



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:19 AM UTC

PDB ID : 1G82 / pdb_00001g82
Title : STRUCTURE OF FIBROBLAST GROWTH FACTOR 9
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Deposited on : 2000-11-16
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

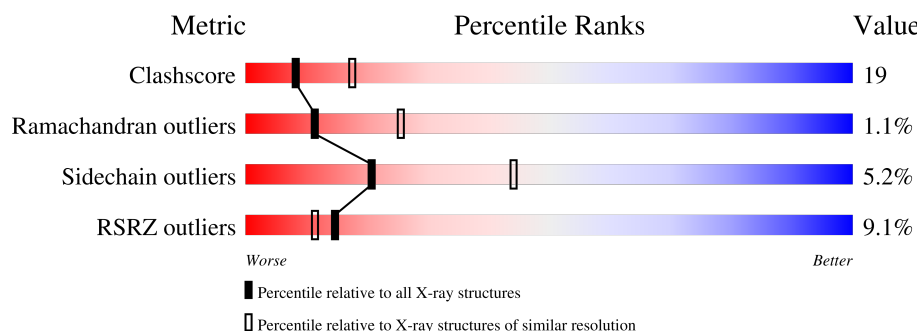
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	160	2% 52% 33% 11% ..
1	B	160	25% 40% 44% 12% ..
1	C	160	6% 54% 32% 9% ..
1	D	160	3% 48% 37% 10% ..
2	E	3	100%
2	F	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	G	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	E	2	X	-	-	-
2	NAG	G	2	X	-	-	-
2	FUC	G	3	X	-	-	-

2 Entry composition [i](#)

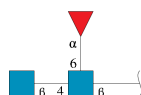
There are 5 unique types of molecules in this entry. The entry contains 5480 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FIBROBLAST GROWTH FACTOR 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	0	0
			1295	819	234	239	3			
1	B	157	Total	C	N	O	S	0	0	0
			1295	821	234	237	3			
1	C	155	Total	C	N	O	S	0	0	0
			1279	811	231	234	3			
1	D	155	Total	C	N	O	S	0	0	0
			1276	809	231	233	3			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	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		
3	C	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	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: C₈H₁₅NO₆).



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

- Molecule 5 is water.

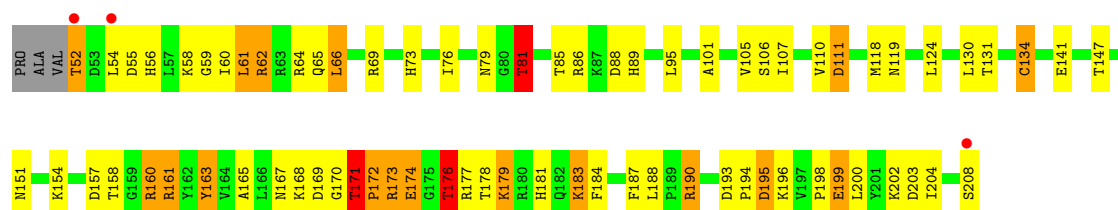
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	4	Total	O	0	0
			4	4		
5	C	35	Total	O	0	0
			35	35		
5	D	49	Total	O	0	0
			49	49		

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.

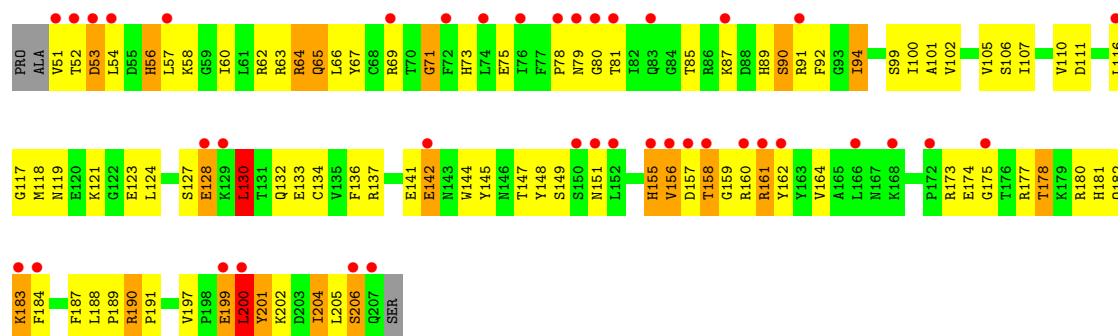
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain A: 



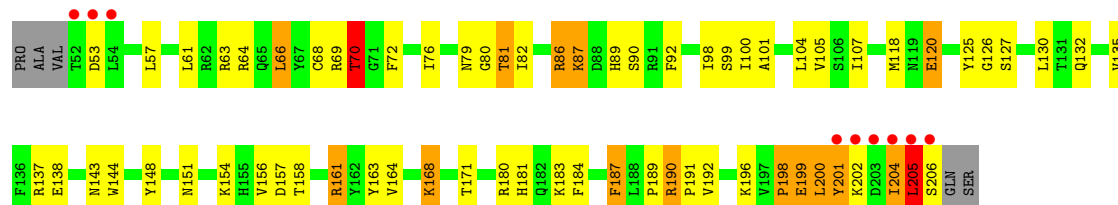
• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain B: 



• Molecule 1: FIBROBLAST GROWTH FACTOR 9

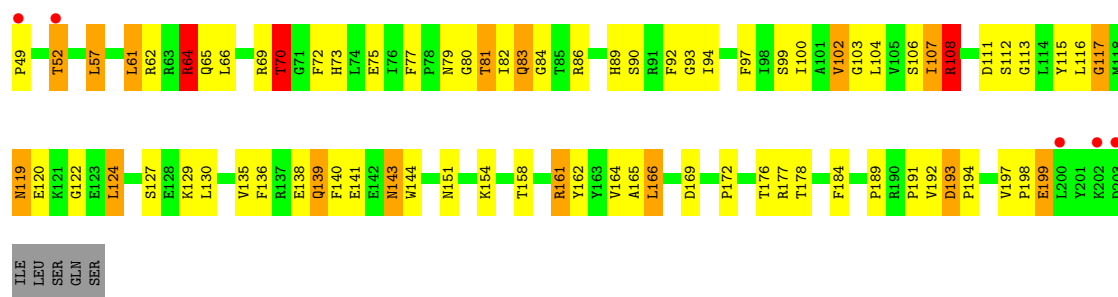
Chain C: 



• Molecule 1: FIBROBLAST GROWTH FACTOR 9

Chain D: 





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

Chain E: 100%



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

Chain F: 33% 67%



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

Chain G: 33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	151.95Å 151.95Å 117.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.60) 100.0 (50.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.52 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.248 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5480	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	2.22	46/1325 (3.5%)	1.67	16/1783 (0.9%)
1	B	1.55	10/1325 (0.8%)	1.43	13/1785 (0.7%)
1	C	2.09	43/1309 (3.3%)	1.62	16/1763 (0.9%)
1	D	2.29	53/1307 (4.1%)	1.70	18/1761 (1.0%)
All	All	2.06	152/5266 (2.9%)	1.61	63/7092 (0.9%)

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	PRO	C-O	-12.18	1.10	1.23
1	D	164	VAL	CA-CB	-9.81	1.44	1.54
1	B	190	ARG	C-O	-9.44	1.14	1.24
1	C	82	ILE	C-O	-9.43	1.14	1.24
1	C	98	ILE	CA-CB	-9.04	1.43	1.54
1	A	118	MET	SD-CE	-9.01	1.57	1.79
1	D	102	VAL	CA-CB	8.99	1.64	1.54
1	A	174	GLU	CA-C	-8.94	1.41	1.52
1	D	64	ARG	CD-NE	-8.75	1.34	1.46
1	D	116	LEU	N-CA	-8.60	1.35	1.46
1	D	154	LYS	C-O	-8.59	1.13	1.23
1	A	173	ARG	C-O	8.54	1.34	1.23
1	A	147	THR	CA-C	-8.41	1.42	1.52
1	D	111	ASP	C-O	-8.31	1.14	1.24
1	D	135	VAL	CA-CB	-8.15	1.43	1.54
1	A	154	LYS	C-O	-7.83	1.14	1.23
1	D	130	LEU	C-O	-7.64	1.14	1.24
1	A	101	ALA	C-O	-7.51	1.16	1.24
1	D	189	PRO	C-O	-7.50	1.15	1.23
1	D	172	PRO	C-O	-7.47	1.15	1.23
1	D	176	THR	CA-C	-7.46	1.42	1.52
1	C	138	GLU	C-O	-7.46	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	GLY	C-O	-7.35	1.14	1.24
1	C	126	GLY	C-O	-7.34	1.15	1.23
1	D	66	LEU	N-CA	-7.32	1.37	1.46
1	A	190	ARG	CD-NE	-7.32	1.36	1.46
1	C	154	LYS	C-O	-7.14	1.15	1.23
1	A	173	ARG	N-CA	-7.11	1.37	1.45
1	C	137	ARG	CA-C	-7.11	1.44	1.52
1	A	107	ILE	N-CA	-7.08	1.37	1.46
1	C	148	TYR	C-O	-6.97	1.16	1.24
1	D	141	GLU	CA-C	6.97	1.59	1.52
1	D	161	ARG	CD-NE	-6.95	1.36	1.46
1	D	158	THR	CA-CB	-6.93	1.42	1.53
1	D	112	SER	CA-C	-6.84	1.43	1.52
1	A	195	ASP	CB-CG	6.82	1.69	1.52
1	A	160	ARG	CB-CG	-6.80	1.32	1.52
1	A	59	GLY	N-CA	-6.79	1.37	1.45
1	C	130	LEU	C-O	-6.68	1.15	1.24
1	C	201	TYR	CA-C	6.68	1.61	1.52
1	C	151	ASN	C-O	-6.68	1.15	1.24
1	A	76	ILE	CA-CB	-6.67	1.45	1.53
1	A	179	LYS	CE-NZ	6.66	1.69	1.49
1	C	99	SER	C-O	-6.63	1.15	1.23
1	C	66	LEU	CA-C	-6.62	1.44	1.52
1	A	134	CYS	N-CA	-6.61	1.38	1.46
1	D	108	ARG	N-CA	-6.52	1.38	1.46
1	B	60	ILE	CA-CB	-6.49	1.46	1.54
1	A	204	ILE	CA-C	-6.47	1.44	1.52
1	A	173	ARG	CA-C	-6.47	1.45	1.52
1	B	155	HIS	CA-C	-6.44	1.44	1.52
1	A	168	LYS	C-O	-6.40	1.16	1.24
1	D	97	PHE	CA-CB	-6.37	1.43	1.53
1	C	190	ARG	NE-CZ	-6.33	1.26	1.33
1	C	87	LYS	CA-C	-6.32	1.44	1.53
1	A	195	ASP	CG-OD2	6.30	1.37	1.25
1	C	135	VAL	C-O	-6.27	1.17	1.24
1	D	178	THR	CA-C	-6.27	1.45	1.52
1	D	151	ASN	C-O	-6.24	1.16	1.24
1	C	86	ARG	N-CA	6.23	1.54	1.46
1	A	110	VAL	C-O	-6.23	1.17	1.24
1	D	86	ARG	C-O	-6.22	1.16	1.24
1	D	119	ASN	CA-C	-6.20	1.45	1.52
1	C	168	LYS	C-O	-6.20	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	ILE	CA-C	-6.17	1.45	1.52
1	A	106	SER	C-O	-6.11	1.16	1.23
1	A	165	ALA	N-CA	-6.09	1.38	1.46
1	C	86	ARG	C-O	-6.09	1.16	1.24
1	D	90	SER	CA-CB	-6.07	1.43	1.53
1	C	192	VAL	CA-CB	-6.05	1.47	1.54
1	B	107	ILE	C-O	-6.01	1.17	1.24
1	C	158	THR	C-O	-5.99	1.16	1.24
1	B	204	ILE	CA-C	-5.97	1.47	1.52
1	C	90	SER	N-CA	-5.95	1.37	1.45
1	A	181	HIS	CA-C	-5.95	1.44	1.52
1	C	164	VAL	C-O	-5.95	1.17	1.24
1	A	107	ILE	C-O	-5.94	1.17	1.24
1	D	82	ILE	CA-CB	-5.89	1.47	1.54
1	D	61	LEU	C-O	-5.89	1.16	1.24
1	B	130	LEU	C-O	-5.86	1.17	1.24
1	A	163	TYR	CA-C	-5.84	1.45	1.52
1	C	198	PRO	C-O	-5.81	1.16	1.24
1	C	156	VAL	CA-CB	-5.80	1.47	1.54
1	D	57	LEU	N-CA	-5.78	1.39	1.46
1	A	173	ARG	CD-NE	-5.76	1.38	1.46
1	D	120	GLU	N-CA	5.76	1.53	1.46
1	D	140	PHE	C-O	-5.74	1.17	1.23
1	A	176	THR	CB-CG2	-5.67	1.33	1.52
1	A	202	LYS	C-O	-5.63	1.16	1.24
1	D	75	GLU	CA-C	-5.63	1.46	1.52
1	D	143	ASN	C-O	-5.58	1.16	1.23
1	C	80	GLY	C-O	-5.57	1.16	1.24
1	D	61	LEU	N-CA	-5.56	1.38	1.46
1	B	107	ILE	CA-CB	-5.55	1.47	1.54
1	A	179	LYS	CD-CE	5.55	1.69	1.52
1	C	161	ARG	CD-NE	-5.52	1.38	1.46
1	D	100	ILE	CA-CB	5.52	1.61	1.54
1	D	166	LEU	CA-C	-5.50	1.46	1.52
1	C	180	ARG	C-O	-5.47	1.17	1.24
1	C	189	PRO	C-O	-5.47	1.16	1.23
1	C	171	THR	CA-C	-5.46	1.46	1.53
1	A	61	LEU	CA-CB	-5.46	1.43	1.53
1	A	141	GLU	CA-C	5.44	1.57	1.52
1	A	105	VAL	N-CA	-5.43	1.39	1.46
1	C	92	PHE	N-CA	-5.41	1.39	1.46
1	B	94	ILE	CA-CB	-5.40	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	LEU	N-CA	-5.40	1.39	1.46
1	D	161	ARG	CZ-NH2	-5.40	1.26	1.33
1	D	65	GLN	CA-CB	-5.39	1.44	1.53
1	A	66	LEU	CA-C	-5.39	1.46	1.53
1	B	199	GLU	C-O	5.37	1.33	1.23
1	A	161	ARG	CD-NE	-5.36	1.38	1.46
1	C	118	MET	SD-CE	-5.35	1.66	1.79
1	D	69	ARG	C-O	-5.35	1.17	1.24
1	A	62	ARG	CD-NE	5.32	1.53	1.46
1	C	164	VAL	CA-C	-5.31	1.46	1.52
1	C	76	ILE	CA-CB	-5.30	1.47	1.53
1	D	83	GLN	CB-CG	-5.28	1.36	1.52
1	C	107	ILE	CA-CB	-5.27	1.47	1.54
1	D	99	SER	C-O	-5.27	1.17	1.24
1	D	193	ASP	C-N	-5.27	1.26	1.33
1	C	120	GLU	CD-OE2	5.27	1.35	1.25
1	C	130	LEU	N-CA	-5.25	1.39	1.46
1	C	104	LEU	N-CA	-5.25	1.39	1.46
1	A	64	ARG	N-CA	-5.24	1.39	1.45
1	C	181	HIS	CA-C	-5.24	1.45	1.52
1	D	119	ASN	C-O	5.24	1.30	1.23
1	A	160	ARG	C-O	5.22	1.30	1.23
1	A	65	GLN	CA-C	5.21	1.58	1.52
1	C	70	THR	C-O	-5.21	1.17	1.24
1	D	93	GLY	C-O	-5.20	1.18	1.23
1	A	181	HIS	C-O	-5.19	1.17	1.24
1	C	132	GLN	C-O	-5.18	1.17	1.24
1	D	161	ARG	CG-CD	-5.17	1.36	1.52
1	D	136	PHE	N-CA	-5.17	1.39	1.45
1	D	192	VAL	N-CA	-5.17	1.40	1.46
1	D	130	LEU	N-CA	-5.16	1.40	1.46
1	A	178	THR	C-O	-5.15	1.17	1.23
1	C	187	PHE	C-O	-5.13	1.17	1.23
1	D	135	VAL	N-CA	-5.13	1.39	1.46
1	A	81	THR	CB-OG1	5.10	1.51	1.43
1	D	92	PHE	N-CA	-5.08	1.39	1.46
1	D	82	ILE	N-CA	-5.08	1.40	1.46
1	D	139	GLN	CA-C	-5.06	1.46	1.52
1	A	89	HIS	C-O	-5.05	1.17	1.23
1	B	116	LEU	N-CA	-5.05	1.40	1.46
1	A	95	LEU	CA-C	-5.05	1.46	1.52
1	A	199	GLU	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	PHE	CG-CD1	-5.04	1.28	1.38
1	C	120	GLU	C-O	-5.04	1.17	1.24
1	D	65	GLN	C-O	-5.04	1.17	1.23
1	A	160	ARG	CA-C	5.01	1.59	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ASN	N-CA-C	-9.22	101.56	113.17
1	B	200	LEU	N-CA-C	-9.02	104.33	114.62
1	A	171	THR	CA-C-N	-7.66	112.02	120.14
1	A	171	THR	C-N-CA	-7.66	112.02	120.14
1	C	53	ASP	N-CA-C	7.63	120.42	110.43
1	A	173	ARG	CG-CD-NE	-7.52	95.46	112.00
1	A	188	LEU	N-CA-CB	-7.46	100.46	110.23
1	C	201	TYR	CA-C-O	7.43	129.56	121.02
1	B	204	ILE	CB-CA-C	-7.25	103.81	110.91
1	C	201	TYR	CB-CA-C	7.21	122.42	110.88
1	C	191	PRO	CA-C-N	-7.02	114.48	123.19
1	C	191	PRO	C-N-CA	-7.02	114.48	123.19
1	B	65	GLN	N-CA-C	-6.86	99.50	110.14
1	A	165	ALA	N-CA-C	6.83	119.56	108.76
1	B	204	ILE	N-CA-C	-6.79	106.42	112.12
1	C	191	PRO	CA-C-O	6.79	130.53	122.12
1	A	176	THR	N-CA-CB	-6.60	99.64	110.40
1	A	176	THR	OG1-CB-CG2	6.59	122.49	109.30
1	C	105	VAL	CB-CA-C	-6.33	101.45	110.82
1	D	64	ARG	CB-CG-CD	6.09	125.30	111.30
1	D	102	VAL	N-CA-CB	6.05	118.24	110.13
1	D	189	PRO	CA-C-O	-5.96	113.95	120.92
1	B	206	SER	N-CA-C	-5.89	102.34	110.35
1	D	70	THR	N-CA-CB	-5.82	100.20	110.39
1	C	205	LEU	CB-CA-C	-5.82	98.85	110.42
1	C	190	ARG	CG-CD-NE	5.78	124.71	112.00
1	D	64	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	A	170	GLY	CA-C-O	5.68	125.33	119.02
1	D	117	GLY	N-CA-C	-5.60	102.33	110.90
1	A	188	LEU	N-CA-C	5.59	117.01	109.24
1	D	193	ASP	CA-C-O	5.54	124.19	119.71
1	D	191	PRO	CB-CA-C	-5.49	103.75	110.95
1	A	62	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	B	178	THR	N-CA-C	5.43	117.44	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	HIS	CA-C-N	-5.37	112.48	121.39
1	D	89	HIS	C-N-CA	-5.37	112.48	121.39
1	A	81	THR	N-CA-CB	-5.37	102.13	110.29
1	C	199	GLU	CA-C-O	5.35	125.97	119.49
1	B	56	HIS	N-CA-C	-5.35	105.11	111.69
1	B	71	GLY	CA-C-N	-5.33	114.10	122.73
1	B	71	GLY	C-N-CA	-5.33	114.10	122.73
1	D	94	ILE	CB-CA-C	-5.31	104.53	110.96
1	D	162	TYR	CB-CA-C	-5.31	102.13	110.79
1	C	164	VAL	N-CA-C	-5.29	102.76	109.58
1	D	103	GLY	CA-C-N	-5.28	114.18	122.73
1	D	103	GLY	C-N-CA	-5.28	114.18	122.73
1	D	124	LEU	CA-C-O	-5.27	115.41	121.47
1	A	190	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	C	204	ILE	CG1-CB-CG2	-5.24	94.97	110.70
1	B	158	THR	N-CA-C	5.24	117.39	111.11
1	B	159	GLY	N-CA-C	-5.24	107.57	115.32
1	C	206	SER	N-CA-C	5.23	125.65	111.00
1	D	107	ILE	N-CA-CB	-5.23	104.71	111.82
1	C	205	LEU	CA-CB-CG	5.21	134.54	116.30
1	D	165	ALA	N-CA-C	5.18	116.94	108.76
1	A	111	ASP	CB-CA-C	-5.17	102.74	110.90
1	B	79	ASN	N-CA-C	-5.15	106.26	113.37
1	B	201	TYR	N-CA-C	-5.11	106.31	112.54
1	A	170	GLY	N-CA-C	-5.09	108.59	115.36
1	D	52	THR	OG1-CB-CG2	-5.09	99.11	109.30
1	C	89	HIS	N-CA-C	5.08	118.60	111.90
1	A	85	THR	OG1-CB-CG2	-5.03	99.25	109.30
1	C	105	VAL	N-CA-C	5.02	116.14	108.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1295	0	1272	34	0
1	B	1295	0	1275	106	0
1	C	1279	0	1259	29	0
1	D	1276	0	1254	37	0
2	E	38	0	34	0	0
2	F	38	0	34	4	0
2	G	38	0	34	1	0
3	A	15	0	0	1	0
3	B	10	0	0	1	0
3	C	20	0	0	0	0
3	D	15	0	0	1	0
4	B	14	0	13	0	0
5	A	59	0	0	2	0
5	B	4	0	0	0	0
5	C	35	0	0	0	0
5	D	49	0	0	4	0
All	All	5480	0	5175	203	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 19.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LYS:CE	1:A:179:LYS:NZ	1.69	1.49
1:B:158:THR:CG2	1:B:160:ARG:HG2	1.61	1.30
1:B:64:ARG:HH11	1:B:64:ARG:CG	1.43	1.27
1:B:155:HIS:HD2	1:B:162:TYR:CE1	1.62	1.16
1:B:158:THR:HG21	1:B:160:ARG:HG2	1.19	1.09
1:B:64:ARG:HG2	1:B:64:ARG:NH1	1.56	1.05
1:B:158:THR:HG21	1:B:160:ARG:CG	1.85	1.05
1:B:63:ARG:O	1:B:64:ARG:CD	2.07	1.03
1:B:63:ARG:O	1:B:64:ARG:HD3	1.58	1.02
1:B:155:HIS:CD2	1:B:162:TYR:CE1	2.48	1.01
1:B:63:ARG:C	1:B:64:ARG:HD3	1.88	0.98
1:B:64:ARG:HH11	1:B:64:ARG:HG2	0.80	0.94
1:B:155:HIS:HD2	1:B:162:TYR:HE1	1.03	0.94
1:B:155:HIS:CD2	1:B:162:TYR:HE1	1.86	0.88
1:D:119:ASN:O	1:D:122:GLY:N	2.05	0.88
1:B:158:THR:HG22	1:B:160:ARG:HG2	1.55	0.86
1:B:158:THR:CG2	1:B:160:ARG:CG	2.48	0.86
1:B:137:ARG:HE	1:B:151:ASN:ND2	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:HIS:CD2	1:B:162:TYR:CD1	2.67	0.83
1:D:49:PRO:O	1:D:52:THR:HG22	1.78	0.83
1:B:63:ARG:O	1:B:64:ARG:HD2	1.80	0.80
1:B:67:TYR:HB2	1:B:73:HIS:CD2	2.16	0.80
1:D:49:PRO:C	1:D:52:THR:HG22	2.06	0.80
1:D:64:ARG:HD2	5:D:431:HOH:O	1.80	0.80
1:A:167:ASN:HD22	1:A:171:THR:HG22	1.48	0.79
1:B:204:ILE:HD12	1:C:57:LEU:HD21	1.64	0.78
1:B:156:VAL:HG13	1:B:157:ASP:H	1.49	0.78
1:B:204:ILE:HD12	1:C:57:LEU:CD2	2.14	0.77
1:A:199:GLU:OE1	1:A:199:GLU:N	2.14	0.76
1:A:161:ARG:NH2	3:A:302:SO4:O4	2.19	0.76
2:F:1:NAG:O3	2:F:1:NAG:H83	1.86	0.75
1:B:137:ARG:HE	1:B:151:ASN:HD22	1.34	0.75
1:B:155:HIS:ND1	1:B:160:ARG:HB2	2.01	0.74
1:B:64:ARG:CG	1:B:64:ARG:NH1	2.20	0.74
1:C:79:ASN:OD1	1:C:81:THR:HB	1.88	0.73
1:B:75:GLU:OE1	1:B:85:THR:HG23	1.88	0.73
1:B:156:VAL:HG13	1:B:157:ASP:N	2.03	0.72
1:B:118:MET:HE1	1:B:162:TYR:O	1.90	0.71
1:A:195:ASP:OD2	1:D:62:ARG:NH1	2.23	0.69
1:D:49:PRO:HA	1:D:52:THR:CG2	2.22	0.69
1:D:49:PRO:HA	1:D:52:THR:HG22	1.73	0.69
2:F:2:NAG:O3	2:F:2:NAG:H82	1.91	0.69
1:C:66:LEU:HD22	1:C:187:PHE:HB3	1.75	0.68
1:C:70:THR:HG23	1:C:72:PHE:HD1	1.60	0.67
1:D:199:GLU:H	1:D:199:GLU:CD	2.02	0.67
1:A:79:ASN:OD1	1:A:81:THR:HB	1.93	0.67
1:D:49:PRO:CA	1:D:52:THR:HG22	2.25	0.67
1:D:77:PHE:HE1	1:D:83:GLN:CG	2.07	0.66
1:B:58:LYS:O	1:B:62:ARG:HG3	1.97	0.65
1:C:143:ASN:O	1:C:144:TRP:HB2	1.94	0.65
1:D:79:ASN:OD1	1:D:81:THR:HB	1.95	0.65
1:B:119:ASN:HA	1:B:133:GLU:CD	2.20	0.65
1:B:51:VAL:HB	1:C:205:LEU:HD21	1.77	0.65
1:B:148:TYR:O	1:B:164:VAL:HG23	1.97	0.65
1:C:199:GLU:O	1:C:201:TYR:N	2.30	0.64
1:B:85:THR:HB	1:B:87:LYS:HG3	1.80	0.64
1:B:201:TYR:HD1	1:B:205:LEU:HD12	1.64	0.63
1:C:199:GLU:O	1:C:200:LEU:C	2.38	0.62
1:B:180:ARG:HD2	1:B:181:HIS:CE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:OD1	1:A:171:THR:HB	2.01	0.60
1:B:78:PRO:C	1:B:80:GLY:H	2.08	0.60
1:A:54:LEU:HG	1:A:58:LYS:HE3	1.85	0.59
1:B:141:GLU:HG2	1:B:147:THR:HG23	1.83	0.59
1:B:156:VAL:CG1	1:B:157:ASP:H	2.14	0.59
1:B:100:ILE:O	1:B:101:ALA:HB2	2.02	0.58
1:B:54:LEU:HA	1:B:57:LEU:HD12	1.86	0.57
1:B:155:HIS:CD2	1:B:162:TYR:HD1	2.23	0.57
2:F:1:NAG:O3	2:F:1:NAG:C8	2.53	0.57
1:A:88:ASP:OD1	1:A:190:ARG:NH2	2.36	0.56
1:B:64:ARG:HH11	1:B:64:ARG:HG3	1.57	0.56
1:B:118:MET:HA	1:B:123:GLU:O	2.06	0.56
1:B:52:THR:HG23	1:B:56:HIS:HD2	1.71	0.56
1:B:173:ARG:HD3	1:B:184:PHE:CE2	2.41	0.56
1:B:52:THR:CG2	1:B:56:HIS:HD2	2.19	0.55
1:B:201:TYR:CD1	1:B:205:LEU:HD12	2.40	0.55
1:B:180:ARG:O	1:B:181:HIS:HB2	2.06	0.55
1:B:173:ARG:HG2	1:B:174:GLU:H	1.72	0.55
1:B:118:MET:O	1:B:133:GLU:HG3	2.07	0.55
1:C:161:ARG:HB2	1:C:163:TYR:CE1	2.42	0.54
1:A:193:ASP:CG	1:A:194:PRO:HD2	2.33	0.54
1:B:67:TYR:CE1	1:B:71:GLY:HA2	2.43	0.53
1:D:77:PHE:CE1	1:D:83:GLN:CG	2.91	0.53
1:B:92:PHE:CE1	1:B:111:ASP:OD2	2.62	0.53
1:B:101:ALA:O	1:B:102:VAL:C	2.51	0.53
1:D:197:VAL:N	1:D:198:PRO:HD3	2.24	0.53
1:B:94:ILE:O	1:B:110:VAL:HG23	2.10	0.52
2:G:1:NAG:H61	2:G:2:NAG:H82	1.90	0.52
1:A:86:ARG:NH1	5:A:403:HOH:O	2.41	0.51
1:B:156:VAL:CG1	1:B:157:ASP:N	2.71	0.51
1:A:176:THR:HG22	1:A:177:ARG:HG3	1.92	0.51
1:C:68:CYS:HB2	1:C:187:PHE:CE2	2.45	0.51
1:C:199:GLU:C	1:C:201:TYR:N	2.67	0.51
1:B:199:GLU:CD	1:B:202:LYS:NZ	2.69	0.51
1:A:160:ARG:HG2	5:A:417:HOH:O	2.11	0.50
1:A:66:LEU:HD22	1:A:187:PHE:HB3	1.93	0.50
1:D:106:SER:C	1:D:107:ILE:HG13	2.36	0.50
1:A:60:ILE:CG2	1:D:61:LEU:HD21	2.42	0.50
1:A:119:ASN:OD1	1:A:119:ASN:C	2.53	0.50
1:A:161:ARG:HB2	1:A:163:TYR:CE1	2.47	0.50
1:B:69:ARG:O	1:B:69:ARG:HG3	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:C	1:B:71:GLY:H	2.19	0.50
1:C:125:TYR:CE2	1:C:127:SER:HB2	2.47	0.50
1:D:108:ARG:HD3	1:D:115:TYR:CE2	2.47	0.50
1:B:78:PRO:C	1:B:80:GLY:N	2.70	0.50
1:B:199:GLU:CD	1:B:202:LYS:HZ1	2.19	0.50
1:D:193:ASP:O	1:D:194:PRO:C	2.54	0.50
1:B:137:ARG:NE	1:B:151:ASN:HD22	2.08	0.49
1:B:190:ARG:HB3	1:B:191:PRO:HD2	1.93	0.49
1:A:69:ARG:HG2	1:A:183:LYS:HG3	1.93	0.49
1:C:69:ARG:HG3	1:C:183:LYS:HE3	1.94	0.49
1:C:100:ILE:O	1:C:101:ALA:HB2	2.12	0.49
1:B:51:VAL:HB	1:C:205:LEU:CD2	2.42	0.49
1:D:161:ARG:HD3	5:D:407:HOH:O	2.12	0.49
1:B:155:HIS:HB2	1:B:160:ARG:H	1.79	0.48
1:A:171:THR:HG23	1:A:172:PRO:N	2.28	0.48
1:D:177:ARG:NH1	3:D:303:SO4:O2	2.36	0.48
1:C:86:ARG:NH1	1:C:86:ARG:HG2	2.28	0.48
1:B:67:TYR:CZ	1:B:71:GLY:HA2	2.49	0.47
1:B:91:ARG:HG3	1:B:91:ARG:NH1	2.27	0.47
1:A:52:THR:HG23	1:A:55:ASP:HB2	1.96	0.47
1:D:117:GLY:O	1:D:124:LEU:HA	2.14	0.47
1:B:66:LEU:O	1:B:73:HIS:HA	2.14	0.47
1:B:161:ARG:NH2	3:B:303:SO4:O2	2.48	0.47
1:C:204:ILE:HD13	1:C:204:ILE:HG21	1.61	0.47
1:B:117:GLY:O	1:B:124:LEU:HA	2.15	0.47
1:D:77:PHE:HE1	1:D:83:GLN:HG2	1.78	0.47
1:D:77:PHE:CE1	1:D:83:GLN:HG2	2.50	0.47
1:B:63:ARG:C	1:B:64:ARG:CD	2.67	0.46
1:B:65:GLN:NE2	1:B:89:HIS:CE1	2.83	0.46
1:B:105:VAL:HG22	1:B:106:SER:N	2.30	0.46
1:B:173:ARG:CG	1:B:174:GLU:H	2.27	0.46
1:D:64:ARG:CD	5:D:431:HOH:O	2.52	0.46
1:A:124:LEU:O	1:C:157:ASP:HB3	2.16	0.46
1:C:63:ARG:C	1:C:64:ARG:HG2	2.39	0.46
1:D:49:PRO:HA	1:D:52:THR:HG21	1.96	0.46
1:A:176:THR:HG22	1:A:177:ARG:CG	2.46	0.46
1:B:118:MET:O	1:B:133:GLU:CG	2.64	0.46
1:A:58:LYS:HA	1:A:61:LEU:HD12	1.97	0.46
1:B:182:GLN:O	1:B:183:LYS:C	2.59	0.46
2:F:2:NAG:H82	2:F:2:NAG:C3	2.46	0.45
1:D:77:PHE:HE1	1:D:83:GLN:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:ARG:HD3	1:D:115:TYR:CZ	2.51	0.45
1:A:130:LEU:C	1:A:130:LEU:HD23	2.41	0.45
1:B:65:GLN:HE22	1:B:89:HIS:CE1	2.35	0.45
1:D:49:PRO:O	1:D:52:THR:CG2	2.56	0.45
1:A:52:THR:CG2	1:A:55:ASP:HB2	2.46	0.45
1:B:136:PHE:CD1	1:B:136:PHE:N	2.84	0.45
1:D:108:ARG:HD2	1:D:113:GLY:O	2.17	0.45
1:A:131:THR:O	1:A:134:CYS:HB2	2.17	0.45
1:A:208:SER:O	1:A:208:SER:OG	2.27	0.45
1:B:67:TYR:HB2	1:B:73:HIS:HD2	1.73	0.45
1:C:161:ARG:HA	1:C:161:ARG:HD3	1.81	0.45
1:C:143:ASN:O	1:C:144:TRP:CB	2.65	0.45
1:B:158:THR:CG2	1:B:160:ARG:NE	2.80	0.44
1:A:199:GLU:O	1:A:200:LEU:C	2.59	0.44
1:B:90:SER:O	1:B:91:ARG:C	2.60	0.44
1:B:132:GLN:C	1:B:134:CYS:H	2.26	0.44
1:D:73:HIS:O	1:D:84:GLY:HA2	2.18	0.44
1:B:85:THR:CB	1:B:87:LYS:HG3	2.47	0.44
1:B:173:ARG:NE	1:B:177:ARG:O	2.50	0.44
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.82	0.44
1:B:63:ARG:HH11	1:B:200:LEU:HD12	1.83	0.43
1:B:178:THR:HG22	1:B:184:PHE:HE2	1.83	0.43
1:B:121:LYS:HE3	1:B:123:GLU:CD	2.44	0.43
1:B:161:ARG:HD3	1:B:161:ARG:HA	1.86	0.43
1:D:79:ASN:CG	5:D:424:HOH:O	2.61	0.43
1:B:144:TRP:HB3	1:C:190:ARG:NH1	2.33	0.43
1:B:182:GLN:OE1	1:B:184:PHE:CZ	2.72	0.43
1:B:128:GLU:H	1:B:128:GLU:CD	2.27	0.42
1:B:174:GLU:O	1:B:177:ARG:N	2.50	0.42
1:B:142:GLU:O	1:B:145:TYR:HB2	2.20	0.42
1:B:155:HIS:NE2	1:B:162:TYR:HD1	2.18	0.42
1:B:158:THR:CG2	1:B:160:ARG:HE	2.32	0.42
1:C:69:ARG:HG3	1:C:69:ARG:O	2.19	0.42
1:D:138:GLU:C	1:D:139:GLN:HG3	2.44	0.42
1:D:143:ASN:O	1:D:144:TRP:HB2	2.20	0.42
1:B:137:ARG:HB2	1:B:149:SER:OG	2.20	0.42
1:B:57:LEU:O	1:B:58:LYS:C	2.58	0.42
1:C:196:LYS:O	1:C:198:PRO:HD3	2.20	0.41
1:C:57:LEU:O	1:C:61:LEU:HG	2.20	0.41
1:C:87:LYS:H	1:C:87:LYS:HG2	1.74	0.41
1:B:119:ASN:HA	1:B:133:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:THR:HG21	1:D:166:LEU:O	2.20	0.41
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.68	0.41
1:B:66:LEU:CD1	1:B:187:PHE:HB3	2.50	0.41
1:D:169:ASP:OD1	1:D:169:ASP:C	2.63	0.41
1:A:157:ASP:OD1	1:A:158:THR:N	2.54	0.41
1:A:196:LYS:C	1:A:198:PRO:HD3	2.46	0.41
1:B:52:THR:O	1:B:53:ASP:C	2.64	0.41
1:B:127:SER:OG	1:B:128:GLU:N	2.53	0.41
1:B:130:LEU:C	1:B:130:LEU:CD2	2.94	0.41
1:C:68:CYS:HB3	1:C:70:THR:HG22	2.02	0.41
1:C:86:ARG:HG2	1:C:86:ARG:HH11	1.85	0.41
1:A:66:LEU:O	1:A:73:HIS:HA	2.21	0.41
1:B:158:THR:HG21	1:B:160:ARG:HG3	1.91	0.41
1:B:188:LEU:HA	1:B:189:PRO:HD3	1.85	0.41
1:D:57:LEU:HD12	1:D:57:LEU:HA	1.83	0.41
1:B:174:GLU:O	1:B:175:GLY:C	2.64	0.40
1:A:56:HIS:HD1	1:A:203:ASP:CG	2.28	0.40
1:A:173:ARG:HG2	1:A:174:GLU:N	2.35	0.40
1:B:197:VAL:HG23	1:B:197:VAL:O	2.21	0.40
1:D:119:ASN:OD1	1:D:119:ASN:C	2.64	0.40
1:D:127:SER:OG	1:D:129:LYS:O	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	155/160 (97%)	149 (96%)	6 (4%)	0	100	100
1	B	155/160 (97%)	136 (88%)	16 (10%)	3 (2%)	6	13
1	C	153/160 (96%)	142 (93%)	7 (5%)	4 (3%)	4	7
1	D	153/160 (96%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	616/640 (96%)	574 (93%)	35 (6%)	7 (1%)	11	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	ASP
1	B	156	VAL
1	C	200	LEU
1	B	183	LYS
1	C	202	LYS
1	C	205	LEU
1	C	168	LYS

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	141/143 (99%)	133 (94%)	8 (6%)	18	40
1	B	141/143 (99%)	131 (93%)	10 (7%)	13	31
1	C	139/143 (97%)	135 (97%)	4 (3%)	37	65
1	D	138/143 (96%)	131 (95%)	7 (5%)	21	45
All	All	559/572 (98%)	530 (95%)	29 (5%)	21	44

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	THR
1	A	62	ARG
1	A	81	THR
1	A	111	ASP
1	A	171	THR
1	A	176	THR
1	A	183	LYS
1	A	184	PHE

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Mol	Chain	Res	Type
1	B	64	ARG
1	B	81	THR
1	B	90	SER
1	B	99	SER
1	B	128	GLU
1	B	130	LEU
1	B	142	GLU
1	B	161	ARG
1	B	200	LEU
1	B	206	SER
1	C	70	THR
1	C	81	THR
1	C	120	GLU
1	C	184	PHE
1	D	64	ARG
1	D	70	THR
1	D	81	THR
1	D	102	VAL
1	D	108	ARG
1	D	184	PHE
1	D	199	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	167	ASN
1	B	56	HIS
1	B	139	GLN
1	B	151	ASN
1	B	155	HIS
1	B	181	HIS
1	B	207	GLN
1	C	186	HIS

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 ⓘ

9 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	2.68	5 (35%)	17,19,21	4.40	11 (64%)
2	NAG	E	2	2	14,14,15	0.95	0	17,19,21	2.69	6 (35%)
2	FUC	E	3	2	10,10,11	1.39	3 (30%)	14,14,16	1.61	3 (21%)
2	NAG	F	1	1,2	14,14,15	1.25	1 (7%)	17,19,21	2.84	9 (52%)
2	NAG	F	2	2	14,14,15	1.42	2 (14%)	17,19,21	4.10	10 (58%)
2	FUC	F	3	2	10,10,11	1.40	1 (10%)	14,14,16	2.89	5 (35%)
2	NAG	G	1	1,2	14,14,15	1.82	2 (14%)	17,19,21	3.47	6 (35%)
2	NAG	G	2	2	14,14,15	1.20	1 (7%)	17,19,21	2.09	5 (29%)
2	FUC	G	3	2	10,10,11	0.92	1 (10%)	14,14,16	2.12	7 (50%)

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	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	6/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
2	NAG	G	1	1,2	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	FUC	G	3	2	1/1/4/5	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C2-N2	-7.46	1.33	1.46
2	G	1	NAG	O7-C7	5.05	1.34	1.23
2	E	1	NAG	C4-C5	-4.11	1.44	1.53
2	F	2	NAG	C1-C2	3.99	1.57	1.52
2	E	1	NAG	C4-C3	-3.43	1.43	1.52
2	F	3	FUC	O5-C1	-3.23	1.38	1.43
2	G	1	NAG	C1-C2	3.20	1.56	1.52
2	G	2	NAG	O5-C5	2.77	1.48	1.43
2	E	3	FUC	C2-C3	-2.52	1.48	1.52
2	E	1	NAG	C1-C2	-2.28	1.49	1.52
2	F	2	NAG	O5-C5	2.20	1.47	1.43
2	E	1	NAG	O5-C1	-2.14	1.40	1.43
2	F	1	NAG	C2-N2	-2.12	1.42	1.46
2	G	3	FUC	O5-C1	-2.10	1.40	1.43
2	E	3	FUC	O5-C5	-2.03	1.39	1.43
2	E	3	FUC	O4-C4	-2.02	1.38	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O5-C1-C2	10.61	127.70	111.29
2	E	1	NAG	C8-C7-N2	10.37	133.31	116.12
2	F	3	FUC	C2-C3-C4	-7.87	97.02	110.86
2	E	1	NAG	C3-C4-C5	-7.42	96.78	110.23
2	G	1	NAG	C8-C7-N2	-7.23	104.13	116.12
2	F	2	NAG	O5-C5-C6	6.91	121.10	107.66
2	G	1	NAG	C1-C2-N2	6.57	120.79	110.43
2	G	1	NAG	O7-C7-N2	6.22	132.96	121.98
2	F	1	NAG	C2-N2-C7	-6.16	114.65	122.90
2	E	1	NAG	O7-C7-C8	-5.93	111.50	122.05
2	E	1	NAG	O4-C4-C3	-5.86	96.56	110.38
2	G	1	NAG	O4-C4-C5	5.67	123.30	109.32
2	E	2	NAG	C1-C2-N2	-5.58	101.63	110.43
2	E	2	NAG	C1-O5-C5	5.50	119.56	112.19
2	E	1	NAG	O5-C5-C6	5.43	118.23	107.66
2	F	2	NAG	C8-C7-N2	5.37	125.03	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	C1-C2-N2	4.83	118.05	110.43
2	F	3	FUC	C3-C4-C5	-4.73	102.62	109.81
2	G	2	NAG	O5-C1-C2	4.59	118.40	111.29
2	G	2	NAG	O5-C5-C6	4.39	116.22	107.66
2	F	1	NAG	O7-C7-N2	4.39	129.73	121.98
2	E	2	NAG	O5-C1-C2	4.29	117.93	111.29
2	G	1	NAG	C4-C3-C2	-3.93	105.25	111.02
2	F	1	NAG	O4-C4-C3	-3.92	101.13	110.38
2	F	2	NAG	C2-N2-C7	-3.86	117.72	122.90
2	E	1	NAG	O7-C7-N2	-3.85	115.18	121.98
2	G	3	FUC	C3-C4-C5	-3.73	104.14	109.81
2	E	2	NAG	O7-C7-N2	3.71	128.54	121.98
2	E	1	NAG	C6-C5-C4	-3.69	103.95	113.02
2	F	2	NAG	O7-C7-C8	-3.66	115.54	122.05
2	G	1	NAG	O4-C4-C3	-3.64	101.79	110.38
2	F	1	NAG	C8-C7-N2	-3.56	110.22	116.12
2	F	1	NAG	C1-O5-C5	3.55	116.94	112.19
2	E	2	NAG	O7-C7-C8	-3.52	115.79	122.05
2	F	2	NAG	C3-C4-C5	3.43	116.45	110.23
2	F	1	NAG	O5-C1-C2	-3.42	105.99	111.29
2	E	1	NAG	C2-N2-C7	-3.35	118.41	122.90
2	E	3	FUC	O4-C4-C3	-3.24	102.73	110.38
2	G	3	FUC	C6-C5-C4	-3.24	107.15	113.08
2	E	1	NAG	C1-O5-C5	-3.23	107.86	112.19
2	F	3	FUC	O3-C3-C2	3.21	116.60	110.05
2	G	2	NAG	C1-O5-C5	3.18	116.44	112.19
2	F	1	NAG	O6-C6-C5	-3.07	100.89	111.33
2	E	2	NAG	O5-C5-C4	3.01	118.15	110.83
2	F	3	FUC	O5-C1-C2	-2.82	104.07	110.79
2	F	2	NAG	C6-C5-C4	-2.80	106.14	113.02
2	G	3	FUC	O5-C5-C6	2.80	113.47	107.40
2	G	2	NAG	C2-N2-C7	-2.71	119.26	122.90
2	G	3	FUC	O2-C2-C1	2.59	115.16	109.22
2	F	1	NAG	O4-C4-C5	2.59	115.69	109.32
2	G	2	NAG	O3-C3-C2	-2.46	104.29	109.40
2	E	3	FUC	O5-C1-C2	-2.46	104.92	110.79
2	F	2	NAG	C1-O5-C5	2.45	115.47	112.19
2	F	1	NAG	O5-C5-C4	-2.38	105.04	110.83
2	E	1	NAG	C4-C3-C2	-2.35	107.58	111.02
2	G	3	FUC	C1-O5-C5	2.33	118.46	112.97
2	E	3	FUC	O2-C2-C3	-2.31	105.36	110.15
2	G	3	FUC	C1-C2-C3	-2.21	106.43	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O5-C1-C2	-2.18	107.92	111.29
2	F	3	FUC	O5-C5-C4	2.15	113.42	109.55
2	G	3	FUC	O4-C4-C5	2.14	114.46	109.74
2	F	2	NAG	C4-C3-C2	-2.02	108.05	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
2	G	2	NAG	C1
2	G	3	FUC	C1

All (22) torsion outliers are listed below:

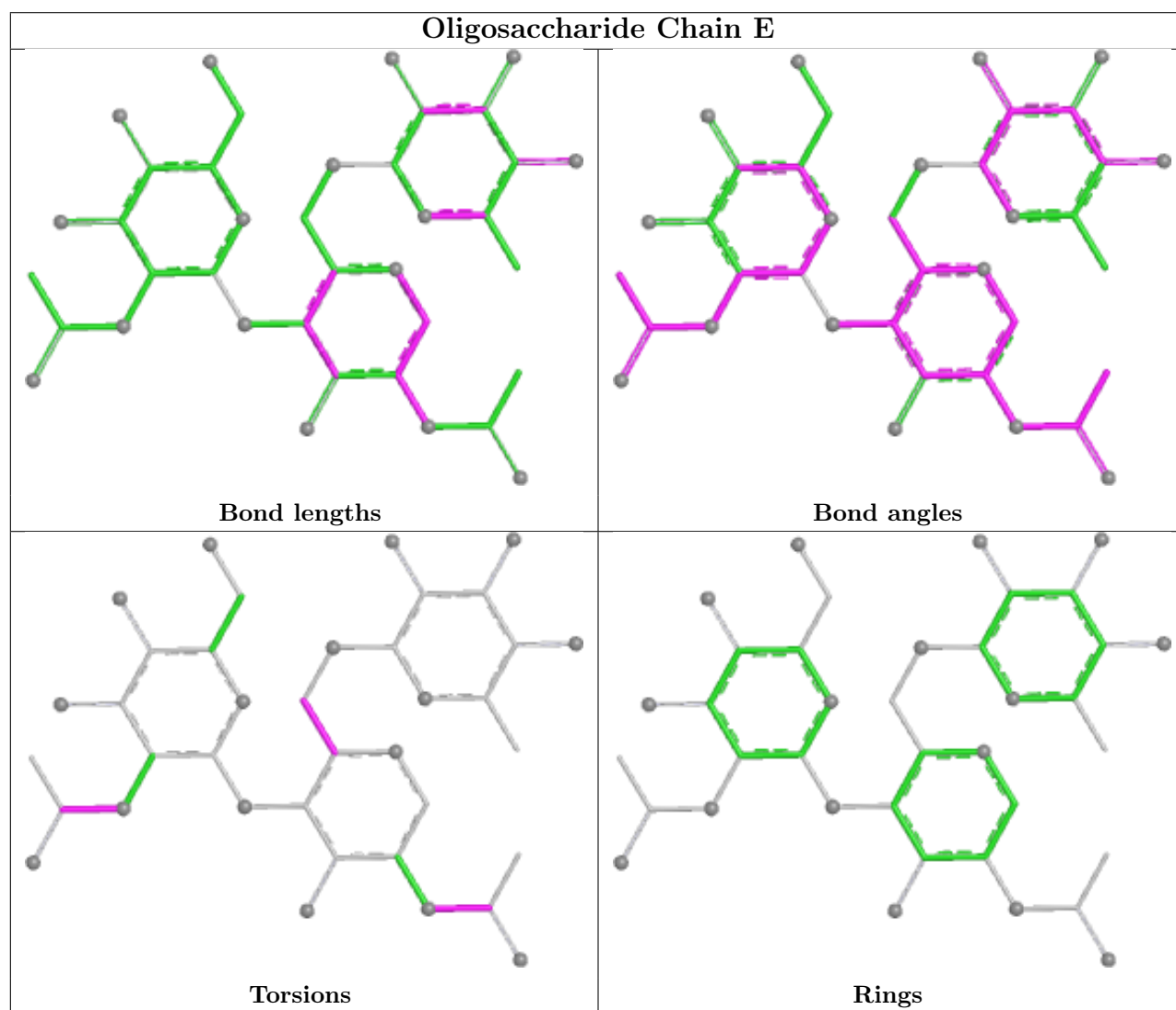
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C3-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6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

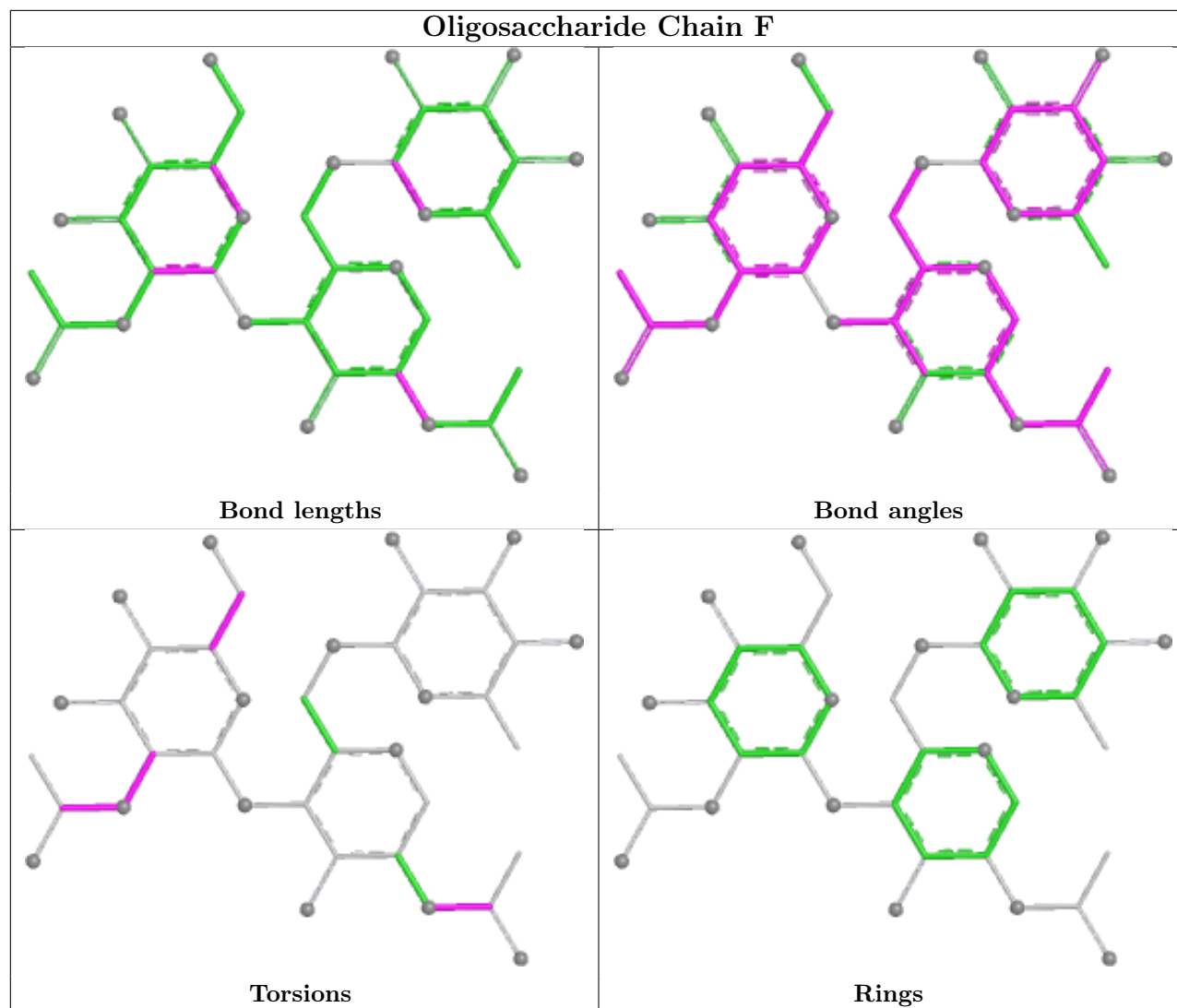
There are no ring outliers.

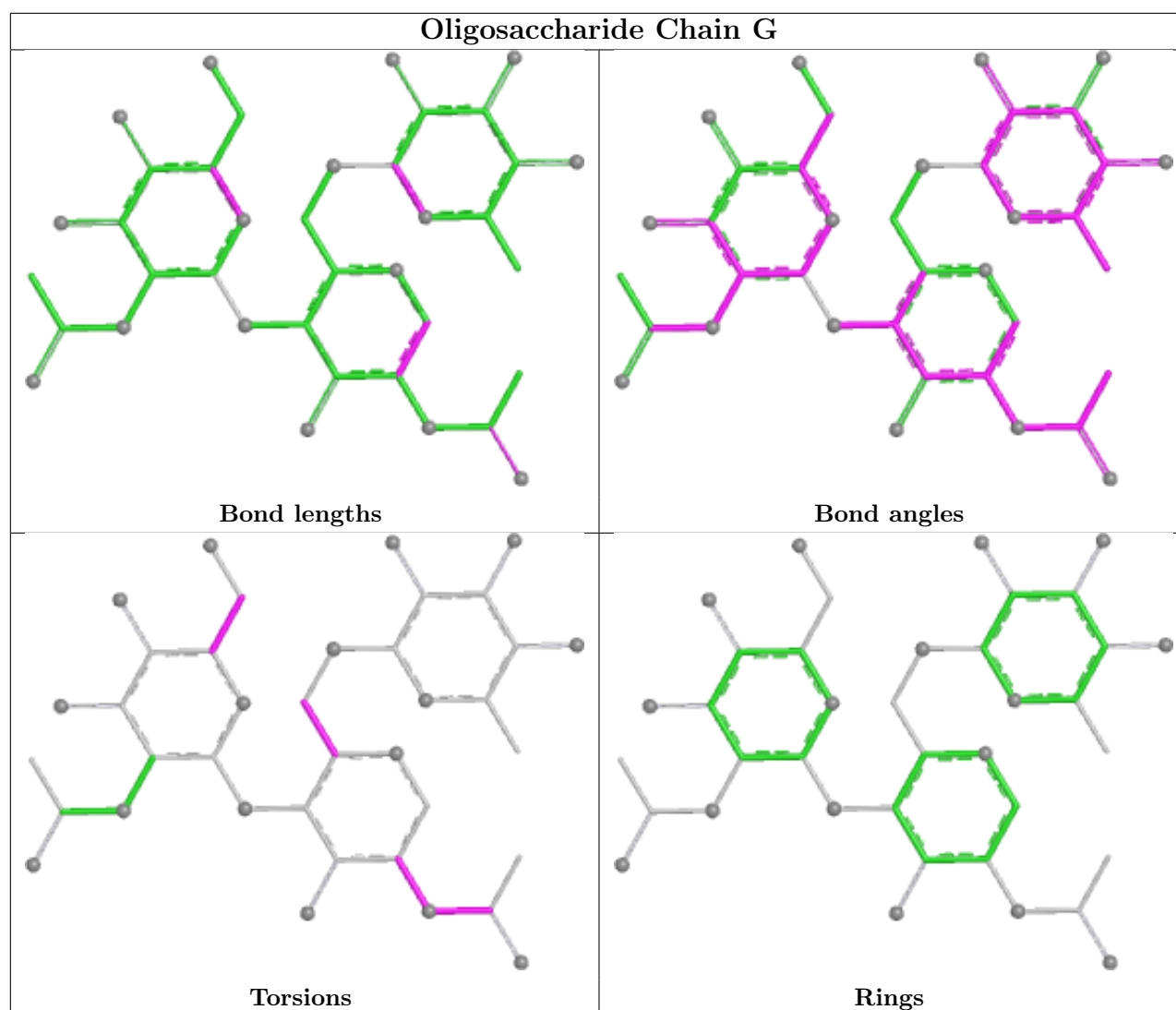
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	F	1	NAG	2	0
2	G	1	NAG	1	0
2	F	2	NAG	2	0

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







5.6 Ligand geometry [i](#)

13 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	D	303	-	4,4,4	0.29	0	6,6,6	0.44	0
3	SO4	A	303	-	4,4,4	0.46	0	6,6,6	0.63	0
3	SO4	B	302	-	4,4,4	0.32	0	6,6,6	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	303	-	4,4,4	0.64	0	6,6,6	1.02	0
3	SO4	C	304	-	4,4,4	0.21	0	6,6,6	0.26	0
3	SO4	D	301	-	4,4,4	0.64	0	6,6,6	1.49	1 (16%)
3	SO4	A	301	-	4,4,4	0.75	0	6,6,6	0.79	0
3	SO4	D	302	-	4,4,4	0.32	0	6,6,6	1.06	1 (16%)
3	SO4	C	302	-	4,4,4	0.22	0	6,6,6	0.59	0
4	NAG	B	301	1	14,14,15	1.15	1 (7%)	17,19,21	1.98	3 (17%)
3	SO4	A	302	-	4,4,4	0.39	0	6,6,6	1.16	0
3	SO4	C	303	-	4,4,4	0.45	0	6,6,6	0.66	0
3	SO4	C	301	-	4,4,4	0.69	0	6,6,6	0.65	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	B	301	1	-	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)
4	B	301	NAG	C1-C2	3.82	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAG	O5-C1-C2	5.14	119.24	111.29
4	B	301	NAG	C1-O5-C5	4.69	118.47	112.19
3	D	301	SO4	O4-S-O1	-3.18	92.95	109.56
4	B	301	NAG	O5-C5-C6	2.20	111.95	107.66
3	D	302	SO4	O3-S-O2	-2.13	98.45	109.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	C8-C7-N2-C2
4	B	301	NAG	O7-C7-N2-C2
4	B	301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	301	NAG	C4-C5-C6-O6
4	B	301	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	SO4	1	0
3	B	303	SO4	1	0
3	A	302	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	157/160 (98%)	-0.13	3 (1%) 66 61	29, 41, 60, 87	0
1	B	157/160 (98%)	1.53	40 (25%) 1 1	51, 79, 103, 110	0
1	C	155/160 (96%)	0.20	9 (5%) 29 23	34, 47, 77, 108	0
1	D	155/160 (96%)	-0.04	5 (3%) 50 44	30, 42, 66, 100	0
All	All	624/640 (97%)	0.39	57 (9%) 15 11	29, 47, 96, 110	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	VAL	7.9
1	B	156	VAL	6.3
1	B	155	HIS	5.4
1	C	52	THR	5.2
1	B	83	GLN	4.9
1	B	87	LYS	4.0
1	C	201	TYR	4.0
1	D	203	ASP	3.9
1	B	207	GLN	3.8
1	B	184	PHE	3.7
1	B	52	THR	3.6
1	B	157	ASP	3.6
1	C	206	SER	3.6
1	C	202	LYS	3.5
1	B	183	LYS	3.5
1	C	203	ASP	3.4
1	B	168	LYS	3.4
1	B	160	ARG	3.3
1	B	54	LEU	3.3
1	B	91	ARG	3.2
1	B	158	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	162	TYR	3.2
1	C	205	LEU	3.2
1	A	54	LEU	3.1
1	C	204	ILE	3.0
1	B	172	PRO	3.0
1	A	52	THR	3.0
1	B	152	LEU	2.9
1	C	53	ASP	2.7
1	B	161	ARG	2.7
1	B	81	THR	2.7
1	B	78	PRO	2.7
1	B	200	LEU	2.6
1	B	129	LYS	2.5
1	B	166	LEU	2.5
1	B	206	SER	2.5
1	B	175	GLY	2.5
1	B	116	LEU	2.5
1	B	128	GLU	2.4
1	B	53	ASP	2.4
1	B	199	GLU	2.3
1	B	150	SER	2.3
1	D	202	LYS	2.3
1	C	54	LEU	2.2
1	B	69	ARG	2.2
1	B	151	ASN	2.2
1	B	80	GLY	2.2
1	D	200	LEU	2.2
1	B	72	PHE	2.2
1	B	142	GLU	2.2
1	D	52	THR	2.2
1	B	57	LEU	2.2
1	B	76	ILE	2.1
1	B	74	LEU	2.1
1	B	79	ASN	2.1
1	A	208	SER	2.1
1	D	49	PRO	2.1

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

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

6.3 Carbohydrates

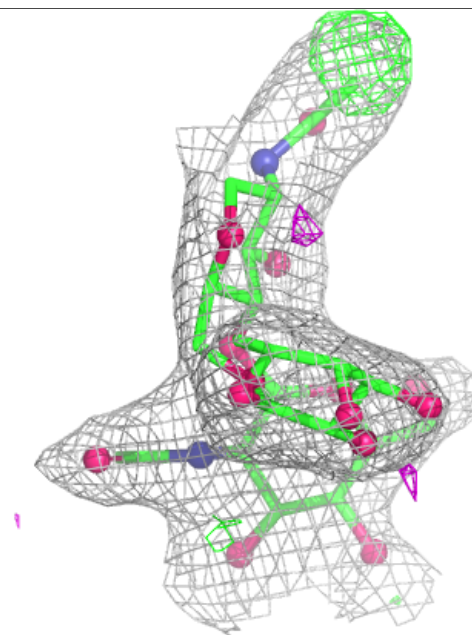
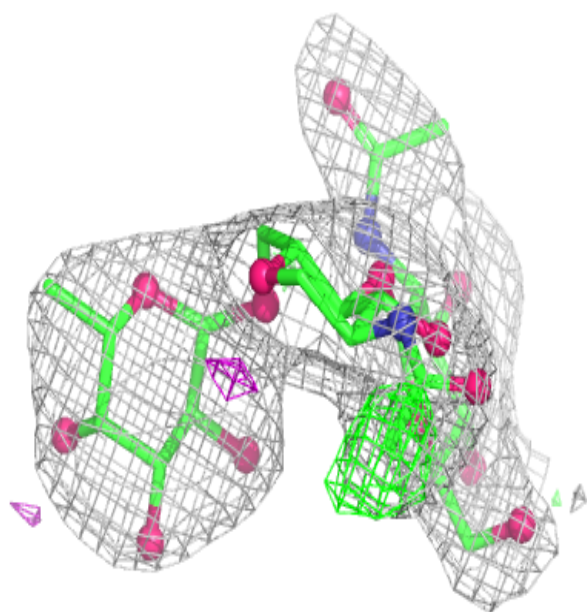
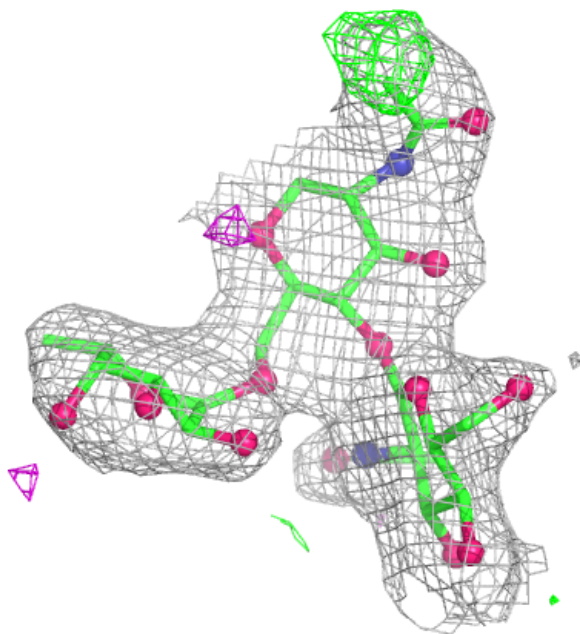
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	2	14/15	0.52	0.19	82,90,99,103	0
2	NAG	E	2	14/15	0.76	0.16	67,76,85,88	0
2	NAG	G	2	14/15	0.78	0.15	69,87,92,93	0
2	NAG	E	1	14/15	0.82	0.13	56,60,71,73	0
2	NAG	G	1	14/15	0.83	0.15	60,69,74,80	0
2	FUC	G	3	10/11	0.90	0.10	63,69,72,72	0
2	NAG	F	1	14/15	0.91	0.10	57,67,75,81	0
2	FUC	F	3	10/11	0.92	0.10	59,66,69,69	0
2	FUC	E	3	10/11	0.92	0.11	60,68,71,74	0

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

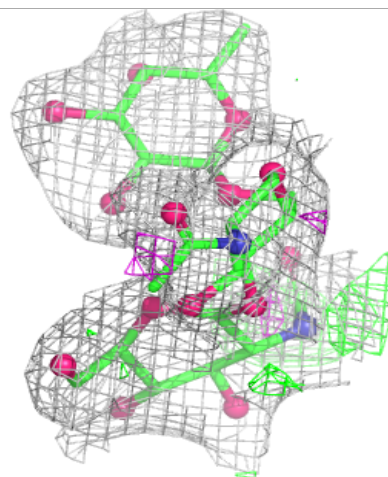
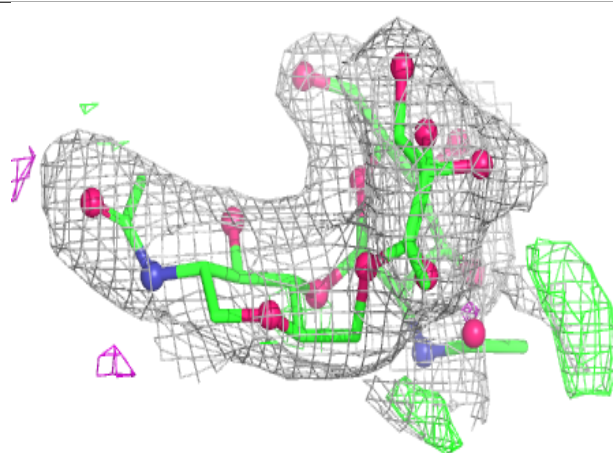
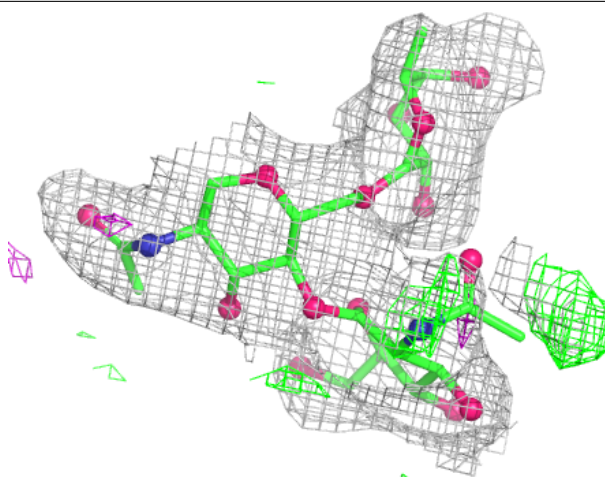
Electron density around Chain E:

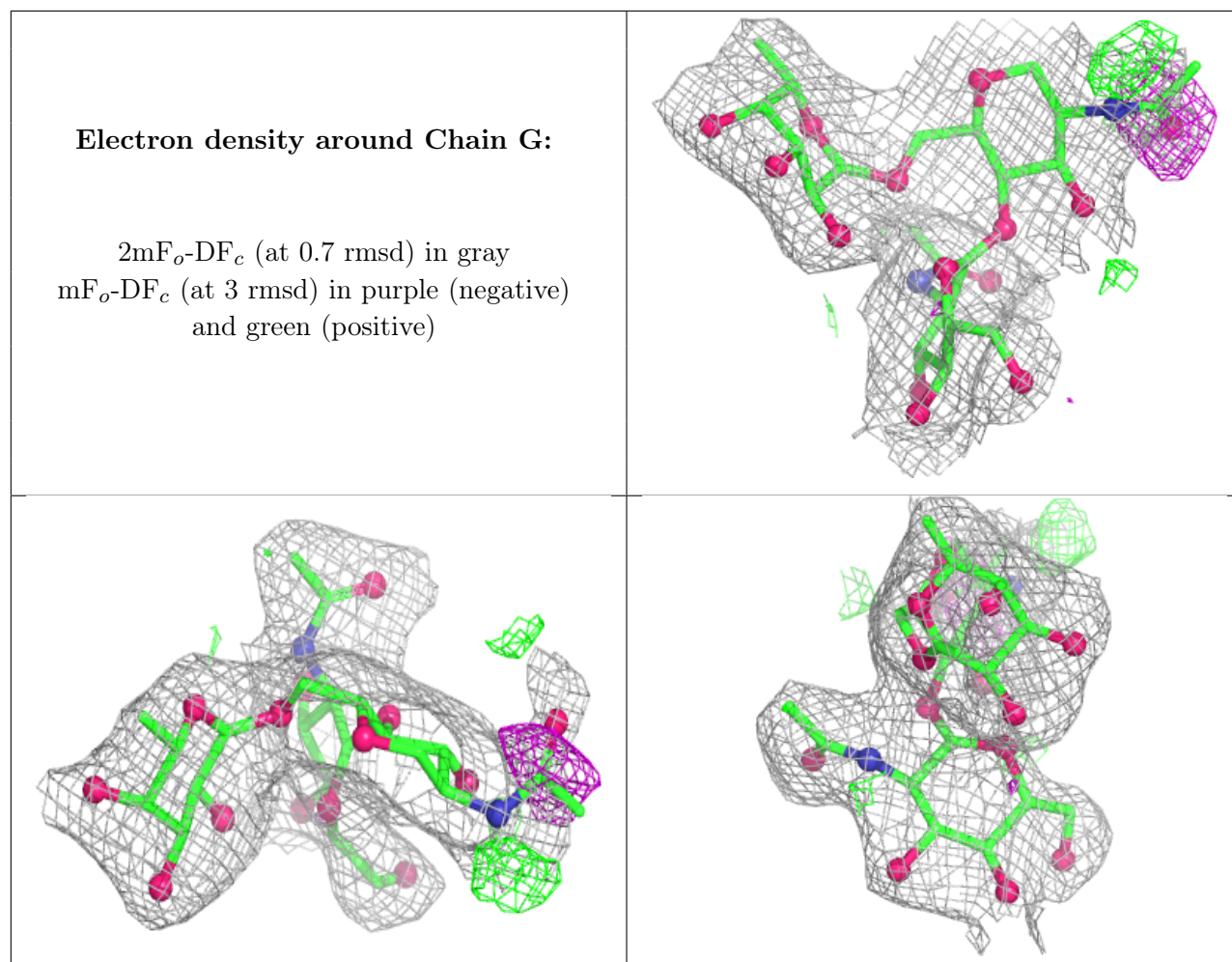
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	303	5/5	0.56	0.15	97,97,102,102	0
3	SO4	C	304	5/5	0.58	0.14	118,120,120,123	0
4	NAG	B	301	14/15	0.59	0.25	120,124,126,126	0
3	SO4	C	303	5/5	0.71	0.27	89,90,91,95	0
3	SO4	D	303	5/5	0.72	0.17	125,126,127,129	0
3	SO4	A	303	5/5	0.77	0.19	80,86,88,93	0
3	SO4	A	302	5/5	0.78	0.16	66,68,78,81	0
3	SO4	C	302	5/5	0.80	0.20	82,88,89,90	0
3	SO4	B	302	5/5	0.89	0.13	83,83,86,86	0
3	SO4	D	302	5/5	0.91	0.21	64,68,71,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	301	5/5	0.96	0.11	48,49,51,56	0
3	SO4	D	301	5/5	0.98	0.08	41,45,51,53	0
3	SO4	C	301	5/5	0.98	0.09	52,54,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.