



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:28 PM UTC

PDB ID : 1UHG / pdb_00001uhg
Title : Crystal Structure of S-Ovalbumin At 1.9 Angstrom Resolution
Authors : Yamasaki, M.; Takahashi, N.; Hirose, M.
Deposited on : 2003-07-03
Resolution : 1.90 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

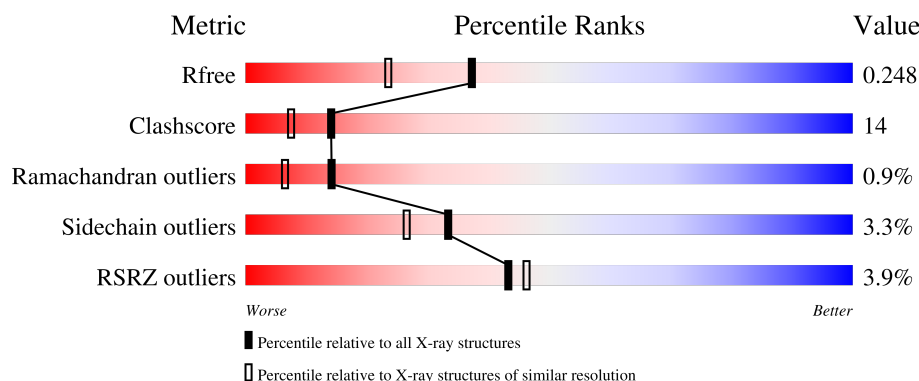
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	6% 72% 25% ..
1	B	385	3% 73% 25% .
1	C	385	4% 69% 24% ..
1	D	385	3% 74% 24% .
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	
2	G	2	

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
1	DSN	D	164	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12910 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 Ovalbumin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	P	S	0	0	0
			2987	1891	496	576	2	22			
1	B	385	Total	C	N	O	P	S	0	0	0
			3001	1901	499	578	1	22			
1	C	374	Total	C	N	O	P	S	0	0	0
			2933	1865	488	558		22			
1	D	385	Total	C	N	O	P	S	0	0	0
			3005	1901	499	581	2	22			

There are 20 discrepancies between the modelled and reference sequences:

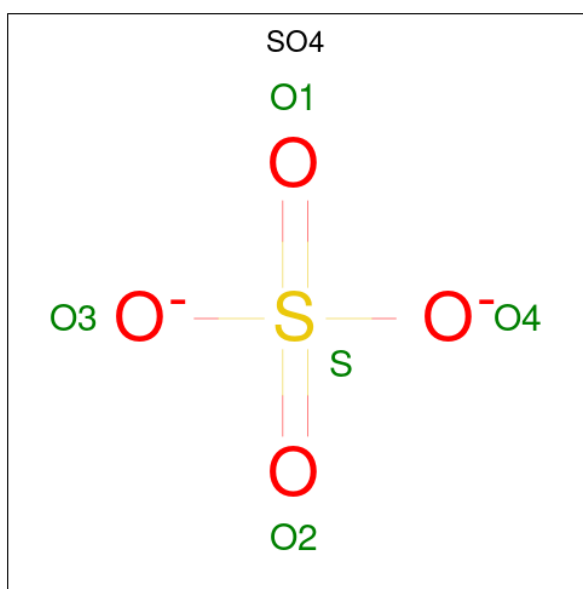
Chain	Residue	Modelled	Actual	Comment	Reference
A	68	SEP	SER	modified residue	UNP P01012
A	164	DSN	SER	modified residue	UNP P01012
A	236	DSN	SER	modified residue	UNP P01012
A	320	DSN	SER	modified residue	UNP P01012
A	344	SEP	SER	modified residue	UNP P01012
B	68	SEP	SER	modified residue	UNP P01012
B	164	DSN	SER	modified residue	UNP P01012
B	236	DSN	SER	modified residue	UNP P01012
B	320	DSN	SER	modified residue	UNP P01012
B	344	SEP	SER	modified residue	UNP P01012
C	68	SEP	SER	modified residue	UNP P01012
C	164	DSN	SER	modified residue	UNP P01012
C	236	DSN	SER	modified residue	UNP P01012
C	320	DSN	SER	modified residue	UNP P01012
C	344	SEP	SER	modified residue	UNP P01012
D	68	SEP	SER	modified residue	UNP P01012
D	164	DSN	SER	modified residue	UNP P01012
D	236	DSN	SER	modified residue	UNP P01012
D	320	DSN	SER	modified residue	UNP P01012
D	344	SEP	SER	modified residue	UNP P01012

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



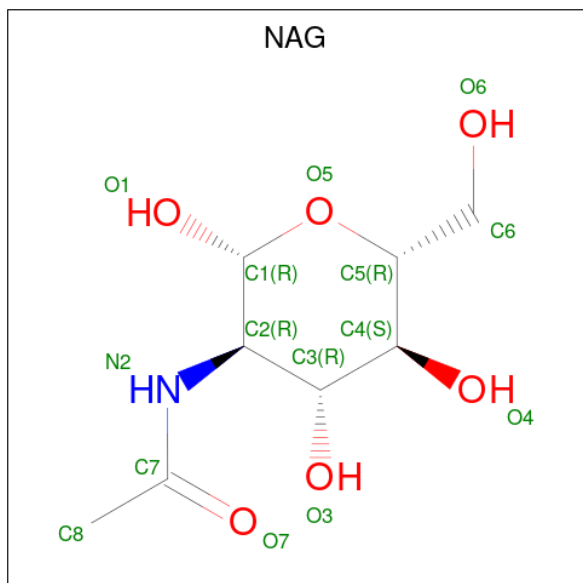
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

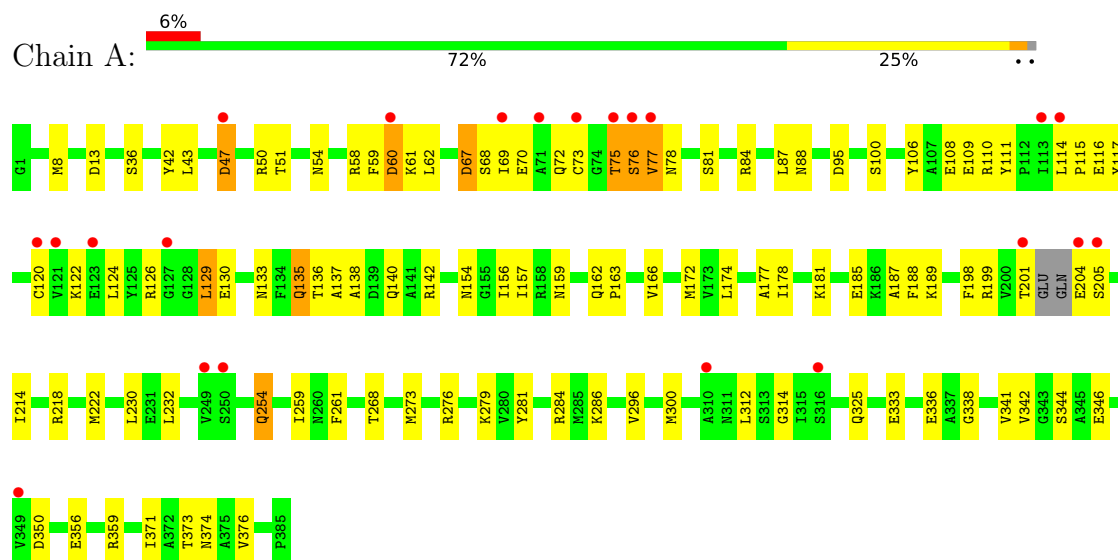
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	218	Total	O	0	0
			218	218		
5	B	219	Total	O	0	0
			219	219		
5	C	206	Total	O	0	0
			206	206		
5	D	208	Total	O	0	0
			208	208		

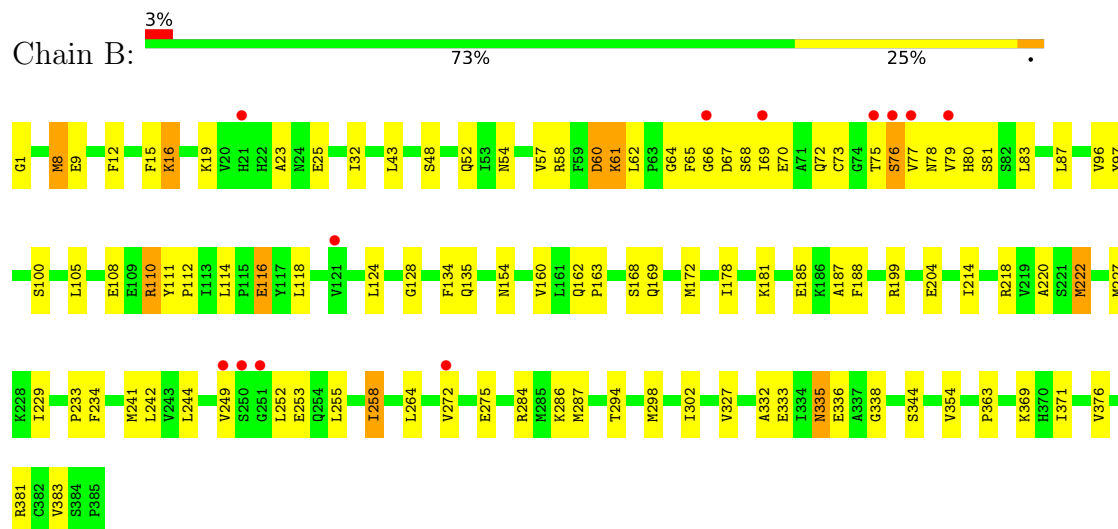
3 Residue-property plots

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: Ovalbumin

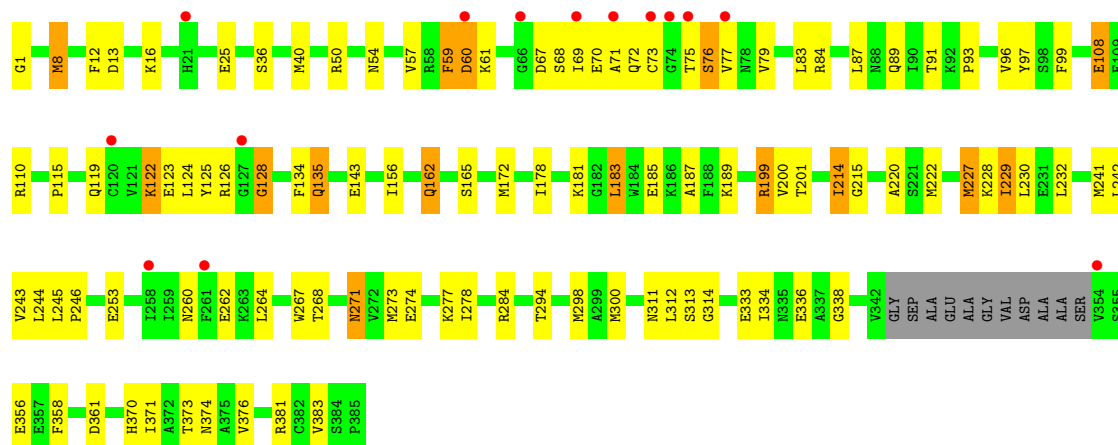


• Molecule 1: Ovalbumin

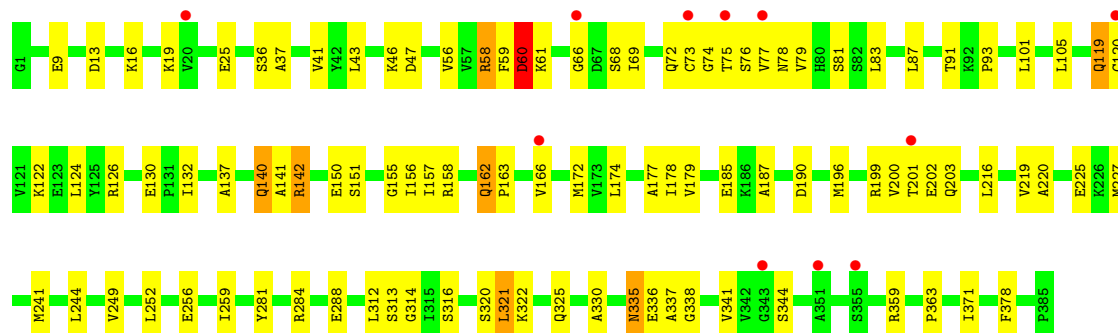
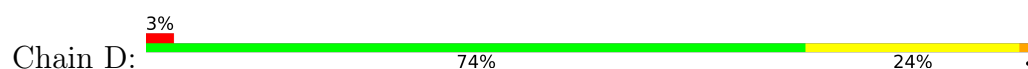


• Molecule 1: Ovalbumin





• Molecule 1: Ovalbumin



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.65Å 70.91Å 83.39Å 87.24° 71.73° 75.95°	Depositor
Resolution (Å)	14.89 – 1.90 14.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (14.89-1.90) 96.0 (14.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.247 0.198 , 0.248	Depositor DCC
R_{free} test set	10051 reflections (8.66%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 53.5	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	0.95	EDS
Total number of atoms	12910	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% 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, DSN, NAG, SEP

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	0.60	0/2999	1.00	11/4043 (0.3%)
1	B	0.60	1/3018 (0.0%)	0.98	10/4070 (0.2%)
1	C	0.61	0/2960	0.96	9/3991 (0.2%)
1	D	0.63	1/3018 (0.0%)	0.96	9/4070 (0.2%)
All	All	0.61	2/11995 (0.0%)	0.97	39/16174 (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	D	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	MET	SD-CE	-7.88	1.59	1.79
1	B	241	MET	SD-CE	-6.43	1.63	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	ARG	N-CA-C	-8.01	98.43	110.28
1	A	371	ILE	N-CA-C	7.78	117.89	110.42
1	A	284	ARG	N-CA-C	-7.74	98.83	110.28
1	B	185	GLU	N-CA-C	-7.47	103.22	111.36
1	D	185	GLU	N-CA-C	-7.46	103.22	111.36
1	D	284	ARG	N-CA-C	-7.44	99.27	110.28
1	B	336	GLU	N-CA-C	7.27	120.25	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ILE	N-CA-C	7.15	117.92	110.62
1	C	371	ILE	N-CA-C	6.95	117.71	110.62
1	D	371	ILE	N-CA-C	6.84	116.98	110.42
1	A	336	GLU	N-CA-C	6.83	119.74	111.82
1	A	62	LEU	N-CA-C	6.55	118.15	109.83
1	D	336	GLU	N-CA-C	6.52	119.38	111.82
1	B	284	ARG	N-CA-C	-6.32	100.93	110.28
1	B	128	GLY	N-CA-C	6.19	121.66	114.16
1	C	135	GLN	N-CA-C	6.18	118.52	111.11
1	B	188	PHE	N-CA-C	-6.07	100.67	110.32
1	B	354	VAL	N-CA-C	6.07	116.85	107.99
1	C	128	GLY	N-CA-C	6.07	120.54	112.77
1	C	336	GLU	N-CA-C	6.05	118.84	111.82
1	A	185	GLU	N-CA-C	-6.04	104.61	111.14
1	A	259	ILE	N-CA-C	6.04	117.37	109.58
1	A	59	PHE	N-CA-C	-6.00	105.79	113.23
1	B	234	PHE	N-CA-C	-5.86	101.85	110.52
1	B	62	LEU	N-CA-C	5.75	117.06	109.93
1	D	56	VAL	N-CA-C	5.72	116.50	110.72
1	A	188	PHE	N-CA-C	-5.69	100.43	109.76
1	D	81	SER	N-CA-C	5.68	117.92	111.11
1	C	185	GLU	N-CA-C	-5.56	105.14	111.14
1	C	156	ILE	N-CA-C	5.41	116.06	110.82
1	A	156	ILE	N-CA-C	5.34	116.00	110.82
1	D	337	ALA	N-CA-C	5.30	118.03	110.24
1	D	314	GLY	N-CA-C	-5.23	108.18	114.66
1	C	314	GLY	N-CA-C	-5.20	108.51	115.32
1	C	59	PHE	N-CA-C	-5.18	106.47	112.89
1	B	214	ILE	N-CA-C	-5.12	100.94	108.11
1	A	47	ASP	CB-CA-C	-5.12	110.65	116.54
1	A	81	SER	N-CA-C	5.06	117.45	111.33
1	D	13	ASP	N-CA-C	-5.04	105.86	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

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	2987	0	2964	86	0
1	B	3001	0	2978	87	0
1	C	2933	0	2924	100	0
1	D	3005	0	2979	86	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	D	14	0	13	3	0
5	A	218	0	0	10	0
5	B	219	0	0	3	0
5	C	206	0	0	1	0
5	D	208	0	0	6	0
All	All	12910	0	11933	344	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 14.

All (344) 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:C:99:PHE:CZ	1:C:178:ILE:HD11	1.92	1.04
1:B:199:ARG:HG2	1:B:249:VAL:HG21	1.54	0.89
1:D:162:GLN:H	1:D:162:GLN:NE2	1.72	0.86
1:B:100:SER:O	1:B:178:ILE:HD12	1.76	0.85
1:D:178:ILE:HD13	1:D:378:PHE:HE1	1.40	0.84
1:A:43:LEU:HD13	1:A:120:CYS:SG	2.17	0.84
1:B:286:LYS:HG3	1:B:333:GLU:HG2	1.63	0.81
1:D:312:LEU:HD12	1:D:321:LEU:HD22	1.61	0.81
1:A:100:SER:O	1:A:178:ILE:HD12	1.82	0.80
1:A:218:ARG:HH21	1:A:273:MET:HB2	1.45	0.80
1:D:172:MET:HE2	1:D:321:LEU:HD21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:C	1:B:110:ARG:HD3	2.07	0.79
1:C:199:ARG:HD3	1:C:199:ARG:N	1.99	0.78
1:C:278:ILE:HG22	1:C:356:GLU:HG2	1.65	0.77
1:B:8:MET:HG2	1:B:376:VAL:HG23	1.66	0.77
1:B:58:ARG:HB3	1:B:61:LYS:NZ	2.00	0.76
1:B:69:ILE:HG12	1:B:79:VAL:HG12	1.67	0.76
1:B:286:LYS:HE3	1:B:333:GLU:CD	2.11	0.74
1:B:108:GLU:OE1	1:B:110:ARG:HG3	1.86	0.74
1:D:172:MET:CE	1:D:321:LEU:HD21	2.17	0.73
1:C:8:MET:HE3	1:C:376:VAL:HG21	1.70	0.72
1:B:287:MET:HE2	1:B:332:ALA:HB3	1.69	0.72
1:C:122:LYS:NZ	1:C:123:GLU:HB2	2.04	0.72
1:D:341:VAL:HG22	5:D:4145:HOH:O	1.89	0.72
1:B:222:MET:HE3	1:B:222:MET:H	1.56	0.71
1:D:162:GLN:H	1:D:162:GLN:CD	1.97	0.71
1:B:58:ARG:HB3	1:B:61:LYS:HZ1	1.56	0.71
1:C:220:ALA:HB3	1:C:229:ILE:CG2	2.21	0.71
1:A:254:GLN:C	1:A:254:GLN:HE21	1.98	0.71
1:B:199:ARG:HH21	1:B:204:GLU:C	2.00	0.69
1:A:114:LEU:HD23	1:A:116:GLU:H	1.58	0.69
1:C:162:GLN:HE22	1:C:165:SER:HB3	1.57	0.69
1:B:8:MET:HG2	1:B:376:VAL:CG2	2.23	0.69
1:D:325:GLN:HE22	4:D:386:NAG:H82	1.58	0.69
1:A:325:GLN:HE22	2:E:1:NAG:HN2	1.39	0.69
1:C:214:ILE:C	1:C:214:ILE:HD13	2.18	0.68
1:D:43:LEU:HD13	1:D:120:CYS:SG	2.34	0.68
1:A:122:LYS:O	1:A:122:LYS:HD3	1.93	0.68
1:C:264:LEU:C	1:C:264:LEU:HD13	2.18	0.68
1:C:1:GLY:HA3	1:C:61:LYS:HD3	1.76	0.67
1:D:178:ILE:HD11	1:D:330:ALA:HB1	1.74	0.67
1:C:91:THR:O	1:D:93:PRO:HG2	1.94	0.67
1:B:116:GLU:CD	1:B:116:GLU:H	2.03	0.67
1:C:99:PHE:CE1	1:C:178:ILE:HD11	2.30	0.67
1:D:178:ILE:HD13	1:D:378:PHE:CE1	2.28	0.67
1:D:178:ILE:HD11	1:D:330:ALA:CB	2.25	0.66
1:B:1:GLY:N	1:B:61:LYS:HD2	2.11	0.66
1:A:163:PRO:HD3	1:C:75:THR:HG21	1.79	0.65
1:A:129:LEU:HD13	1:A:129:LEU:C	2.22	0.64
1:B:72:GLN:O	1:B:79:VAL:HG11	1.98	0.64
1:D:66:GLY:O	1:D:69:ILE:HG22	1.98	0.63
1:D:142:ARG:HG3	1:D:166:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:GLY:HA3	5:D:2082:HOH:O	1.98	0.63
1:D:178:ILE:HD12	1:D:178:ILE:O	1.98	0.63
1:A:117:TYR:O	1:A:120:CYS:HB3	1.98	0.63
1:C:122:LYS:HD3	1:C:123:GLU:N	2.14	0.63
1:A:142:ARG:NH1	1:A:163:PRO:HD3	2.15	0.62
1:B:12:PHE:O	1:B:16:LYS:HD3	1.99	0.62
1:D:321:LEU:HD23	1:D:322:LYS:N	2.15	0.62
1:C:99:PHE:CZ	1:C:178:ILE:CD1	2.77	0.62
1:B:168:SER:OG	1:B:169:GLN:NE2	2.33	0.61
1:B:58:ARG:CB	1:B:61:LYS:HZ1	2.12	0.61
1:B:163:PRO:HG2	1:D:119:GLN:HG3	1.82	0.61
2:G:2:NAG:O7	2:G:2:NAG:H3	2.00	0.61
1:A:109:GLU:OE2	1:A:133:ASN:HB2	2.01	0.61
1:A:214:ILE:HG21	1:A:350:ASP:HB3	1.83	0.61
1:B:48:SER:O	1:B:52:GLN:HG3	2.00	0.60
1:C:214:ILE:HD13	1:C:215:GLY:N	2.16	0.60
1:D:79:VAL:HB	1:D:124:LEU:HD11	1.84	0.60
1:A:122:LYS:HD3	1:A:122:LYS:C	2.27	0.60
1:C:222:MET:HG2	1:C:227:MET:HE2	1.84	0.60
1:A:47:ASP:O	1:A:51:THR:HG23	2.02	0.59
1:C:222:MET:HE2	1:C:267:TRP:CD1	2.38	0.59
1:A:126:ARG:NH2	5:A:1212:HOH:O	2.35	0.59
1:C:162:GLN:NE2	1:C:165:SER:HB3	2.18	0.59
1:A:198:PHE:O	1:A:205:SER:HB2	2.02	0.59
1:C:189:LYS:HZ3	1:D:140:GLN:HG3	1.68	0.59
1:D:200:VAL:HG23	1:D:201:THR:HG23	1.85	0.59
1:C:57:VAL:HG12	1:C:57:VAL:O	2.03	0.59
1:B:64:GLY:HA2	1:B:69:ILE:HD13	1.84	0.59
1:B:58:ARG:HB2	5:B:2107:HOH:O	2.03	0.59
1:C:8:MET:HG2	1:C:376:VAL:CG2	2.33	0.58
1:C:172:MET:HE1	1:C:312:LEU:HD13	1.84	0.58
1:C:244:LEU:N	1:C:244:LEU:HD12	2.18	0.58
1:C:311:ASN:C	1:C:311:ASN:HD22	2.11	0.58
1:C:199:ARG:HD3	1:C:199:ARG:H	1.68	0.58
1:A:230:LEU:HD21	1:A:232:LEU:HD21	1.85	0.57
4:D:386:NAG:O3	4:D:386:NAG:H83	2.03	0.57
1:B:110:ARG:HD2	1:B:111:TYR:CD1	2.38	0.57
1:B:199:ARG:HG2	1:B:249:VAL:CG2	2.30	0.57
1:A:58:ARG:HB2	5:A:1238:HOH:O	2.04	0.57
1:C:220:ALA:HB2	1:C:273:MET:HG2	1.87	0.57
1:B:218:ARG:HG2	1:B:275:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:SER:HB3	1:D:321:LEU:HD12	1.85	0.57
1:D:75:THR:O	1:D:77:VAL:N	2.39	0.56
1:B:1:GLY:H1	1:B:61:LYS:HD2	1.70	0.56
1:A:114:LEU:CD2	1:A:116:GLU:HB3	2.36	0.56
1:B:381:ARG:HD3	1:B:383:VAL:HG13	1.88	0.56
1:C:8:MET:HG2	1:C:376:VAL:HG23	1.88	0.56
1:D:101:LEU:HD13	1:D:178:ILE:CG2	2.36	0.56
1:D:335:ASN:HD22	1:D:335:ASN:C	2.13	0.55
1:B:110:ARG:HG2	1:B:135:GLN:OE1	2.07	0.55
1:C:271:ASN:N	1:C:271:ASN:HD22	2.04	0.55
1:A:13:ASP:HB3	1:A:300:MET:HE3	1.88	0.55
1:D:219:VAL:HG22	1:D:220:ALA:N	2.21	0.55
1:D:132:ILE:HD11	1:D:141:ALA:HA	1.88	0.55
1:A:174:LEU:HG	5:A:1178:HOH:O	2.06	0.55
1:A:268:THR:HG22	1:A:273:MET:HE2	1.89	0.55
1:C:91:THR:O	1:D:93:PRO:CG	2.55	0.54
1:B:79:VAL:CG2	1:B:124:LEU:HD21	2.38	0.54
1:A:341:VAL:HG22	1:A:342:VAL:N	2.21	0.54
1:A:137:ALA:HB1	1:A:140:GLN:HB3	1.90	0.54
1:D:155:GLY:O	1:D:158:ARG:NH2	2.36	0.54
1:B:54:ASN:OD1	1:B:60:ASP:HB3	2.07	0.54
1:B:222:MET:SD	1:B:227:MET:HE2	2.48	0.54
1:A:114:LEU:HD23	1:A:116:GLU:N	2.24	0.53
1:C:229:ILE:HD11	1:C:242:LEU:HB3	1.90	0.53
1:A:13:ASP:OD2	1:A:58:ARG:NH2	2.37	0.53
1:A:108:GLU:OE1	1:A:135:GLN:HG3	2.07	0.53
1:A:214:ILE:HG12	1:A:279:LYS:HG2	1.90	0.53
1:A:114:LEU:HD21	1:A:116:GLU:HB3	1.89	0.53
1:D:150:GLU:HG3	1:D:155:GLY:HA2	1.89	0.53
1:B:79:VAL:HG23	1:B:124:LEU:CD2	2.38	0.53
1:A:218:ARG:HD3	5:A:1173:HOH:O	2.09	0.53
1:B:79:VAL:HG23	1:B:124:LEU:HD21	1.90	0.53
1:D:172:MET:HE2	1:D:321:LEU:CD2	2.37	0.52
1:D:178:ILE:CD1	1:D:378:PHE:HE1	2.17	0.52
1:B:70:GLU:C	1:B:72:GLN:H	2.16	0.52
1:A:77:VAL:HG12	1:A:77:VAL:O	2.10	0.52
1:A:8:MET:HG3	1:A:376:VAL:HG23	1.91	0.52
1:C:162:GLN:NE2	1:C:162:GLN:H	2.07	0.52
1:A:189:LYS:HE2	1:A:341:VAL:HG21	1.92	0.52
1:B:60:ASP:O	1:B:61:LYS:HB3	2.09	0.52
1:C:189:LYS:NZ	1:D:140:GLN:HG3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASN:HD22	1:C:313:SER:H	1.58	0.51
1:A:108:GLU:HB3	1:A:111:TYR:HD1	1.75	0.51
1:B:255:LEU:O	1:B:258:ILE:HD13	2.10	0.51
1:C:119:GLN:O	1:C:122:LYS:HD3	2.10	0.51
1:A:138:ALA:HB1	1:A:166:VAL:HG12	1.93	0.51
1:C:199:ARG:NH2	1:C:361:ASP:OD2	2.44	0.51
1:D:36:SER:HA	1:D:83:LEU:HD21	1.91	0.51
1:C:260:ASN:OD1	1:C:262:GLU:HB2	2.10	0.51
1:A:84:ARG:NE	1:A:124:LEU:O	2.44	0.51
1:B:58:ARG:CG	1:B:61:LYS:HZ1	2.23	0.51
1:B:77:VAL:HG22	1:B:77:VAL:O	2.10	0.51
1:B:110:ARG:HD3	1:B:111:TYR:N	2.26	0.51
1:A:73:CYS:SG	1:A:124:LEU:HD12	2.51	0.50
1:A:199:ARG:HD2	1:A:199:ARG:N	2.26	0.50
1:A:373:THR:O	1:A:374:ASN:HB2	2.10	0.50
1:C:13:ASP:HB3	1:C:300:MET:HE3	1.93	0.50
1:A:77:VAL:HG23	5:A:1239:HOH:O	2.11	0.50
1:C:68:SEP:O	1:C:72:GLN:HG3	2.11	0.50
1:A:88:ASN:HB3	5:A:1250:HOH:O	2.10	0.50
1:B:16:LYS:HD2	1:B:16:LYS:N	2.26	0.50
1:B:114:LEU:HB3	1:B:116:GLU:OE1	2.12	0.50
1:C:122:LYS:HZ2	1:C:123:GLU:HB2	1.74	0.50
1:D:162:GLN:NE2	1:D:162:GLN:N	2.53	0.50
1:C:61:LYS:HG2	1:C:61:LYS:O	2.11	0.50
1:B:57:VAL:O	1:B:58:ARG:HB2	2.12	0.49
1:B:65:PHE:CE1	1:B:80:HIS:HA	2.47	0.49
1:C:229:ILE:HD12	1:C:243:VAL:O	2.13	0.49
1:C:122:LYS:HZ3	1:C:123:GLU:HB2	1.77	0.49
1:A:108:GLU:OE2	1:A:110:ARG:N	2.37	0.49
1:C:189:LYS:HZ3	1:D:140:GLN:CG	2.26	0.49
1:A:276:ARG:HE	1:A:356:GLU:CD	2.21	0.49
1:B:381:ARG:HD3	1:B:383:VAL:CG1	2.43	0.49
1:D:187:ALA:HB2	1:D:338:GLY:CA	2.43	0.49
1:C:189:LYS:NZ	1:D:140:GLN:CG	2.76	0.48
1:B:58:ARG:HG3	1:B:61:LYS:HZ1	1.78	0.48
1:C:222:MET:CG	1:C:227:MET:HE2	2.42	0.48
1:D:83:LEU:O	1:D:87:LEU:HD23	2.12	0.48
1:D:187:ALA:HB2	1:D:338:GLY:HA3	1.94	0.48
1:D:172:MET:HE3	5:D:4144:HOH:O	2.12	0.48
1:A:214:ILE:HG21	1:A:350:ASP:CB	2.43	0.48
1:C:12:PHE:O	1:C:16:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:CYS:C	1:B:75:THR:H	2.22	0.48
1:D:162:GLN:CD	1:D:162:GLN:N	2.69	0.48
1:B:187:ALA:HB2	1:B:338:GLY:HA3	1.95	0.48
1:D:16:LYS:HE3	5:D:4106:HOH:O	2.12	0.48
1:A:187:ALA:HB2	1:A:338:GLY:HA3	1.96	0.48
1:C:264:LEU:C	1:C:264:LEU:CD1	2.87	0.48
1:D:78:ASN:CG	1:D:78:ASN:O	2.56	0.48
1:D:225:GLU:HB2	1:D:227:MET:HG2	1.95	0.48
1:D:312:LEU:CD1	1:D:321:LEU:HD22	2.38	0.48
1:A:73:CYS:SG	1:A:124:LEU:CD1	3.02	0.47
1:C:181:LYS:HE2	1:D:151:SER:OG	2.14	0.47
1:A:54:ASN:HD21	1:A:60:ASP:N	2.12	0.47
1:A:129:LEU:HD22	1:A:130:GLU:N	2.30	0.47
1:B:335:ASN:C	1:B:335:ASN:HD22	2.21	0.47
1:C:162:GLN:H	1:C:162:GLN:CD	2.21	0.47
1:A:106:TYR:O	1:A:172:MET:HG3	2.15	0.47
1:B:23:ALA:O	1:B:25:GLU:HG3	2.14	0.47
1:B:187:ALA:HB2	1:B:338:GLY:CA	2.45	0.47
1:C:119:GLN:O	1:C:122:LYS:CD	2.63	0.47
1:D:101:LEU:HD13	1:D:178:ILE:HG22	1.97	0.47
1:C:75:THR:OG1	1:C:76:SER:N	2.46	0.47
1:D:199:ARG:O	1:D:363:PRO:HD3	2.15	0.47
1:D:252:LEU:O	1:D:256:GLU:HG3	2.14	0.47
1:A:129:LEU:HD22	1:A:130:GLU:H	1.80	0.47
1:A:187:ALA:HB2	1:A:338:GLY:CA	2.44	0.47
1:A:218:ARG:HH21	1:A:273:MET:CB	2.21	0.47
1:C:230:LEU:HD21	1:C:232:LEU:HD21	1.97	0.47
1:D:178:ILE:HD12	1:D:178:ILE:C	2.39	0.47
1:B:78:ASN:O	1:B:81:SER:HB3	2.15	0.47
1:B:83:LEU:O	1:B:87:LEU:HD23	2.15	0.47
1:C:222:MET:HE2	1:C:267:TRP:HD1	1.80	0.47
1:D:142:ARG:HG3	1:D:166:VAL:CG2	2.45	0.47
1:B:162:GLN:HB3	1:D:75:THR:CG2	2.46	0.46
1:C:227:MET:HE3	1:C:228:LYS:C	2.39	0.46
1:B:66:GLY:O	1:B:68:SEP:N	2.49	0.46
1:A:341:VAL:HG12	5:A:1226:HOH:O	2.16	0.46
1:D:69:ILE:O	1:D:72:GLN:HB2	2.16	0.46
1:D:320:DSN:HA	5:D:4167:HOH:O	2.14	0.46
1:C:334:ILE:N	1:C:334:ILE:HD12	2.31	0.46
1:D:321:LEU:HD23	1:D:321:LEU:C	2.40	0.46
1:D:325:GLN:NE2	4:D:386:NAG:H82	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:HB2	1:A:87:LEU:HD11	1.98	0.46
1:B:244:LEU:HD12	1:B:244:LEU:N	2.31	0.46
1:D:47:ASP:HB3	5:D:4132:HOH:O	2.14	0.45
1:A:95:ASP:HB3	5:A:1150:HOH:O	2.15	0.45
1:B:294:THR:O	1:B:298:MET:HG3	2.17	0.45
1:C:1:GLY:CA	1:C:61:LYS:HD3	2.44	0.45
1:C:278:ILE:CG2	1:C:356:GLU:HG2	2.42	0.45
1:C:69:ILE:HD12	5:C:3166:HOH:O	2.16	0.45
1:A:108:GLU:HB3	1:A:111:TYR:CD1	2.51	0.45
1:C:50:ARG:HH22	1:C:70:GLU:CD	2.22	0.45
1:A:154:ASN:ND2	1:B:154:ASN:ND2	2.65	0.45
1:C:187:ALA:HB2	1:C:338:GLY:HA3	1.99	0.45
1:D:157:ILE:CD1	1:D:177:ALA:HB1	2.47	0.45
1:C:8:MET:HE2	1:C:8:MET:HA	1.99	0.45
1:C:93:PRO:HG3	1:D:91:THR:O	2.17	0.45
1:B:60:ASP:O	1:B:61:LYS:CB	2.65	0.44
1:C:241:MET:HE1	1:C:334:ILE:HG12	1.98	0.44
1:D:219:VAL:CG2	1:D:220:ALA:N	2.81	0.44
1:A:114:LEU:HA	1:A:115:PRO:HD2	1.88	0.44
1:B:162:GLN:HB3	1:D:75:THR:HG23	1.98	0.44
1:D:137:ALA:HB1	1:D:140:GLN:HB3	1.99	0.44
1:B:58:ARG:CB	1:B:61:LYS:NZ	2.73	0.44
1:A:281:TYR:HB2	1:A:359:ARG:HA	1.99	0.44
1:A:341:VAL:HG22	1:A:342:VAL:O	2.16	0.44
1:B:70:GLU:C	1:B:72:GLN:N	2.73	0.44
1:B:112:PRO:HG3	5:B:2148:HOH:O	2.17	0.44
1:A:76:SER:C	1:A:78:ASN:H	2.25	0.44
1:A:199:ARG:N	1:A:199:ARG:CD	2.80	0.44
1:C:68:SEP:C	1:C:71:ALA:H	2.31	0.44
1:C:96:VAL:HG23	1:C:97:TYR:CD2	2.53	0.44
1:A:142:ARG:HH11	1:A:163:PRO:HD3	1.82	0.44
1:B:220:ALA:HB1	1:B:272:VAL:HG12	2.00	0.44
1:C:162:GLN:CA	1:C:162:GLN:HE21	2.31	0.44
1:A:286:LYS:HG3	1:A:333:GLU:HG2	1.99	0.44
1:B:252:LEU:HD22	1:B:363:PRO:HB3	1.99	0.44
1:C:373:THR:O	1:C:374:ASN:HB2	2.17	0.44
1:D:288:GLU:HA	1:D:330:ALA:O	2.18	0.43
1:A:8:MET:SD	1:A:261:PHE:HD1	2.41	0.43
1:C:89:GLN:NE2	1:C:370:HIS:NE2	2.65	0.43
1:D:196:MET:HE1	1:D:281:TYR:CD1	2.53	0.43
1:A:137:ALA:O	1:A:140:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:GLU:OE2	1:B:58:ARG:NH2	2.51	0.43
1:B:15:PHE:O	1:B:19:LYS:HG3	2.17	0.43
1:C:381:ARG:HD3	1:C:383:VAL:CG1	2.48	0.43
1:D:46:LYS:HD2	1:D:313:SER:OG	2.19	0.43
1:A:61:LYS:O	1:A:61:LYS:HG2	2.18	0.43
1:A:296:VAL:O	1:A:300:MET:HG3	2.18	0.43
1:B:75:THR:O	1:B:76:SER:HB2	2.18	0.43
1:C:228:LYS:HE3	1:C:358:PHE:HD2	1.83	0.43
1:A:42:TYR:OH	1:A:50:ARG:NH1	2.51	0.43
1:D:73:CYS:SG	1:D:124:LEU:CD1	3.06	0.43
1:A:189:LYS:CE	1:A:341:VAL:HG21	2.49	0.43
1:A:222:MET:HE2	1:A:222:MET:HB2	1.94	0.43
1:B:298:MET:HA	1:B:302:ILE:O	2.19	0.43
1:C:143:GLU:HG3	1:D:190:ASP:OD2	2.19	0.43
1:C:214:ILE:HD11	1:C:277:LYS:CG	2.49	0.43
1:A:69:ILE:HG23	1:A:70:GLU:N	2.34	0.42
1:C:183:LEU:HD12	1:C:338:GLY:CA	2.49	0.42
1:D:59:PHE:O	1:D:60:ASP:C	2.62	0.42
1:B:96:VAL:HG23	1:B:97:TYR:CD2	2.54	0.42
1:B:58:ARG:HB3	1:B:61:LYS:HZ3	1.81	0.42
1:C:93:PRO:HD3	1:D:93:PRO:HD3	2.00	0.42
1:D:244:LEU:HD22	1:D:259:ILE:HD12	2.02	0.42
1:D:321:LEU:CD2	1:D:321:LEU:C	2.93	0.42
1:A:36:SER:HB2	1:A:87:LEU:CD1	2.50	0.42
1:C:40:MET:SD	1:C:128:GLY:HA3	2.60	0.42
1:B:227:MET:HE1	1:B:229:ILE:HD11	2.01	0.42
1:C:8:MET:HE1	1:C:12:PHE:CE2	2.55	0.42
1:A:136:THR:HG23	5:A:1214:HOH:O	2.20	0.42
1:B:43:LEU:HD21	1:B:80:HIS:CE1	2.54	0.42
1:B:79:VAL:HG21	1:B:124:LEU:HD11	2.01	0.42
1:C:77:VAL:HG23	1:C:79:VAL:HG23	2.01	0.42
1:D:9:GLU:OE2	1:D:58:ARG:HD2	2.19	0.42
1:D:202:GLU:OE2	1:D:249:VAL:HG23	2.19	0.42
1:B:57:VAL:O	1:B:57:VAL:HG12	2.19	0.42
1:B:69:ILE:HG23	1:B:70:GLU:N	2.34	0.42
1:C:162:GLN:OE1	2:G:1:NAG:H81	2.20	0.42
1:B:105:LEU:HD22	1:B:172:MET:HG2	2.02	0.42
1:C:84:ARG:HD2	1:C:124:LEU:HB3	2.01	0.41
1:C:115:PRO:O	1:C:119:GLN:HG3	2.20	0.41
1:C:242:LEU:HD13	1:C:268:THR:HG21	2.02	0.41
1:D:156:ILE:HD12	1:D:179:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:GLU:CD	1:D:202:GLU:H	2.28	0.41
1:B:108:GLU:HG2	1:B:134:PHE:HB2	2.02	0.41
1:A:159:ASN:HD21	1:C:76:SER:HB3	1.85	0.41
1:B:252:LEU:HD22	1:B:363:PRO:CB	2.51	0.41
1:C:36:SER:HA	1:C:83:LEU:HD21	2.01	0.41
1:C:75:THR:O	1:C:76:SER:HB2	2.20	0.41
1:C:294:THR:O	1:C:298:MET:HG3	2.21	0.41
1:A:199:ARG:CD	1:A:199:ARG:H	2.32	0.41
1:C:108:GLU:OE1	1:C:134:PHE:N	2.51	0.41
1:A:341:VAL:CG2	1:A:342:VAL:N	2.83	0.41
1:B:242:LEU:HD11	1:B:369:LYS:HE2	2.03	0.41
1:C:110:ARG:NH1	1:C:135:GLN:NE2	2.68	0.41
1:A:75:THR:OG1	1:A:76:SER:N	2.53	0.41
1:A:181:LYS:HE3	5:A:2157:HOH:O	2.19	0.41
1:D:41:VAL:HG22	1:D:105:LEU:HD11	2.02	0.41
1:A:342:VAL:HG12	1:A:346:GLU:HB2	2.02	0.41
1:C:69:ILE:HA	1:C:72:GLN:NE2	2.35	0.41
1:C:93:PRO:CG	1:D:91:THR:O	2.69	0.41
1:A:312:LEU:C	1:A:314:GLY:H	2.28	0.41
1:B:32:ILE:HG13	1:B:87:LEU:HD21	2.02	0.41
1:C:214:ILE:C	1:C:214:ILE:CD1	2.88	0.41
1:C:311:ASN:ND2	1:C:313:SER:H	2.18	0.41
1:D:60:ASP:HB2	1:D:61:LYS:H	1.54	0.41
1:A:70:GLU:C	1:A:72:GLN:N	2.77	0.41
1:A:204:GLU:HG2	1:A:205:SER:N	2.35	0.41
1:D:19:LYS:HB3	1:D:19:LYS:HE2	1.94	0.41
1:B:181:LYS:HD2	1:B:181:LYS:HA	1.78	0.41
1:C:73:CYS:SG	1:C:124:LEU:HD11	2.60	0.41
1:C:125:TYR:O	1:C:126:ARG:C	2.64	0.41
1:C:245:LEU:HA	1:C:246:PRO:HD3	1.91	0.41
1:B:233:PRO:HG3	5:B:2094:HOH:O	2.21	0.40
1:C:59:PHE:O	1:C:60:ASP:C	2.63	0.40
1:C:200:VAL:HG12	1:C:201:THR:HG23	2.03	0.40
1:D:150:GLU:CD	1:D:158:ARG:HG2	2.46	0.40
1:D:281:TYR:HB2	1:D:359:ARG:HA	2.02	0.40
1:A:70:GLU:C	1:A:72:GLN:H	2.29	0.40
1:B:160:VAL:HG22	1:B:327:VAL:HG21	2.03	0.40
1:C:333:GLU:C	1:C:334:ILE:HD12	2.46	0.40
1:A:157:ILE:HD13	1:A:177:ALA:HB1	2.03	0.40
1:C:54:ASN:HD22	1:C:59:PHE:HB2	1.87	0.40
1:B:8:MET:SD	1:B:264:LEU:HD23	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ILE:HD13	1:B:258:ILE:H	1.86	0.40
1:C:199:ARG:N	1:C:199:ARG:CD	2.78	0.40
1:D:37:ALA:HB1	1:D:174:LEU:HD11	2.02	0.40
1:D:79:VAL:HB	1:D:124:LEU:CD1	2.51	0.40
1:D:122:LYS:HE2	1:D:126:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/385 (97%)	361 (96%)	9 (2%)	4 (1%)	11	4
1	B	378/385 (98%)	363 (96%)	11 (3%)	4 (1%)	11	4
1	C	366/385 (95%)	347 (95%)	16 (4%)	3 (1%)	16	8
1	D	378/385 (98%)	368 (97%)	8 (2%)	2 (0%)	24	16
All	All	1496/1540 (97%)	1439 (96%)	44 (3%)	13 (1%)	14	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	67	ASP
1	B	61	LYS
1	C	60	ASP
1	C	67	ASP
1	C	76	SER
1	D	60	ASP
1	D	76	SER
1	B	60	ASP
1	A	76	SER

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Mol	Chain	Res	Type
1	B	67	ASP
1	B	76	SER
1	A	77	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	324/326 (99%)	317 (98%)	7 (2%)	45	42
1	B	326/326 (100%)	317 (97%)	9 (3%)	38	32
1	C	322/326 (99%)	308 (96%)	14 (4%)	26	18
1	D	326/326 (100%)	313 (96%)	13 (4%)	28	20
All	All	1298/1304 (100%)	1255 (97%)	43 (3%)	33	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ASP
1	A	75	THR
1	A	129	LEU
1	A	135	GLN
1	A	162	GLN
1	A	201	THR
1	A	254	GLN
1	B	8	MET
1	B	16	LYS
1	B	110	ARG
1	B	116	GLU
1	B	118	LEU
1	B	222	MET
1	B	253	GLU
1	B	258	ILE
1	B	335	ASN
1	C	8	MET
1	C	25	GLU

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Mol	Chain	Res	Type
1	C	87	LEU
1	C	108	GLU
1	C	122	LYS
1	C	162	GLN
1	C	183	LEU
1	C	199	ARG
1	C	214	ILE
1	C	227	MET
1	C	229	ILE
1	C	253	GLU
1	C	271	ASN
1	C	274	GLU
1	D	25	GLU
1	D	58	ARG
1	D	60	ASP
1	D	119	GLN
1	D	130	GLU
1	D	140	GLN
1	D	142	ARG
1	D	162	GLN
1	D	163	PRO
1	D	203	GLN
1	D	216	LEU
1	D	321	LEU
1	D	335	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	54	ASN
1	A	89	GLN
1	A	119	GLN
1	A	135	GLN
1	A	154	ASN
1	A	159	ASN
1	A	162	GLN
1	A	213	GLN
1	A	254	GLN
1	A	325	GLN
1	B	89	GLN
1	B	152	GLN

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Mol	Chain	Res	Type
1	B	154	ASN
1	B	169	GLN
1	B	203	GLN
1	B	254	GLN
1	B	271	ASN
1	B	335	ASN
1	C	54	ASN
1	C	72	GLN
1	C	88	ASN
1	C	89	GLN
1	C	135	GLN
1	C	140	GLN
1	C	154	ASN
1	C	162	GLN
1	C	169	GLN
1	C	194	GLN
1	C	203	GLN
1	C	213	GLN
1	C	254	GLN
1	C	271	ASN
1	C	311	ASN
1	D	119	GLN
1	D	135	GLN
1	D	140	GLN
1	D	152	GLN
1	D	154	ASN
1	D	162	GLN
1	D	194	GLN
1	D	203	GLN
1	D	271	ASN
1	D	335	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

19 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	$\# Z > 2$
1	SEP	C	68	1	4,5,10	0.68	0	1,5,14	0.60	0
1	SEP	D	68	1	8,9,10	1.04	1 (12%)	7,12,14	1.49	1 (14%)
1	SEP	D	344	1	8,9,10	1.06	1 (12%)	7,12,14	1.89	1 (14%)
1	SEP	B	68	1	4,5,10	0.62	0	1,5,14	0.60	0
1	SEP	B	344	1	8,9,10	1.06	1 (12%)	7,12,14	1.49	1 (14%)
1	SEP	A	68	1	8,9,10	1.02	1 (12%)	7,12,14	1.26	1 (14%)
1	SEP	A	344	1	8,9,10	0.87	0	7,12,14	1.29	1 (14%)

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
1	DSN	D	164	1	1/1/1/2	-	-
1	SEP	C	68	1	-	0/2/4/10	-
1	SEP	D	68	1	-	0/6/8/10	-
1	SEP	D	344	1	-	1/6/8/10	-
1	SEP	B	68	1	-	0/2/4/10	-
1	SEP	B	344	1	-	2/6/8/10	-
1	SEP	A	68	1	-	2/6/8/10	-
1	SEP	A	344	1	-	4/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	344	SEP	P-O1P	2.15	1.57	1.50
1	A	68	SEP	P-O1P	2.13	1.57	1.50
1	D	68	SEP	P-O1P	2.06	1.56	1.50
1	B	344	SEP	P-O1P	2.03	1.56	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	SEP	OG-CB-CA	4.45	112.48	108.14
1	D	68	SEP	OG-CB-CA	3.01	111.08	108.14
1	B	344	SEP	OG-CB-CA	2.70	110.78	108.14
1	A	344	SEP	OG-CB-CA	2.63	110.70	108.14
1	A	68	SEP	OG-CB-CA	2.35	110.44	108.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	164	DSN	CA

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	SEP	N-CA-CB-OG
1	A	68	SEP	C-CA-CB-OG
1	A	344	SEP	N-CA-CB-OG
1	A	344	SEP	CB-OG-P-O1P
1	A	344	SEP	CB-OG-P-O2P
1	A	344	SEP	CB-OG-P-O3P
1	B	344	SEP	N-CA-CB-OG
1	B	344	SEP	C-CA-CB-OG
1	D	344	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	68	SEP	2	0
1	B	68	SEP	1	0

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	E	1	1,2	14,14,15	0.62	0	17,19,21	0.96	1 (5%)
2	NAG	E	2	2	14,14,15	0.56	0	17,19,21	0.64	0
2	NAG	F	1	1,2	14,14,15	0.76	0	17,19,21	0.67	0
2	NAG	F	2	2	14,14,15	0.59	0	17,19,21	1.08	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.67	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.04	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	O5-C5	2.00	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C2-N2-C7	-3.47	118.25	122.90
2	E	1	NAG	C2-N2-C7	-3.32	118.45	122.90
2	G	2	NAG	C2-N2-C7	-2.32	119.79	122.90
2	G	2	NAG	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2

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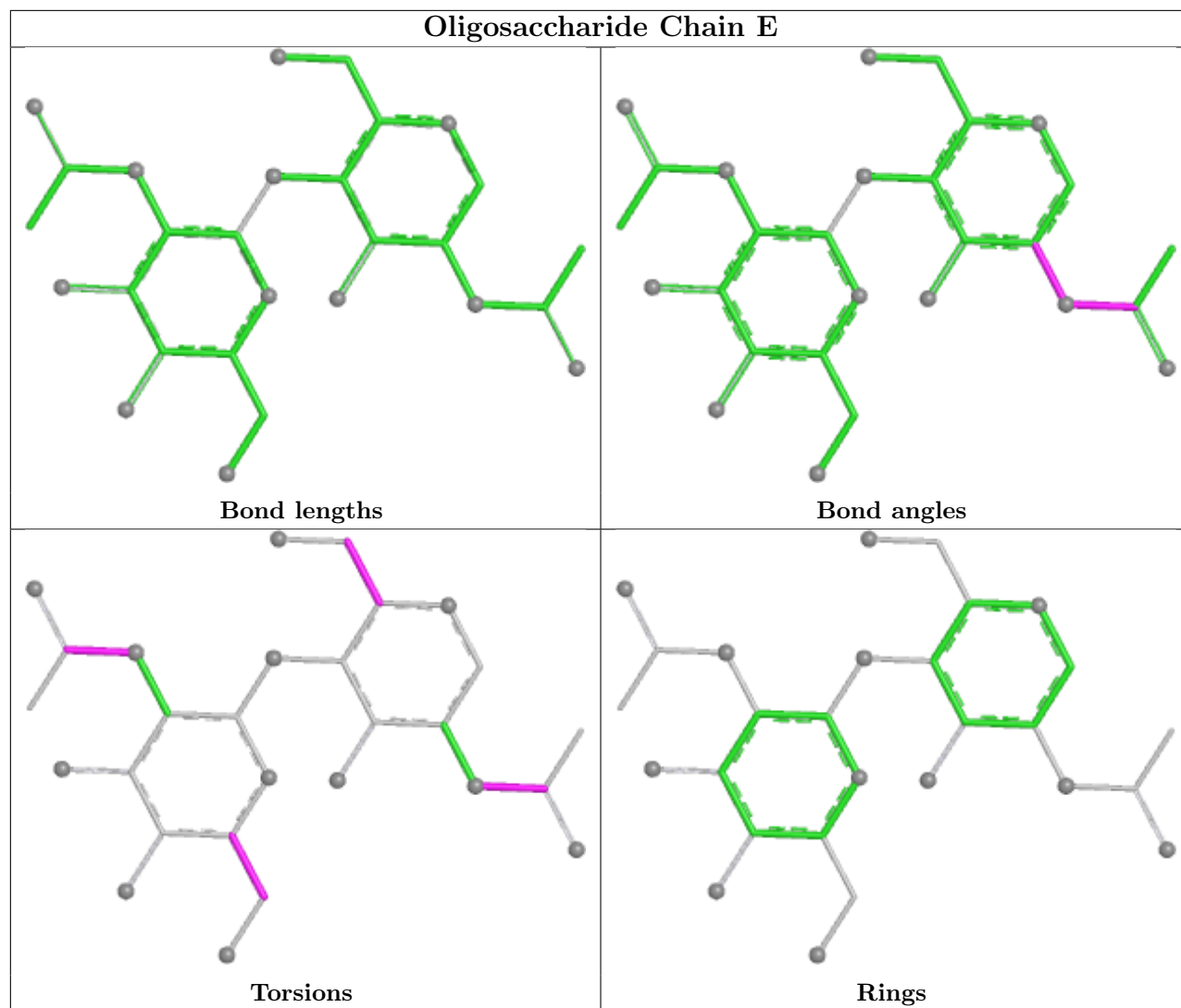
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

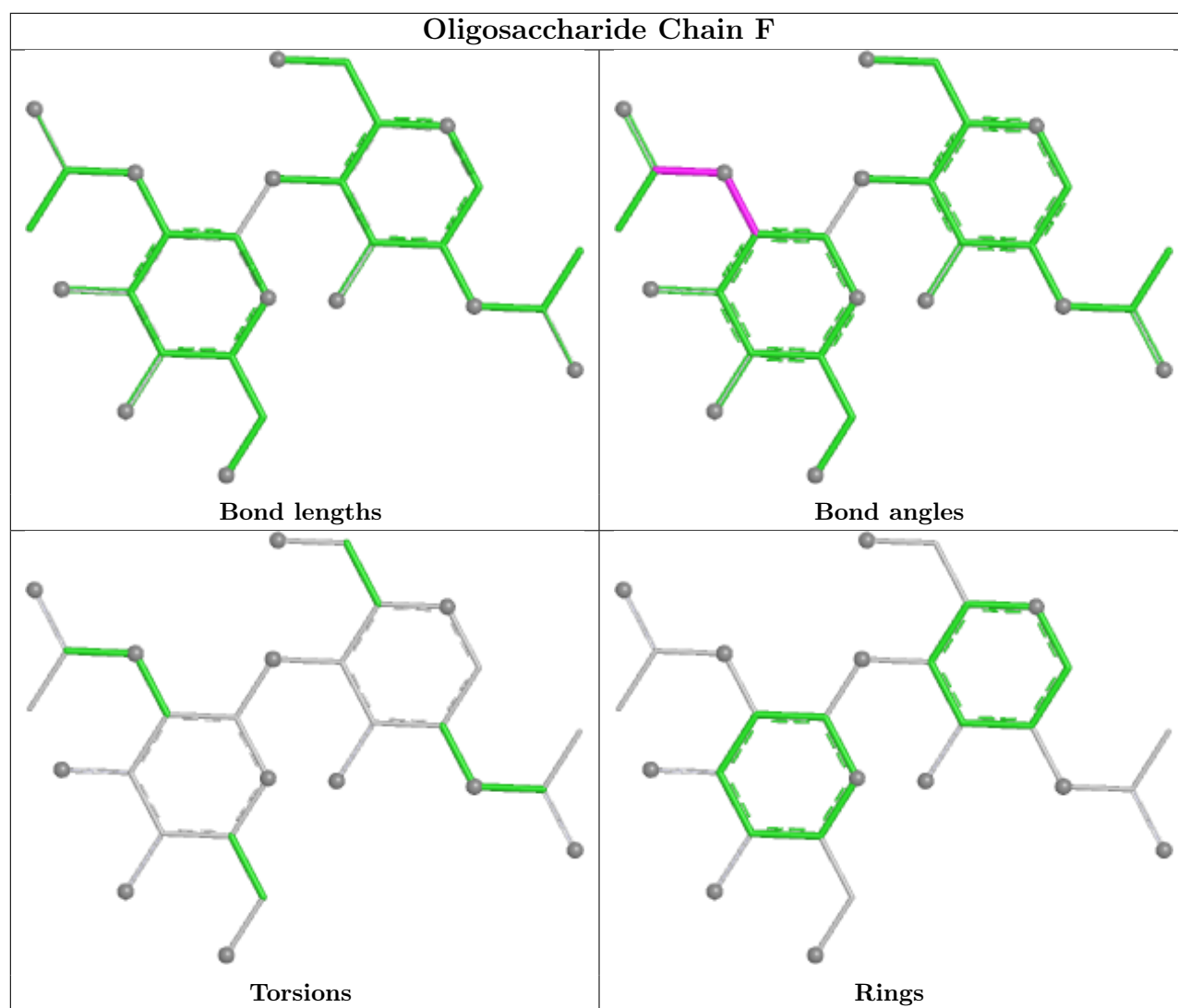
There are no ring outliers.

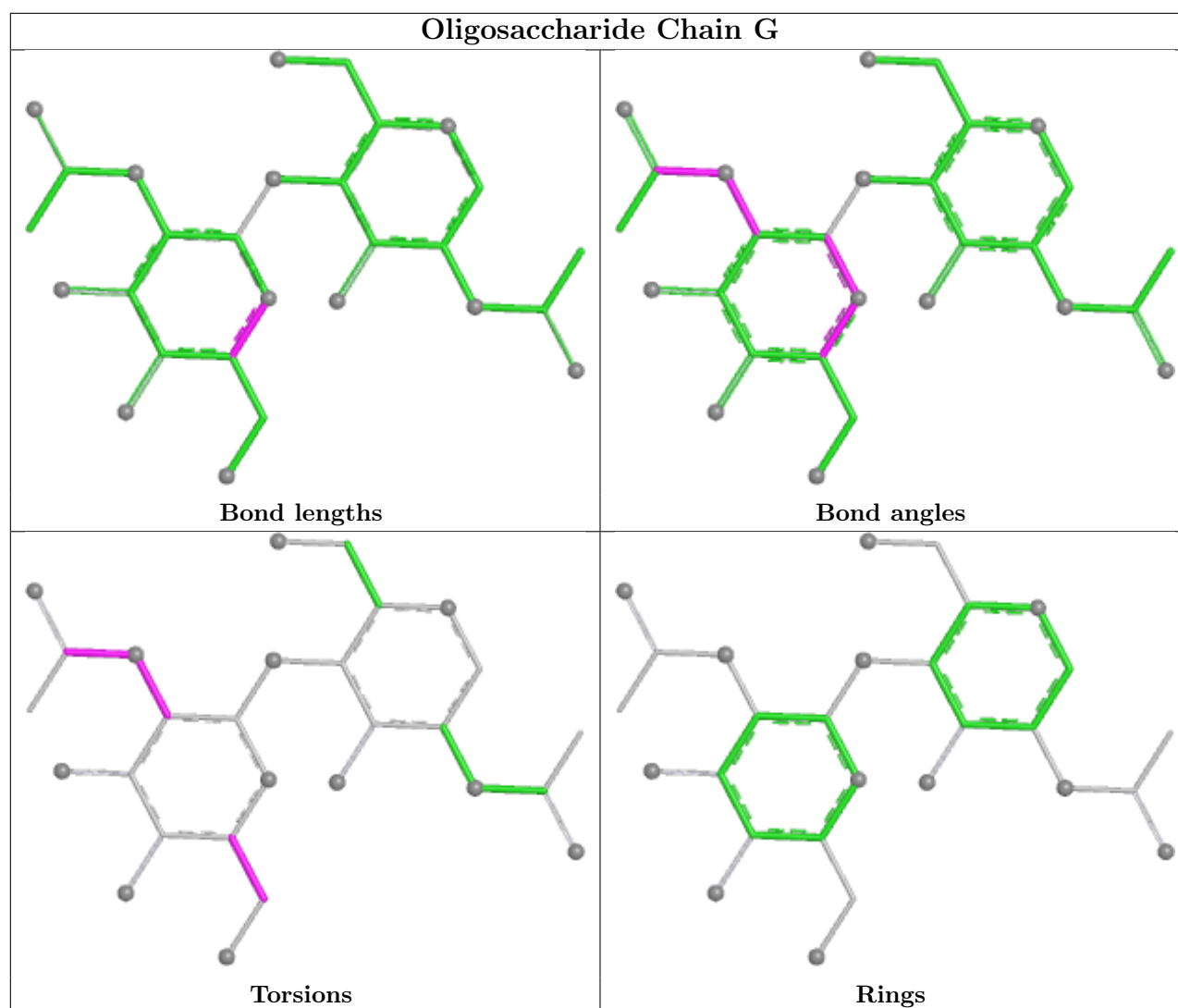
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	G	2	NAG	1	0
2	E	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](#)

8 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	$\# Z > 2$
3	SO4	A	401	-	4,4,4	0.39	0	6,6,6	0.13	0
3	SO4	D	3401	-	4,4,4	0.39	0	6,6,6	0.08	0
3	SO4	B	1402	-	4,4,4	0.34	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	1401	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	A	402	-	4,4,4	0.39	0	6,6,6	0.06	0
4	NAG	D	386	1	14,14,15	0.71	0	17,19,21	0.81	0
3	SO4	D	3402	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	C	2401	-	4,4,4	0.44	0	6,6,6	0.10	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	D	386	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	386	NAG	C8-C7-N2-C2
4	D	386	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	386	NAG	3	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	378/385 (98%)	0.30	22 (5%)	29 30	13, 28, 50, 62	0
1	B	380/385 (98%)	0.21	12 (3%)	50 54	14, 26, 50, 75	0
1	C	370/385 (96%)	0.20	14 (3%)	44 47	12, 25, 48, 67	0
1	D	380/385 (98%)	0.14	11 (2%)	53 57	14, 26, 43, 56	0
All	All	1508/1540 (97%)	0.21	59 (3%)	43 46	12, 26, 49, 75	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	CYS	4.8
1	B	77	VAL	4.1
1	A	75	THR	3.6
1	D	75	THR	3.6
1	B	66	GLY	3.5
1	D	66	GLY	3.5
1	A	77	VAL	3.3
1	A	76	SER	3.3
1	C	69	ILE	3.2
1	C	127	GLY	3.2
1	B	250	SER	3.1
1	D	166	VAL	2.8
1	C	73	CYS	2.7
1	D	201	THR	2.7
1	A	127	GLY	2.7
1	A	114	LEU	2.7
1	C	74	GLY	2.6
1	C	71	ALA	2.6
1	C	77	VAL	2.6
1	B	251	GLY	2.6
1	A	121	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	120	CYS	2.5
1	A	113	ILE	2.5
1	C	75	THR	2.5
1	A	349	VAL	2.5
1	A	60	ASP	2.5
1	A	47	ASP	2.5
1	A	249	VAL	2.4
1	C	66	GLY	2.4
1	C	60	ASP	2.4
1	B	75	THR	2.4
1	A	123	GLU	2.4
1	B	272	VAL	2.4
1	A	73	CYS	2.4
1	D	351	ALA	2.4
1	A	310	ALA	2.3
1	B	76	SER	2.3
1	A	204	GLU	2.3
1	A	71	ALA	2.3
1	D	77	VAL	2.3
1	C	120	CYS	2.3
1	A	205	SER	2.2
1	A	69	ILE	2.2
1	A	120	CYS	2.2
1	A	316	SER	2.2
1	C	261	PHE	2.2
1	B	249	VAL	2.2
1	D	355	SER	2.2
1	C	21	HIS	2.1
1	A	250	SER	2.1
1	B	21	HIS	2.1
1	B	121	VAL	2.1
1	D	20	VAL	2.1
1	B	69	ILE	2.0
1	A	201	THR	2.0
1	B	79	VAL	2.0
1	C	258	ILE	2.0
1	D	343	GLY	2.0
1	C	354	VAL	2.0

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
1	SEP	C	68	6/11	0.41	0.25	63,65,65,65	0
1	SEP	B	68	6/11	0.66	0.12	67,68,68,69	0
1	SEP	D	344	10/11	0.69	0.16	25,36,52,53	0
1	DSN	D	164	6/7	0.70	0.17	37,38,41,45	0
1	SEP	D	68	10/11	0.70	0.14	53,57,64,64	0
1	DSN	A	320	6/7	0.71	0.12	45,49,51,53	0
1	DSN	B	320	6/7	0.71	0.13	32,37,40,44	0
1	DSN	D	320	6/7	0.76	0.12	34,37,39,42	0
1	SEP	A	68	10/11	0.76	0.11	50,55,60,61	0
1	DSN	C	320	6/7	0.77	0.12	31,36,38,41	0
1	DSN	A	164	6/7	0.82	0.10	38,39,42,45	0
1	DSN	C	164	6/7	0.85	0.08	29,31,33,36	0
1	DSN	B	164	6/7	0.86	0.09	27,30,32,37	0
1	SEP	B	344	10/11	0.87	0.11	23,30,46,48	0
1	SEP	A	344	10/11	0.88	0.09	40,44,51,51	0
1	DSN	B	236	6/7	0.89	0.07	23,29,31,35	0
1	DSN	A	236	6/7	0.91	0.08	19,20,22,27	0
1	DSN	D	236	6/7	0.91	0.07	18,22,25,27	0
1	DSN	C	236	6/7	0.94	0.05	20,24,26,28	0

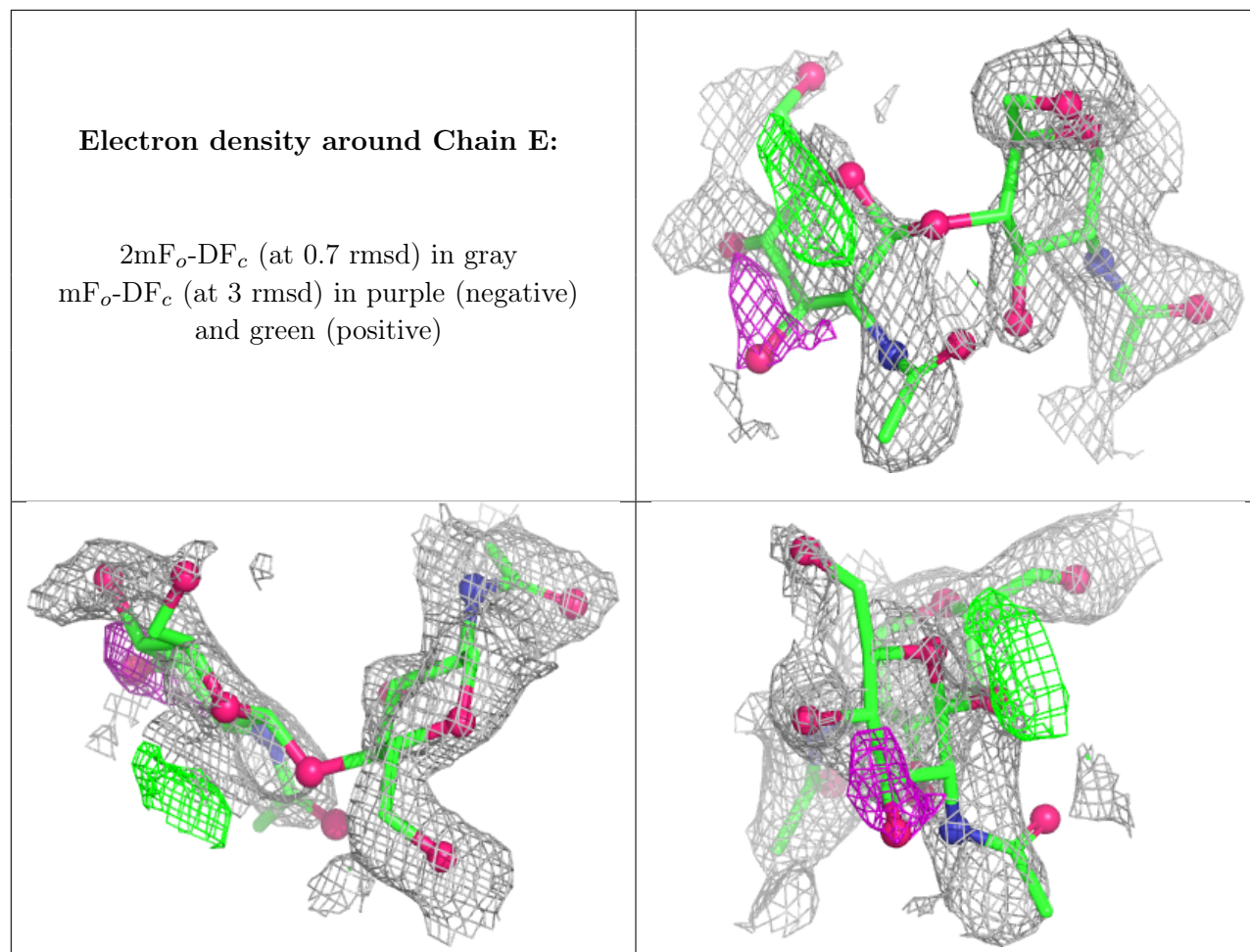
6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.50	0.17	58,61,64,64	0
2	NAG	G	2	14/15	0.61	0.18	40,44,49,49	0
2	NAG	F	2	14/15	0.63	0.14	41,46,47,51	0
2	NAG	E	1	14/15	0.75	0.11	38,42,47,53	0
2	NAG	G	1	14/15	0.90	0.08	19,21,24,31	0
2	NAG	F	1	14/15	0.90	0.08	21,26,30,35	0

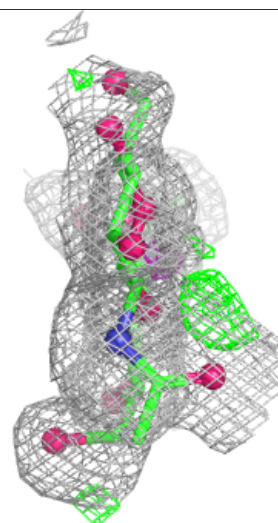
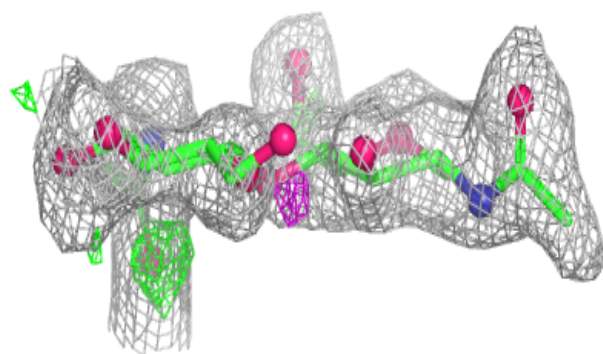
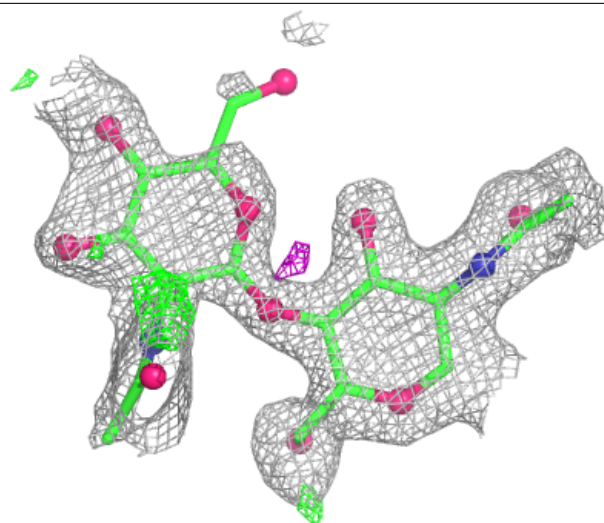
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

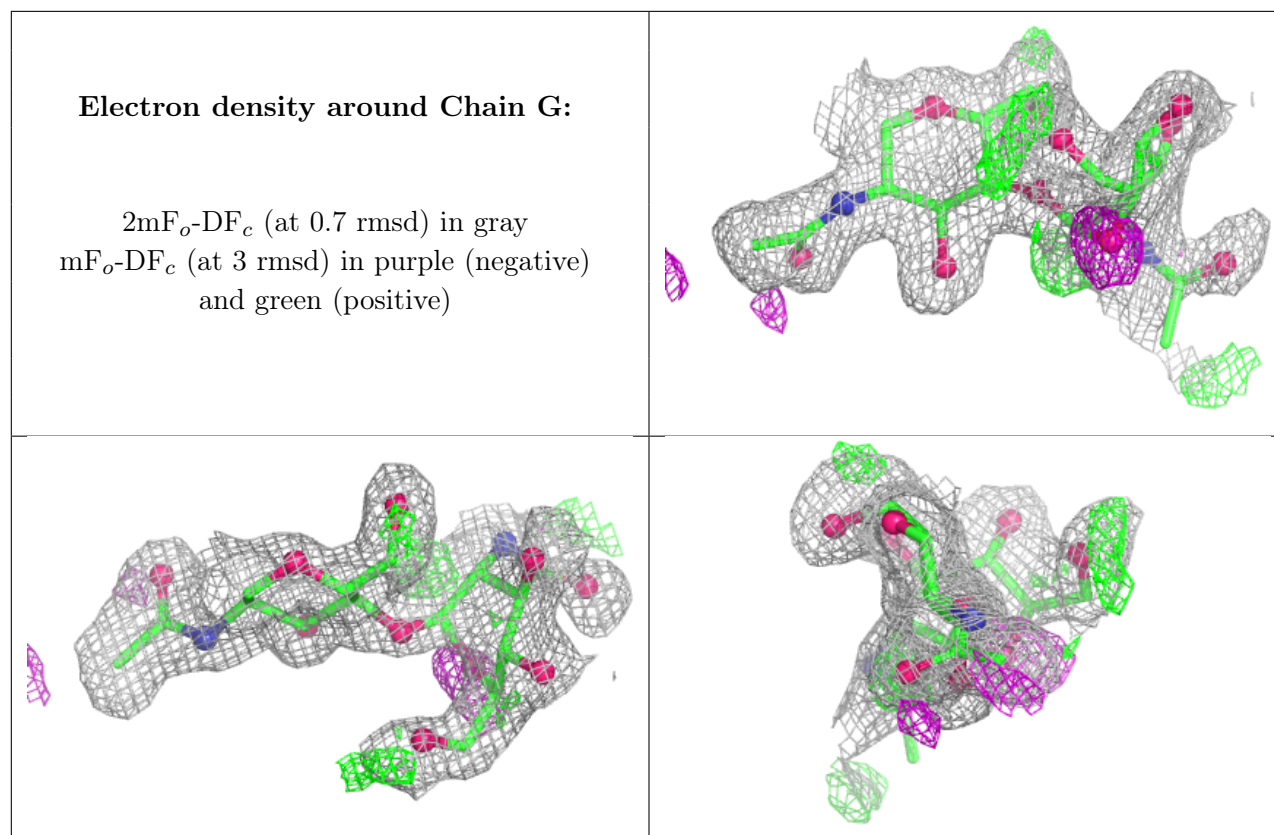
charide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

$2mF_o-DF_c$ (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
3	SO4	B	1401	5/5	0.65	0.10	99,99,99,99	0
3	SO4	D	3402	5/5	0.72	0.12	74,74,74,74	0
3	SO4	B	1402	5/5	0.77	0.14	89,89,90,90	0
3	SO4	A	401	5/5	0.81	0.14	52,52,53,54	0
3	SO4	D	3401	5/5	0.82	0.10	78,78,79,79	0
4	NAG	D	386	14/15	0.82	0.10	32,37,41,41	0
3	SO4	A	402	5/5	0.85	0.11	56,56,58,58	0
3	SO4	C	2401	5/5	0.91	0.10	52,52,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.