1	E	164	THR	2.0
1	A	244	ARG	2.0
1	C	197	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

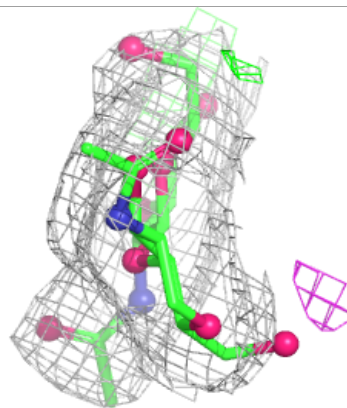
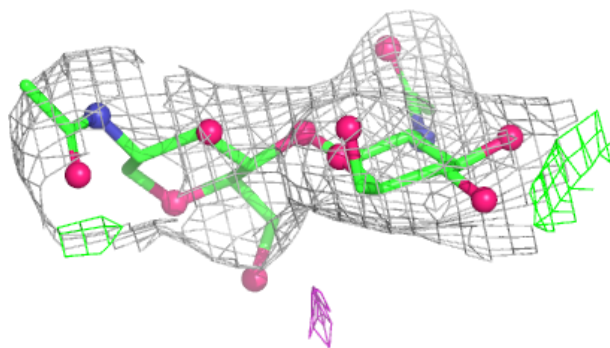
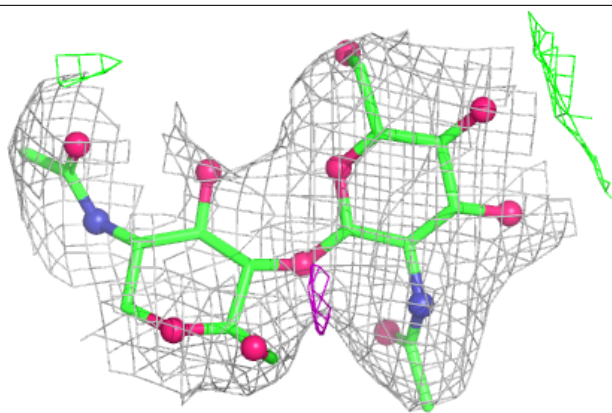
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.17	0.15	156,169,176,185	0
2	NAG	G	2	14/15	0.77	0.11	79,86,99,100	0
2	NAG	I	1	14/15	0.77	0.17	66,92,103,111	0
2	NAG	I	2	14/15	0.83	0.10	74,90,109,124	0
2	NAG	H	1	14/15	0.84	0.10	83,109,134,154	0
2	NAG	G	1	14/15	0.87	0.12	63,78,95,101	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.

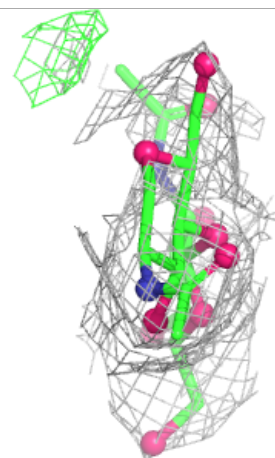
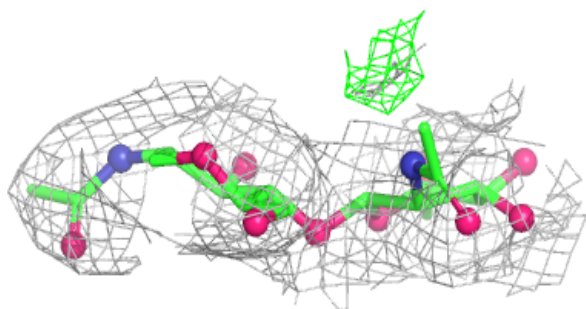
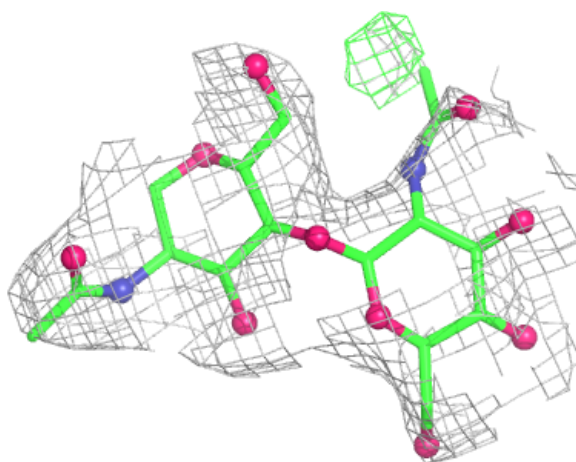
Electron density around Chain G:

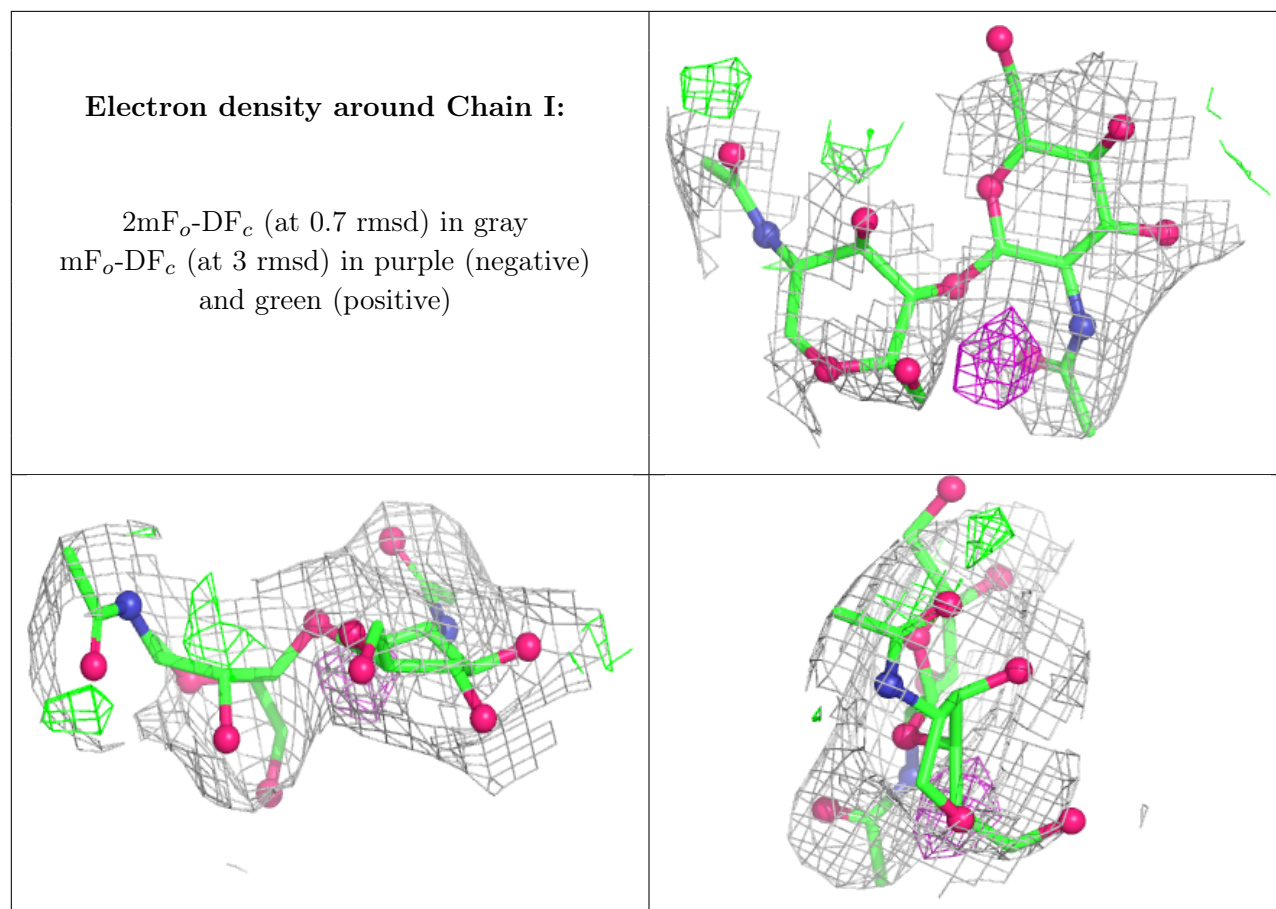
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	601	14/15	0.55	0.18	103,132,141,146	0
4	NAG	A	602	14/15	0.61	0.13	108,123,132,139	0
4	NAG	E	601	14/15	0.63	0.13	100,128,139,142	0
4	NAG	E	603	14/15	0.65	0.16	110,134,146,149	0
4	NAG	F	601	14/15	0.67	0.13	116,132,146,150	0
4	NAG	C	603	14/15	0.69	0.14	90,111,122,123	0
4	NAG	E	602	14/15	0.69	0.12	122,149,159,160	0
4	NAG	E	604	14/15	0.73	0.16	110,132,162,162	0
4	NAG	F	602	14/15	0.73	0.16	98,112,127,129	0
4	NAG	D	602	14/15	0.74	0.11	130,150,165,168	0
4	NAG	A	601	14/15	0.78	0.13	113,129,140,146	0
3	SO4	B	603	5/5	0.87	0.10	125,127,137,140	0
4	NAG	D	605	14/15	0.87	0.11	102,122,135,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	606	5/5	0.89	0.12	111,124,131,137	0
3	SO4	F	603	5/5	0.93	0.09	53,66,68,68	0
3	SO4	C	604	5/5	0.94	0.11	38,50,56,61	0
3	SO4	E	605	5/5	0.96	0.09	59,59,69,75	0
3	SO4	A	603	5/5	0.96	0.07	51,52,68,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.