



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:05 PM UTC

PDB ID : 3FBY / pdb_00003fby
Title : The crystal structure of the signature domain of cartilage oligomeric matrix protein.
Authors : Tan, K.; Lawler, J.
Deposited on : 2008-11-20
Resolution : 3.15 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:

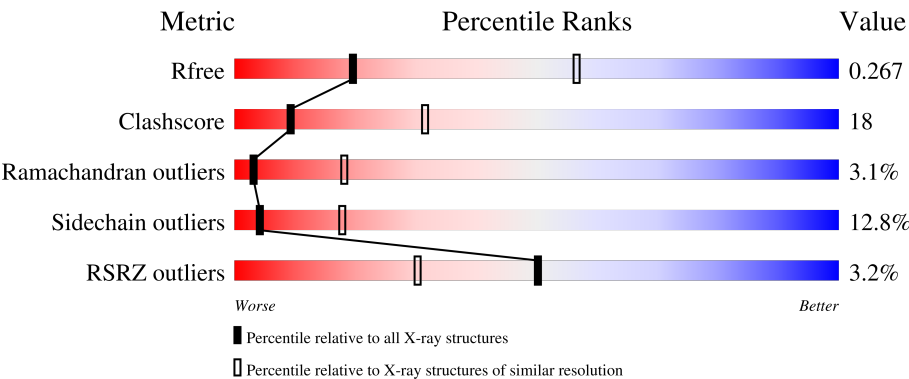
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	551	% 61%29%7% .
1	B	551	5% 52%38%6% . .
1	C	551	3% 60%30%7% .
2	D	4	50%50%
3	E	3	100%

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Mol	Chain	Length	Quality of chain
4	F	5	 100%

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	MAN	D	3	X	-	-	-
3	NAG	E	1	X	-	-	-
3	MAN	E	3	X	-	-	-
4	MAN	F	3	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12777 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 Cartilage oligomeric matrix protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	B	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			
1	C	535	Total	C	N	O	S	0	0	0
			4161	2495	749	888	29			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ARG	-	expression tag	UNP P49747
A	210	SER	-	expression tag	UNP P49747
A	211	PRO	-	expression tag	UNP P49747
A	212	TRP	-	expression tag	UNP P49747
A	213	PRO	-	expression tag	UNP P49747
A	214	GLY	-	expression tag	UNP P49747
A	215	VAL	-	expression tag	UNP P49747
A	216	PRO	-	expression tag	UNP P49747
A	217	THR	-	expression tag	UNP P49747
A	218	SER	-	expression tag	UNP P49747
A	219	PRO	-	expression tag	UNP P49747
A	220	VAL	-	expression tag	UNP P49747
A	221	TRP	-	expression tag	UNP P49747
A	222	TRP	-	expression tag	UNP P49747
A	223	ASN	-	expression tag	UNP P49747
A	224	SER	-	expression tag	UNP P49747
A	758	GLY	-	expression tag	UNP P49747
A	759	THR	-	expression tag	UNP P49747
B	209	ARG	-	expression tag	UNP P49747
B	210	SER	-	expression tag	UNP P49747
B	211	PRO	-	expression tag	UNP P49747
B	212	TRP	-	expression tag	UNP P49747
B	213	PRO	-	expression tag	UNP P49747

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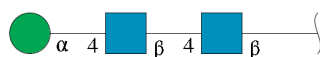
Chain	Residue	Modelled	Actual	Comment	Reference
B	214	GLY	-	expression tag	UNP P49747
B	215	VAL	-	expression tag	UNP P49747
B	216	PRO	-	expression tag	UNP P49747
B	217	THR	-	expression tag	UNP P49747
B	218	SER	-	expression tag	UNP P49747
B	219	PRO	-	expression tag	UNP P49747
B	220	VAL	-	expression tag	UNP P49747
B	221	TRP	-	expression tag	UNP P49747
B	222	TRP	-	expression tag	UNP P49747
B	223	ASN	-	expression tag	UNP P49747
B	224	SER	-	expression tag	UNP P49747
B	758	GLY	-	expression tag	UNP P49747
B	759	THR	-	expression tag	UNP P49747
C	209	ARG	-	expression tag	UNP P49747
C	210	SER	-	expression tag	UNP P49747
C	211	PRO	-	expression tag	UNP P49747
C	212	TRP	-	expression tag	UNP P49747
C	213	PRO	-	expression tag	UNP P49747
C	214	GLY	-	expression tag	UNP P49747
C	215	VAL	-	expression tag	UNP P49747
C	216	PRO	-	expression tag	UNP P49747
C	217	THR	-	expression tag	UNP P49747
C	218	SER	-	expression tag	UNP P49747
C	219	PRO	-	expression tag	UNP P49747
C	220	VAL	-	expression tag	UNP P49747
C	221	TRP	-	expression tag	UNP P49747
C	222	TRP	-	expression tag	UNP P49747
C	223	ASN	-	expression tag	UNP P49747
C	224	SER	-	expression tag	UNP P49747
C	758	GLY	-	expression tag	UNP P49747
C	759	THR	-	expression tag	UNP P49747

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



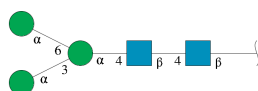
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	30	Total	Ca	0	0
			30	30		
5	B	29	Total	Ca	0	0
			29	29		
5	C	29	Total	Ca	0	0
			29	29		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	3	Total	O	0	0
			3	3		

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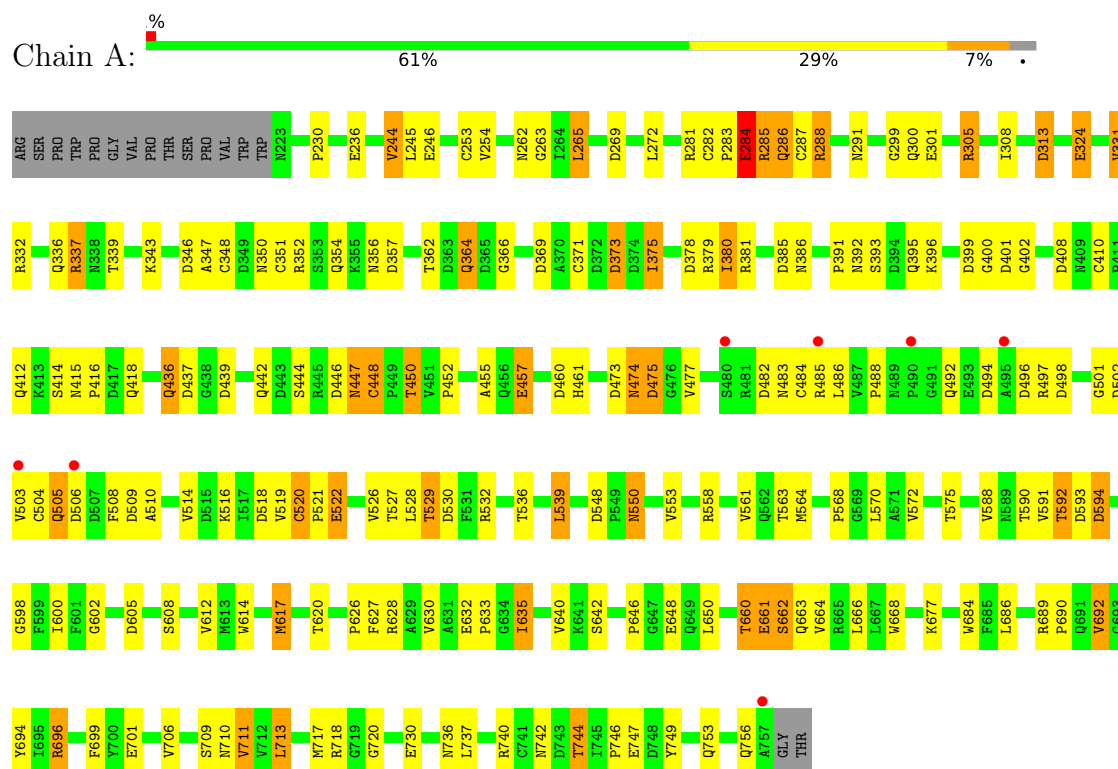
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	O	0	0
			2	2		

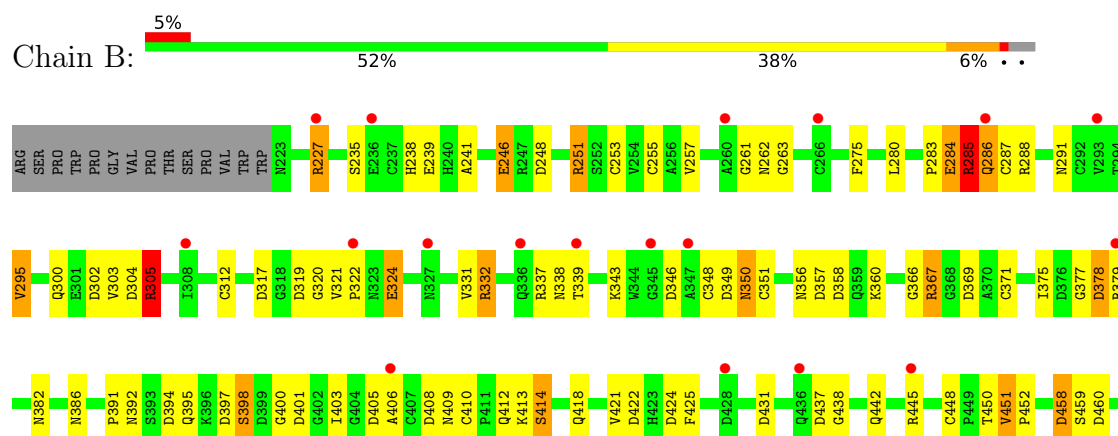
3 Residue-property plots [i](#)

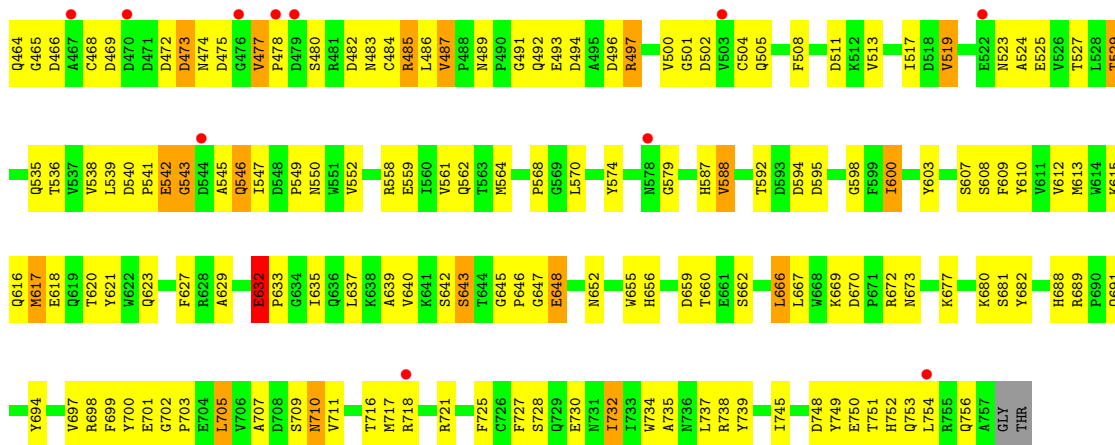
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

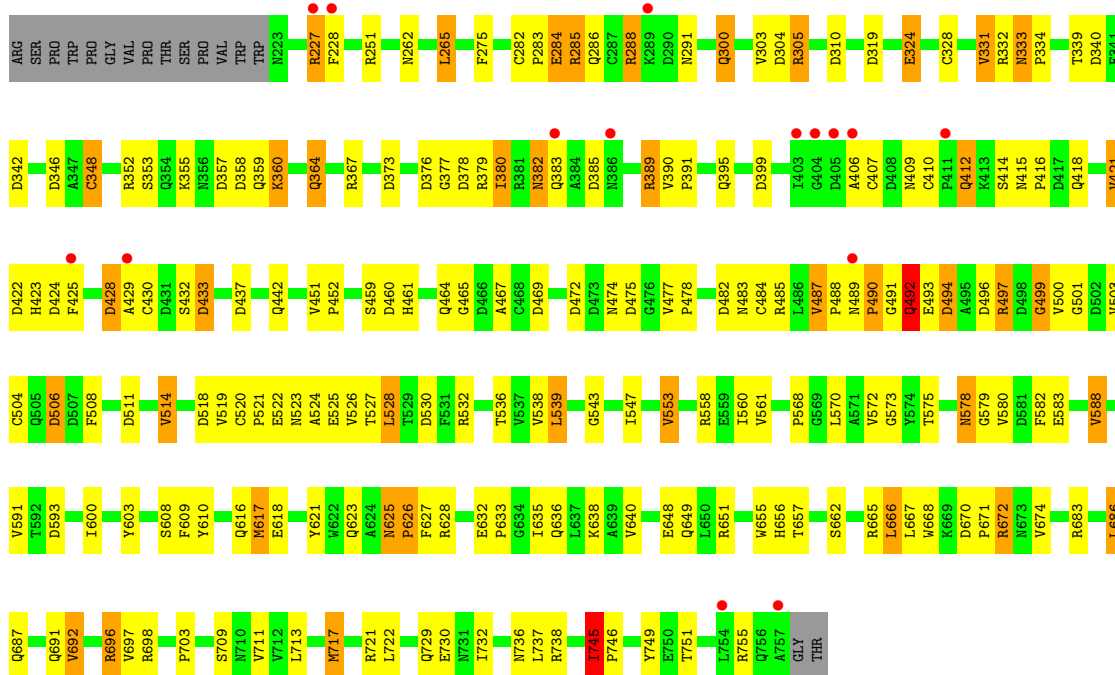


• Molecule 1: Cartilage oligomeric matrix protein





• Molecule 1: Cartilage oligomeric matrix protein



• Molecule 2: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
MAN3

- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:

100%

MAG1
MAG2
MAN3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.24Å 192.24Å 145.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 3.15 39.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.00-3.15) 99.6 (39.00-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.202 , 0.266 0.204 , 0.267	Depositor DCC
R_{free} test set	2735 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12777	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 2.69% 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: CA, NAG, SO4, MAN

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	0.86	1/4245 (0.0%)	1.12	15/5770 (0.3%)
1	B	0.82	2/4245 (0.0%)	1.09	13/5770 (0.2%)
1	C	0.82	3/4245 (0.1%)	1.07	8/5770 (0.1%)
All	All	0.84	6/12735 (0.0%)	1.09	36/17310 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	ARG	C-N	-6.47	1.24	1.33
1	A	285	ARG	C-N	-5.85	1.25	1.33
1	C	275	PHE	CA-C	-5.69	1.48	1.52
1	C	703	PRO	N-CA	-5.20	1.44	1.47
1	C	588	VAL	CA-CB	5.06	1.59	1.53
1	B	588	VAL	CA-CB	5.03	1.59	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	VAL	CB-CA-C	-8.28	101.27	111.04
1	A	520	CYS	CA-C-N	8.16	127.88	119.56
1	A	520	CYS	C-N-CA	8.16	127.88	119.56
1	C	410	CYS	CA-C-N	7.40	129.09	119.84
1	C	410	CYS	C-N-CA	7.40	129.09	119.84
1	B	321	VAL	CA-C-N	7.18	127.22	119.90
1	B	321	VAL	C-N-CA	7.18	127.22	119.90
1	A	661	GLU	CA-C-N	-6.88	111.57	122.79
1	A	661	GLU	C-N-CA	-6.88	111.57	122.79
1	A	284	GLU	CA-C-N	-6.27	111.22	121.19
1	A	284	GLU	C-N-CA	-6.27	111.22	121.19
1	B	477	VAL	N-CA-C	6.20	115.72	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	ASN	N-CA-C	6.05	118.60	108.73
1	B	421	VAL	N-CA-C	5.99	116.45	110.23
1	C	745	ILE	CB-CA-C	-5.84	105.16	110.88
1	B	275	PHE	CA-C-N	5.66	125.57	119.85
1	B	275	PHE	C-N-CA	5.66	125.57	119.85
1	B	632	GLU	CA-C-N	-5.66	114.92	120.52
1	B	632	GLU	C-N-CA	-5.66	114.92	120.52
1	C	310	ASP	N-CA-C	-5.66	105.20	111.71
1	C	339	THR	N-CA-C	5.50	119.09	112.38
1	B	540	ASP	CA-C-N	5.45	125.10	119.05
1	B	540	ASP	C-N-CA	5.45	125.10	119.05
1	C	333	ASN	CA-C-N	5.40	125.05	119.05
1	C	333	ASN	C-N-CA	5.40	125.05	119.05
1	A	548	ASP	CA-C-N	-5.39	114.22	119.78
1	A	548	ASP	C-N-CA	-5.39	114.22	119.78
1	A	448	CYS	CA-C-N	5.38	125.70	119.47
1	A	448	CYS	C-N-CA	5.38	125.70	119.47
1	A	313	ASP	CA-C-N	5.31	126.48	119.84
1	A	313	ASP	C-N-CA	5.31	126.48	119.84
1	A	362	THR	N-CA-CB	5.20	117.86	110.06
1	A	662	SER	N-CA-C	5.16	119.14	111.87
1	C	553	VAL	N-CA-C	5.10	115.20	107.75
1	B	659	ASP	N-CA-C	5.07	117.25	110.35
1	A	371	CYS	CB-CA-C	-5.05	100.54	109.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4161	0	3698	131	0
1	B	4161	0	3698	178	0
1	C	4161	0	3698	127	0
2	D	50	0	43	3	0
3	E	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	61	0	52	0	0
5	A	30	0	0	0	0
5	B	29	0	0	0	0
5	C	29	0	0	0	0
6	A	25	0	0	0	0
6	B	10	0	0	0	0
6	C	15	0	0	1	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	2	0	0	0	0
All	All	12777	0	11223	435	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 18.

All (435) 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:B:251:ARG:HG3	1:B:251:ARG:HH11	1.04	1.17
1:A:617:MET:HE3	1:A:617:MET:HA	1.36	1.02
1:A:253:CYS:HB2	1:A:263:GLY:HA3	1.39	1.01
1:B:749:TYR:O	1:B:753:GLN:HG2	1.69	0.93
1:B:570:LEU:HD22	1:B:600:ILE:CD1	1.99	0.92
1:A:337:ARG:HH21	1:A:337:ARG:HG3	1.35	0.89
1:A:520:CYS:HB2	1:A:526:VAL:HG13	1.56	0.88
1:B:246:GLU:OE1	1:B:246:GLU:HA	1.73	0.87
1:C:482:ASP:HA	1:C:492:GLN:OE1	1.75	0.85
1:C:626:PRO:HD3	1:C:648:GLU:HB3	1.61	0.82
1:B:478:PRO:O	1:B:482:ASP:HB2	1.79	0.82
1:A:253:CYS:CB	1:A:263:GLY:HA3	2.10	0.81
1:A:305:ARG:HB3	1:A:305:ARG:NH1	1.94	0.81
1:B:251:ARG:HG3	1:B:251:ARG:NH1	1.80	0.79
1:C:291:ASN:H	1:C:300:GLN:HE22	1.30	0.79
1:A:339:THR:HG23	1:A:346:ASP:OD1	1.84	0.78
1:A:539:LEU:HB2	1:A:568:PRO:HB2	1.67	0.77
1:A:520:CYS:HB2	1:A:526:VAL:CG1	2.13	0.77
1:B:570:LEU:HD22	1:B:600:ILE:HD12	1.67	0.76
1:C:483:ASN:HB2	1:C:499:GLY:O	1.85	0.76
1:C:424:ASP:O	1:C:425:PHE:HB2	1.84	0.76
1:B:635:ILE:HD12	1:B:635:ILE:H	1.50	0.76
1:A:305:ARG:HB3	1:A:305:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:HB2	1:A:245:LEU:HD22	1.69	0.75
1:B:617:MET:HA	1:B:617:MET:HE2	1.68	0.75
1:C:672:ARG:HB3	1:C:674:VAL:HG23	1.68	0.75
1:A:284:GLU:O	1:A:285:ARG:C	2.29	0.75
1:B:367:ARG:NH2	1:B:371:CYS:HB3	2.03	0.73
1:B:689:ARG:HB2	1:B:694:TYR:HB3	1.71	0.72
1:C:437:ASP:HB2	1:C:452:PRO:HG3	1.70	0.72
1:A:337:ARG:HH21	1:A:337:ARG:CG	2.01	0.72
1:A:337:ARG:NH2	1:A:339:THR:HG22	2.04	0.72
1:A:617:MET:HA	1:A:617:MET:CE	2.16	0.72
1:A:494:ASP:HB3	1:A:496:ASP:O	1.89	0.71
1:B:613:MET:HG2	1:B:725:PHE:CE2	2.26	0.71
1:B:305:ARG:HH11	1:B:305:ARG:HB3	1.56	0.70
1:B:610:TYR:CE1	1:B:717:MET:HB2	2.25	0.70
1:C:227:ARG:HG2	1:C:227:ARG:HH21	1.54	0.70
1:C:573:GLY:O	1:C:721:ARG:HD2	1.90	0.70
1:C:227:ARG:HH21	1:C:227:ARG:CG	2.03	0.69
1:C:331:VAL:HG11	1:C:348:CYS:HB3	1.75	0.69
1:A:497:ARG:HD3	1:A:497:ARG:C	2.18	0.69
1:A:378:ASP:OD2	1:A:391:PRO:HA	1.93	0.69
1:B:295:VAL:HG21	1:B:312:CYS:HB3	1.75	0.68
1:C:415:ASN:HD22	1:C:418:GLN:HA	1.58	0.68
1:A:689:ARG:HB2	1:A:694:TYR:HB3	1.76	0.68
1:B:497:ARG:HA	1:B:497:ARG:HH21	1.59	0.67
1:C:340:ASP:HB3	1:C:353:SER:HA	1.77	0.67
1:C:487:VAL:CG2	1:C:504:CYS:HB3	2.24	0.67
1:A:286:GLN:CD	1:A:286:GLN:H	2.02	0.66
1:A:364:GLN:HA	1:A:364:GLN:NE2	2.11	0.66
1:B:618:GLU:HG2	1:B:633:PRO:HD3	1.78	0.66
1:B:378:ASP:OD2	1:B:391:PRO:HA	1.96	0.66
1:A:473:ASP:O	1:A:474:ASN:HB2	1.94	0.65
1:B:483:ASN:HD21	1:B:492:GLN:HA	1.61	0.65
1:B:547:ILE:HG21	1:B:564:MET:HE2	1.78	0.65
1:B:629:ALA:HB1	1:B:656:HIS:HB2	1.78	0.65
1:C:692:VAL:HG21	1:C:749:TYR:CZ	2.32	0.64
1:C:625:ASN:HA	1:C:627:PHE:N	2.12	0.64
1:A:285:ARG:O	1:A:287:CYS:N	2.30	0.64
1:A:291:ASN:H	1:A:300:GLN:HE22	1.45	0.63
1:B:494:ASP:HA	1:B:502:ASP:OD1	1.98	0.63
1:C:399:ASP:HB3	1:C:412:GLN:O	1.98	0.63
1:C:409:ASN:OD1	1:C:415:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:626:PRO:CD	1:C:648:GLU:HB3	2.29	0.63
1:A:364:GLN:NE2	1:A:364:GLN:CA	2.62	0.62
1:A:369:ASP:CG	1:A:375:ILE:HD12	2.24	0.62
1:C:751:THR:O	1:C:755:ARG:HB2	2.00	0.62
1:A:285:ARG:HA	1:A:288:ARG:HD3	1.80	0.62
1:A:337:ARG:HH22	1:A:339:THR:HG22	1.62	0.62
1:A:262:ASN:HD21	1:A:282:CYS:HB3	1.65	0.62
1:A:642:SER:HB2	1:A:650:LEU:HD13	1.82	0.62
1:C:324:GLU:CD	1:C:324:GLU:H	2.07	0.62
1:C:618:GLU:HB2	1:C:633:PRO:HD3	1.81	0.61
1:A:550:ASN:ND2	1:A:563:THR:OG1	2.30	0.61
1:B:643:SER:HB3	1:B:662:SER:HB3	1.83	0.60
1:C:635:ILE:HD12	1:C:635:ILE:H	1.66	0.60
1:B:392:ASN:ND2	1:B:395:GLN:HA	2.16	0.60
1:B:410:CYS:C	1:B:412:GLN:H	2.08	0.60
1:B:519:VAL:CG2	1:B:739:TYR:O	2.50	0.60
1:B:253:CYS:CB	1:B:263:GLY:HA3	2.32	0.60
1:C:610:TYR:CE1	1:C:717:MET:HG2	2.38	0.59
1:A:627:PHE:CZ	1:A:660:THR:HG21	2.37	0.59
1:A:530:ASP:OD1	1:A:532:ARG:HG2	2.02	0.59
1:B:677:LYS:HE3	1:B:680:LYS:HD2	1.83	0.59
1:A:262:ASN:HD21	1:A:282:CYS:CB	2.16	0.59
1:A:539:LEU:HD21	1:A:570:LEU:HG	1.85	0.59
1:B:511:ASP:HB3	1:B:524:ALA:O	2.03	0.59
1:B:284:GLU:H	1:B:284:GLU:CD	2.11	0.59
1:C:285:ARG:O	1:C:288:ARG:HD3	2.03	0.59
1:A:558:ARG:NH2	1:A:736:ASN:OD1	2.37	0.58
1:C:625:ASN:HA	1:C:626:PRO:C	2.28	0.58
1:B:618:GLU:CG	1:B:633:PRO:HD3	2.33	0.58
1:B:251:ARG:NH1	1:B:251:ARG:CG	2.58	0.58
1:B:570:LEU:CD2	1:B:600:ILE:CD1	2.78	0.58
1:A:594:ASP:HB2	1:A:617:MET:HB2	1.84	0.58
1:B:451:VAL:HG21	1:B:468:CYS:HB3	1.84	0.58
1:B:375:ILE:HG23	1:B:382:ASN:HD21	1.69	0.58
1:A:350:ASN:HB2	1:A:366:GLY:O	2.04	0.58
1:A:401:ASP:HB3	1:A:414:SER:HA	1.86	0.58
1:B:598:GLY:HA3	1:B:612:VAL:O	2.04	0.58
1:B:324:GLU:H	1:B:324:GLU:CD	2.11	0.57
1:C:511:ASP:HB3	1:C:524:ALA:HA	1.84	0.57
1:A:380:ILE:HG22	1:A:385:ASP:HB2	1.86	0.57
1:B:610:TYR:HE1	1:B:717:MET:HB2	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:O	1:A:288:ARG:HG2	2.04	0.57
1:C:608:SER:HA	1:C:640:VAL:O	2.04	0.57
1:A:308:ILE:HG22	1:A:313:ASP:HB2	1.87	0.57
1:A:364:GLN:CA	1:A:364:GLN:HE21	2.17	0.57
1:B:305:ARG:HB3	1:B:305:ARG:NH1	2.19	0.57
1:B:483:ASN:ND2	1:B:492:GLN:HA	2.19	0.57
1:A:455:ALA:HB3	1:A:457:GLU:OE1	2.05	0.56
1:A:436:GLN:HE22	1:A:450:THR:HG23	1.71	0.56
1:B:253:CYS:HB3	1:B:263:GLY:HA3	1.88	0.56
1:B:489:ASN:O	1:B:492:GLN:NE2	2.38	0.56
1:C:465:GLY:O	1:C:469:ASP:HB2	2.06	0.56
1:B:529:THR:HG22	1:B:558:ARG:HG2	1.86	0.56
1:B:477:VAL:HG21	1:B:492:GLN:NE2	2.21	0.56
1:B:694:TYR:CE1	1:B:711:VAL:HG12	2.41	0.56
1:A:475:ASP:OD2	1:A:488:PRO:HA	2.06	0.56
1:C:621:TYR:HB2	1:C:655:TRP:CD1	2.41	0.56
1:B:541:PRO:C	1:B:543:GLY:H	2.14	0.56
1:B:621:TYR:CE2	1:B:623:GLN:HB2	2.41	0.56
1:B:285:ARG:O	1:B:288:ARG:HG2	2.06	0.55
1:C:487:VAL:HG21	1:C:504:CYS:HB3	1.88	0.55
1:C:494:ASP:HB2	1:C:501:GLY:HA2	1.88	0.55
1:A:701:GLU:HG2	1:A:706:VAL:HG11	1.88	0.55
1:B:464:GLN:OE1	1:B:469:ASP:HA	2.07	0.55
1:B:486:LEU:HD12	1:B:508:PHE:HD2	1.72	0.55
1:A:635:ILE:HG21	1:A:699:PHE:CE2	2.41	0.55
1:A:509:ASP:HB3	1:A:522:GLU:HA	1.88	0.55
1:B:607:SER:HB3	1:B:642:SER:HB3	1.90	0.54
1:B:699:PHE:HB2	1:B:707:ALA:HB3	1.89	0.54
1:A:494:ASP:CB	1:A:496:ASP:O	2.55	0.54
1:C:582:PHE:HB3	1:C:686:LEU:HD23	1.88	0.54
1:B:574:TYR:HA	1:B:721:ARG:HH11	1.71	0.54
1:B:543:GLY:O	1:B:546:GLN:NE2	2.40	0.54
1:B:711:VAL:HG21	1:B:752:HIS:CG	2.43	0.54
1:C:415:ASN:ND2	1:C:418:GLN:HA	2.23	0.54
1:A:632:GLU:HB3	1:A:633:PRO:HD2	1.90	0.54
1:B:666:LEU:HD11	1:B:669:LYS:HB2	1.91	0.54
1:C:333:ASN:O	1:C:333:ASN:ND2	2.41	0.53
1:C:390:VAL:HB	1:C:407:CYS:HB3	1.90	0.53
1:B:350:ASN:HB2	1:B:366:GLY:O	2.07	0.53
1:B:317:ASP:O	1:B:332:ARG:HD2	2.08	0.53
1:B:431:ASP:HA	1:B:442:GLN:HE22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ARG:O	1:A:385:ASP:HB2	2.07	0.53
1:B:617:MET:HA	1:B:617:MET:CE	2.37	0.53
1:B:448:CYS:HB2	1:B:465:GLY:HA3	1.90	0.53
1:C:409:ASN:H	1:C:418:GLN:HE22	1.57	0.53
1:C:464:GLN:HG3	1:C:464:GLN:O	2.09	0.53
1:C:527:THR:HG23	1:C:528:LEU:HB2	1.91	0.53
1:A:446:ASP:O	1:A:448:CYS:N	2.40	0.52
1:C:283:PRO:HD2	1:C:284:GLU:OE1	2.09	0.52
1:C:648:GLU:HG2	1:C:651:ARG:HH22	1.74	0.52
1:B:409:ASN:HB2	1:B:425:PHE:O	2.10	0.52
1:A:740:ARG:HD2	2:D:1:NAG:H81	1.92	0.52
1:B:227:ARG:O	1:B:235:SER:HB3	2.10	0.52
1:C:485:ARG:HB3	1:C:508:PHE:HZ	1.75	0.52
1:B:466:ASP:HA	1:B:469:ASP:HB3	1.92	0.52
1:B:549:PRO:HA	1:B:562:GLN:HE21	1.75	0.52
1:B:562:GLN:HE22	1:B:564:MET:HB2	1.74	0.52
1:B:473:ASP:OD2	1:B:485:ARG:O	2.27	0.51
1:A:446:ASP:C	1:A:448:CYS:H	2.18	0.51
1:B:339:THR:HG23	1:B:346:ASP:OD1	2.09	0.51
1:B:408:ASP:HA	1:B:418:GLN:HE22	1.76	0.51
1:C:432:SER:O	1:C:433:ASP:C	2.53	0.51
1:A:439:ASP:HB3	1:A:452:PRO:HA	1.93	0.51
1:B:700:TYR:CE2	1:B:705:LEU:HB2	2.46	0.51
1:C:304:ASP:C	1:C:305:ARG:HG2	2.34	0.51
1:C:428:ASP:C	1:C:430:CYS:H	2.19	0.51
1:A:282:CYS:HB2	1:A:284:GLU:OE1	2.11	0.51
1:B:587:HIS:HD2	1:B:681:SER:OG	1.93	0.51
1:A:502:ASP:C	1:A:504:CYS:H	2.19	0.51
1:A:457:GLU:H	1:A:457:GLU:CD	2.19	0.51
1:A:598:GLY:HA3	1:A:612:VAL:O	2.10	0.50
1:A:460:ASP:O	1:A:461:HIS:HB2	2.10	0.50
1:B:319:ASP:HB3	1:B:332:ARG:HB3	1.92	0.50
1:B:367:ARG:HD3	1:B:371:CYS:HB3	1.92	0.50
1:A:262:ASN:ND2	1:A:282:CYS:CB	2.74	0.50
1:C:603:TYR:HA	1:C:609:PHE:HB3	1.93	0.50
1:A:331:VAL:HG21	1:A:347:ALA:O	2.12	0.50
1:C:459:SER:HB2	1:C:472:ASP:O	2.12	0.50
1:C:478:PRO:O	1:C:482:ASP:HB2	2.11	0.50
1:C:378:ASP:C	1:C:380:ILE:H	2.20	0.50
1:A:709:SER:O	1:A:710:ASN:HB2	2.12	0.49
1:B:732:ILE:HB	1:B:734:TRP:CZ3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASP:HB3	1:C:389:ARG:O	2.12	0.49
1:A:694:TYR:CE2	1:A:746:PRO:HG2	2.46	0.49
1:B:343:LYS:HG3	1:B:357:ASP:OD1	2.12	0.49
1:A:626:PRO:HD3	1:A:648:GLU:HG2	1.95	0.49
1:B:613:MET:HG2	1:B:725:PHE:HE2	1.72	0.49
1:C:291:ASN:N	1:C:300:GLN:HE22	2.06	0.49
1:C:583:GLU:HG2	1:C:738:ARG:HB2	1.94	0.49
1:A:373:ASP:OD1	1:A:373:ASP:N	2.43	0.49
1:A:529:THR:HG22	1:A:558:ARG:HG2	1.94	0.49
1:B:642:SER:HG	1:B:645:GLY:H	1.59	0.49
1:B:392:ASN:O	1:B:392:ASN:CG	2.55	0.49
1:C:520:CYS:C	1:C:522:GLU:H	2.21	0.49
1:B:464:GLN:HG2	1:B:469:ASP:HB2	1.95	0.49
1:B:438:GLY:O	1:B:718:ARG:HG3	2.13	0.49
1:C:570:LEU:HD22	1:C:600:ILE:HG13	1.95	0.49
1:C:483:ASN:OD1	1:C:484:CYS:N	2.46	0.48
1:B:748:ASP:HA	1:B:751:THR:OG1	2.12	0.48
1:C:539:LEU:HB2	1:C:568:PRO:HB2	1.94	0.48
1:A:694:TYR:CE1	1:A:711:VAL:HB	2.48	0.48
1:B:561:VAL:HG23	1:B:732:ILE:O	2.14	0.48
1:C:286:GLN:H	1:C:286:GLN:CD	2.22	0.48
1:C:262:ASN:HB3	1:C:284:GLU:HG3	1.95	0.48
1:A:505:GLN:HG3	1:A:506:ASP:OD2	2.14	0.48
1:A:415:ASN:ND2	1:A:418:GLN:OE1	2.47	0.48
1:A:684:TRP:CD1	1:A:684:TRP:C	2.92	0.48
1:B:483:ASN:OD1	1:B:501:GLY:HA3	2.13	0.48
1:C:415:ASN:O	1:C:416:PRO:C	2.57	0.48
1:B:337:ARG:HH21	1:B:337:ARG:HG3	1.78	0.48
1:C:340:ASP:O	1:C:355:LYS:HE3	2.14	0.48
1:A:660:THR:HB	1:A:663:GLN:HB2	1.96	0.47
1:B:367:ARG:HH21	1:B:371:CYS:HB3	1.75	0.47
1:B:358:ASP:OD2	1:B:360:LYS:HB2	2.14	0.47
1:B:466:ASP:O	1:B:469:ASP:HB3	2.14	0.47
1:B:473:ASP:O	1:B:475:ASP:N	2.42	0.47
1:A:494:ASP:OD1	1:A:501:GLY:HA2	2.14	0.47
1:B:487:VAL:HG11	1:B:504:CYS:HB3	1.97	0.47
1:A:269:ASP:OD1	1:A:272:LEU:N	2.47	0.47
1:A:747:GLU:C	1:A:749:TYR:H	2.23	0.47
1:B:670:ASP:OD1	1:B:672:ARG:HG3	2.14	0.47
1:C:583:GLU:CG	1:C:738:ARG:HB2	2.45	0.47
1:A:527:THR:HG23	1:A:528:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ALA:HA	1:B:255:CYS:HA	1.97	0.47
1:B:691:GLN:CD	1:B:691:GLN:H	2.23	0.47
1:A:324:GLU:CD	1:A:324:GLU:H	2.22	0.47
1:B:285:ARG:C	1:B:287:CYS:H	2.23	0.47
1:C:746:PRO:HB3	6:C:1003:SO4:O1	2.15	0.47
1:C:583:GLU:HG3	1:C:683:ARG:NH2	2.30	0.47
1:C:626:PRO:HG3	1:C:649:GLN:HA	1.97	0.47
1:C:459:SER:C	1:C:461:HIS:H	2.23	0.47
1:A:570:LEU:HD22	1:A:600:ILE:HG13	1.97	0.47
1:A:640:VAL:HG22	1:A:664:VAL:HG22	1.96	0.47
1:B:238:HIS:CG	1:B:239:GLU:H	2.33	0.47
1:B:550:ASN:H	1:B:562:GLN:HE21	1.63	0.47
1:C:638:LYS:HG2	1:C:666:LEU:HA	1.97	0.47
1:C:692:VAL:CG2	1:C:749:TYR:CZ	2.97	0.47
1:B:238:HIS:CG	1:B:239:GLU:N	2.83	0.46
1:B:568:PRO:HG3	1:B:727:PHE:CE2	2.50	0.46
1:B:285:ARG:O	1:B:287:CYS:N	2.49	0.46
1:B:513:VAL:HG21	1:B:527:THR:OG1	2.15	0.46
1:C:560:ILE:HG22	1:C:561:VAL:N	2.29	0.46
1:A:690:PRO:HB3	1:A:718:ARG:C	2.41	0.46
1:B:698:ARG:HB3	1:B:705:LEU:HD11	1.96	0.46
1:B:750:GLU:HA	1:B:753:GLN:HB2	1.97	0.46
1:C:333:ASN:N	1:C:334:PRO:HD3	2.30	0.46
1:C:475:ASP:HB3	1:C:488:PRO:CB	2.46	0.46
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.71	0.46
1:B:248:ASP:N	1:B:248:ASP:OD1	2.47	0.46
1:B:403:ILE:HG21	1:B:418:GLN:NE2	2.30	0.46
1:C:500:VAL:HG23	1:C:504:CYS:SG	2.55	0.46
1:B:542:GLU:N	1:B:542:GLU:OE1	2.48	0.46
1:A:285:ARG:C	1:A:287:CYS:H	2.23	0.46
1:A:337:ARG:CG	1:A:337:ARG:NH2	2.69	0.46
1:B:291:ASN:H	1:B:300:GLN:HE22	1.63	0.46
1:B:302:ASP:CG	1:B:305:ARG:HA	2.41	0.46
1:B:409:ASN:O	1:B:445:ARG:NH2	2.48	0.46
1:C:506:ASP:HB3	1:C:514:VAL:HG13	1.98	0.46
1:A:497:ARG:HD3	1:A:498:ASP:N	2.30	0.46
1:A:520:CYS:CB	1:A:526:VAL:CG1	2.90	0.46
1:B:410:CYS:C	1:B:412:GLN:N	2.74	0.46
1:B:711:VAL:HG21	1:B:752:HIS:CB	2.46	0.46
1:C:464:GLN:HG3	1:C:469:ASP:OD2	2.14	0.46
1:C:489:ASN:HD21	1:C:492:GLN:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLY:O	1:B:322:PRO:HD3	2.17	0.45
1:B:550:ASN:O	1:B:562:GLN:HA	2.16	0.45
1:C:227:ARG:CG	1:C:227:ARG:NH2	2.69	0.45
1:C:692:VAL:HG21	1:C:749:TYR:CE2	2.51	0.45
1:C:319:ASP:HB3	1:C:332:ARG:HB3	1.97	0.45
1:A:482:ASP:OD1	1:A:483:ASN:N	2.49	0.45
1:A:550:ASN:HD21	1:A:563:THR:HG1	1.62	0.45
1:B:239:GLU:HG3	1:C:228:PHE:CE2	2.51	0.45
1:B:483:ASN:CG	1:B:484:CYS:N	2.75	0.45
1:C:686:LEU:HG	1:C:687:GLN:N	2.28	0.45
1:A:692:VAL:HG22	1:A:749:TYR:OH	2.17	0.45
1:B:337:ARG:HG3	1:B:337:ARG:NH2	2.32	0.45
1:B:682:TYR:CE2	1:B:701:GLU:HG3	2.51	0.45
1:C:331:VAL:CG1	1:C:348:CYS:HB3	2.45	0.45
1:A:475:ASP:HB3	1:A:488:PRO:HA	1.98	0.45
1:C:422:ASP:OD2	1:C:422:ASP:N	2.49	0.45
1:A:614:TRP:CD2	1:A:635:ILE:HD13	2.52	0.45
1:B:284:GLU:O	1:B:285:ARG:C	2.59	0.45
1:C:729:GLN:HB3	1:C:732:ILE:HD11	1.97	0.45
1:A:668:TRP:CE2	1:A:709:SER:HA	2.52	0.45
1:B:689:ARG:HB3	1:B:691:GLN:HE21	1.82	0.45
1:C:378:ASP:O	1:C:380:ILE:HG22	2.16	0.45
1:B:482:ASP:O	1:B:483:ASN:C	2.60	0.45
1:A:337:ARG:HG3	1:A:337:ARG:NH2	2.14	0.45
1:C:638:LYS:NZ	1:C:656:HIS:O	2.50	0.45
1:A:518:ASP:OD1	1:A:521:PRO:HA	2.16	0.44
1:B:473:ASP:HB3	1:B:486:LEU:O	2.16	0.44
1:B:727:PHE:C	1:B:727:PHE:CD2	2.94	0.44
1:C:333:ASN:O	1:C:333:ASN:CG	2.60	0.44
1:B:647:GLY:O	1:B:648:GLU:C	2.60	0.44
1:C:378:ASP:O	1:C:380:ILE:N	2.51	0.44
1:C:380:ILE:HG12	1:C:385:ASP:HB2	1.98	0.44
1:B:627:PHE:O	1:B:652:ASN:ND2	2.50	0.44
1:C:475:ASP:HB3	1:C:488:PRO:HA	1.99	0.44
1:C:621:TYR:CE2	1:C:623:GLN:HB2	2.53	0.44
1:A:590:THR:OG1	1:A:592:THR:HG23	2.18	0.44
1:B:261:GLY:HA2	1:B:286:GLN:O	2.17	0.44
1:B:349:ASP:C	1:B:351:CYS:H	2.26	0.44
1:B:410:CYS:O	1:B:412:GLN:N	2.49	0.44
1:B:469:ASP:OD2	1:B:472:ASP:HA	2.18	0.44
1:C:668:TRP:CE2	1:C:709:SER:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:VAL:HG22	1:B:637:LEU:HD23	2.00	0.44
1:B:304:ASP:O	1:B:305:ARG:C	2.60	0.44
1:C:648:GLU:HA	1:C:651:ARG:NH2	2.33	0.44
1:B:351:CYS:HB2	1:B:356:ASN:ND2	2.33	0.44
1:B:637:LEU:HD12	1:B:667:LEU:HB2	2.00	0.44
1:C:358:ASP:C	1:C:358:ASP:OD1	2.61	0.44
1:C:373:ASP:HA	1:C:382:ASN:ND2	2.32	0.44
1:A:386:ASN:H	1:A:395:GLN:HE22	1.65	0.43
1:B:324:GLU:CD	1:B:324:GLU:N	2.75	0.43
1:B:377:GLY:C	1:B:379:ARG:H	2.26	0.43
1:B:552:VAL:HB	1:B:561:VAL:HG13	1.99	0.43
1:C:421:VAL:HG23	1:C:428:ASP:OD2	2.18	0.43
1:C:518:ASP:OD1	1:C:521:PRO:HA	2.18	0.43
1:C:582:PHE:CD2	1:C:722:LEU:HD22	2.53	0.43
1:C:662:SER:O	1:C:662:SER:OG	2.35	0.43
1:A:740:ARG:HH11	2:D:1:NAG:C8	2.31	0.43
1:B:608:SER:HA	1:B:640:VAL:O	2.18	0.43
1:A:503:VAL:HG12	1:A:503:VAL:O	2.18	0.43
1:A:635:ILE:H	1:A:635:ILE:HG12	1.42	0.43
1:B:386:ASN:OD1	1:B:392:ASN:ND2	2.48	0.43
1:B:559:GLU:HG3	1:B:735:ALA:HA	1.99	0.43
1:A:437:ASP:O	1:A:718:ARG:HD2	2.18	0.43
1:C:625:ASN:OD1	1:C:625:ASN:N	2.51	0.43
1:A:265:LEU:HD13	1:A:265:LEU:HA	1.84	0.43
1:B:486:LEU:HD12	1:B:508:PHE:CD2	2.52	0.43
1:A:620:THR:HG21	1:A:628:ARG:NH1	2.34	0.43
1:B:437:ASP:OD2	1:B:452:PRO:HA	2.18	0.43
1:C:583:GLU:HG3	1:C:683:ARG:HH21	1.82	0.43
1:C:399:ASP:HB2	1:C:414:SER:OG	2.19	0.43
1:A:532:ARG:HG2	1:A:532:ARG:H	1.55	0.43
1:A:696:ARG:HG2	1:A:710:ASN:O	2.18	0.43
1:B:424:ASP:O	1:B:425:PHE:HB2	2.18	0.43
1:B:632:GLU:HG2	1:B:673:ASN:OD1	2.18	0.43
1:B:732:ILE:HB	1:B:734:TRP:CH2	2.54	0.43
1:C:460:ASP:HB2	1:C:474:ASN:ND2	2.33	0.43
1:B:574:TYR:HA	1:B:721:ARG:NH1	2.33	0.43
1:B:603:TYR:HA	1:B:609:PHE:HB3	2.01	0.42
1:A:308:ILE:CG2	1:A:313:ASP:HB2	2.48	0.42
1:A:364:GLN:HE21	1:A:364:GLN:N	2.17	0.42
1:B:394:ASP:O	1:B:395:GLN:HB2	2.18	0.42
1:B:612:VAL:HG11	1:B:699:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASN:HB3	1:C:579:GLY:H	1.67	0.42
1:A:460:ASP:HB2	1:A:474:ASN:ND2	2.34	0.42
1:B:262:ASN:OD1	1:B:262:ASN:C	2.62	0.42
1:B:549:PRO:HA	1:B:562:GLN:NE2	2.34	0.42
1:C:342:ASP:HB2	1:C:357:ASP:OD2	2.20	0.42
1:C:670:ASP:HA	1:C:671:PRO:HD3	1.95	0.42
1:B:705:LEU:HD23	1:B:705:LEU:O	2.19	0.42
1:A:484:CYS:O	1:A:486:LEU:N	2.52	0.42
1:A:600:ILE:HD13	1:A:600:ILE:HA	1.87	0.42
1:B:397:ASP:CG	1:B:400:GLY:HA2	2.45	0.42
1:B:401:ASP:HB3	1:B:414:SER:HA	2.01	0.42
1:B:702:GLY:HA3	1:B:703:PRO:HD2	1.88	0.42
1:C:520:CYS:HB2	1:C:526:VAL:HG13	2.01	0.42
1:B:303:VAL:C	1:B:305:ARG:H	2.28	0.42
1:B:484:CYS:HB2	1:B:489:ASN:OD1	2.20	0.42
1:B:491:GLY:C	1:B:493:GLU:OE1	2.63	0.42
1:B:579:GLY:HA2	1:B:688:HIS:O	2.20	0.42
1:B:639:ALA:HB2	1:B:667:LEU:HD11	2.02	0.42
1:C:530:ASP:OD2	1:C:532:ARG:HG2	2.20	0.42
1:A:351:CYS:HB3	1:A:354:GLN:HB3	2.01	0.42
1:B:367:ARG:CZ	1:B:371:CYS:HB3	2.49	0.42
1:C:380:ILE:HG21	1:C:395:GLN:OE1	2.19	0.42
1:C:558:ARG:NH2	1:C:736:ASN:OD1	2.52	0.42
1:C:523:ASN:OD1	1:C:523:ASN:C	2.63	0.42
1:C:530:ASP:OD2	1:C:530:ASP:C	2.63	0.42
1:A:447:ASN:O	1:A:448:CYS:HB2	2.20	0.41
1:B:337:ARG:HG2	1:B:338:ASN:N	2.35	0.41
1:B:616:GLN:HG2	1:B:617:MET:HG2	2.02	0.41
1:C:617:MET:HE2	1:C:617:MET:HB2	1.86	0.41
1:C:618:GLU:OE1	1:C:632:GLU:HG2	2.20	0.41
1:A:284:GLU:O	1:A:285:ARG:O	2.37	0.41
1:B:595:ASP:HB2	1:B:728:SER:O	2.20	0.41
1:B:615:LYS:HE2	1:B:655:TRP:CH2	2.55	0.41
1:C:422:ASP:O	1:C:423:HIS:C	2.62	0.41
1:A:713:LEU:HD12	1:A:713:LEU:HA	1.94	0.41
1:A:747:GLU:HG2	2:D:2:NAG:H83	2.02	0.41
1:B:285:ARG:C	1:B:287:CYS:N	2.79	0.41
1:C:627:PHE:HD2	1:C:628:ARG:O	2.03	0.41
1:B:505:GLN:OE1	1:B:505:GLN:HA	2.20	0.41
1:A:414:SER:C	1:A:416:PRO:HD3	2.45	0.41
1:B:422:ASP:OD2	1:B:422:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ILE:H	1:B:635:ILE:CD1	2.25	0.41
1:C:487:VAL:HG22	1:C:504:CYS:HB3	2.02	0.41
1:A:244:VAL:O	1:A:244:VAL:CG2	2.64	0.41
1:A:378:ASP:C	1:A:380:ILE:H	2.27	0.41
1:A:602:GLY:HA2	1:A:720:GLY:HA3	2.02	0.41
1:B:545:ALA:C	1:B:547:ILE:N	2.79	0.41
1:C:265:LEU:HD13	1:C:265:LEU:HA	1.76	0.41
1:C:378:ASP:OD2	1:C:391:PRO:HA	2.21	0.41
1:A:508:PHE:CD2	1:A:508:PHE:C	2.99	0.41
1:A:742:ASN:OD1	1:A:744:THR:HG23	2.20	0.41
1:C:358:ASP:OD1	1:C:360:LYS:HB2	2.21	0.41
1:C:745:ILE:H	1:C:745:ILE:HG12	1.56	0.41
1:A:299:GLY:C	1:A:301:GLU:H	2.29	0.41
1:B:253:CYS:HB2	1:B:263:GLY:HA3	2.02	0.41
1:B:494:ASP:HB2	1:B:501:GLY:HA2	2.03	0.41
1:C:691:GLN:H	1:C:691:GLN:CD	2.27	0.41
1:A:305:ARG:HB3	1:A:305:ARG:CZ	2.48	0.41
1:A:508:PHE:CD2	1:A:508:PHE:O	2.74	0.41
1:B:369:ASP:C	1:B:371:CYS:H	2.28	0.41
1:B:398:SER:H	1:B:405:ASP:CG	2.28	0.41
1:C:328:CYS:HB2	1:C:333:ASN:OD1	2.21	0.41
1:C:497:ARG:HA	1:C:497:ARG:HD3	1.50	0.41
1:C:636:GLN:CD	1:C:657:THR:HG23	2.46	0.41
1:A:605:ASP:OD1	1:A:608:SER:N	2.53	0.41
1:B:484:CYS:HB2	1:B:489:ASN:ND2	2.36	0.41
1:C:621:TYR:HB2	1:C:655:TRP:NE1	2.35	0.41
1:A:477:VAL:HG21	1:A:492:GLN:NE2	2.36	0.40
1:A:502:ASP:C	1:A:504:CYS:N	2.79	0.40
1:B:549:PRO:CA	1:B:562:GLN:HE21	2.34	0.40
1:B:615:LYS:HE2	1:B:655:TRP:CZ2	2.56	0.40
1:A:400:GLY:C	1:A:402:GLY:H	2.27	0.40
1:A:408:ASP:C	1:A:410:CYS:H	2.29	0.40
1:A:563:THR:C	1:A:564:MET:HE2	2.47	0.40
1:B:709:SER:O	1:B:710:ASN:C	2.64	0.40
1:B:727:PHE:C	1:B:727:PHE:HD2	2.29	0.40
1:C:696:ARG:CZ	1:C:698:ARG:NH2	2.84	0.40
1:A:284:GLU:HB2	1:A:286:GLN:NE2	2.36	0.40
1:A:343:LYS:HG3	1:A:357:ASP:OD1	2.21	0.40
1:B:458:ASP:O	1:B:459:SER:C	2.64	0.40
1:B:485:ARG:NH2	1:B:486:LEU:HD21	2.35	0.40
1:B:412:GLN:O	1:B:413:LYS:HE3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:H	1:C:300:GLN:NE2	2.10	0.40
1:C:490:PRO:HB2	1:C:491:GLY:H	1.71	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	533/551 (97%)	443 (83%)	74 (14%)	16 (3%)	3	19
1	B	533/551 (97%)	435 (82%)	82 (15%)	16 (3%)	3	19
1	C	533/551 (97%)	443 (83%)	72 (14%)	18 (3%)	3	16
All	All	1599/1653 (97%)	1321 (83%)	228 (14%)	50 (3%)	3	18

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ASN
1	B	474	ASN
1	B	543	GLY
1	C	352	ARG
1	C	379	ARG
1	C	490	PRO
1	C	492	GLN
1	A	283	PRO
1	A	286	GLN
1	A	336	GLN
1	A	379	ARG
1	A	485	ARG
1	B	348	CYS
1	B	414	SER
1	B	594	ASP

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Mol	Chain	Res	Type
1	C	406	ALA
1	C	543	GLY
1	A	392	ASN
1	A	399	ASP
1	A	475	ASP
1	A	510	ALA
1	B	305	ARG
1	C	382	ASN
1	C	421	VAL
1	C	429	ALA
1	A	505	GLN
1	B	350	ASN
1	B	458	ASP
1	C	300	GLN
1	C	364	GLN
1	C	428	ASP
1	C	626	PRO
1	A	348	CYS
1	A	474	ASN
1	A	594	ASP
1	A	661	GLU
1	B	286	GLN
1	B	378	ASP
1	B	406	ALA
1	B	648	GLU
1	C	348	CYS
1	C	467	ALA
1	A	356	ASN
1	B	398	SER
1	B	519	VAL
1	C	359	GLN
1	C	499	GLY
1	B	283	PRO
1	B	646	PRO
1	C	377	GLY

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	459/473 (97%)	398 (87%)	61 (13%)	4	17
1	B	459/473 (97%)	408 (89%)	51 (11%)	6	22
1	C	459/473 (97%)	395 (86%)	64 (14%)	3	15
All	All	1377/1419 (97%)	1201 (87%)	176 (13%)	4	18

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	GLU
1	A	244	VAL
1	A	246	GLU
1	A	254	VAL
1	A	265	LEU
1	A	281	ARG
1	A	284	GLU
1	A	288	ARG
1	A	305	ARG
1	A	324	GLU
1	A	331	VAL
1	A	332	ARG
1	A	337	ARG
1	A	352	ARG
1	A	364	GLN
1	A	373	ASP
1	A	375	ILE
1	A	380	ILE
1	A	393	SER
1	A	396	LYS
1	A	412	GLN
1	A	436	GLN
1	A	442	GLN
1	A	444	SER
1	A	450	THR
1	A	457	GLU
1	A	514	VAL
1	A	516	LYS
1	A	519	VAL
1	A	522	GLU
1	A	529	THR
1	A	536	THR

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Mol	Chain	Res	Type
1	A	539	LEU
1	A	550	ASN
1	A	553	VAL
1	A	561	VAL
1	A	572	VAL
1	A	575	THR
1	A	588	VAL
1	A	591	VAL
1	A	592	THR
1	A	593	ASP
1	A	617	MET
1	A	630	VAL
1	A	635	ILE
1	A	646	PRO
1	A	660	THR
1	A	662	SER
1	A	666	LEU
1	A	677	LYS
1	A	686	LEU
1	A	692	VAL
1	A	696	ARG
1	A	711	VAL
1	A	713	LEU
1	A	717	MET
1	A	730	GLU
1	A	737	LEU
1	A	744	THR
1	A	753	GLN
1	A	756	GLN
1	B	227	ARG
1	B	246	GLU
1	B	251	ARG
1	B	257	VAL
1	B	280	LEU
1	B	284	GLU
1	B	285	ARG
1	B	305	ARG
1	B	324	GLU
1	B	331	VAL
1	B	332	ARG
1	B	367	ARG
1	B	450	THR

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Mol	Chain	Res	Type
1	B	451	VAL
1	B	460	ASP
1	B	473	ASP
1	B	480	SER
1	B	485	ARG
1	B	487	VAL
1	B	496	ASP
1	B	497	ARG
1	B	500	VAL
1	B	517	ILE
1	B	525	GLU
1	B	529	THR
1	B	535	GLN
1	B	536	THR
1	B	538	VAL
1	B	539	LEU
1	B	542	GLU
1	B	546	GLN
1	B	588	VAL
1	B	592	THR
1	B	600	ILE
1	B	617	MET
1	B	620	THR
1	B	632	GLU
1	B	643	SER
1	B	660	THR
1	B	666	LEU
1	B	697	VAL
1	B	705	LEU
1	B	710	ASN
1	B	716	THR
1	B	730	GLU
1	B	732	ILE
1	B	737	LEU
1	B	738	ARG
1	B	745	ILE
1	B	754	LEU
1	B	756	GLN
1	C	227	ARG
1	C	251	ARG
1	C	265	LEU
1	C	282	CYS

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Mol	Chain	Res	Type
1	C	284	GLU
1	C	285	ARG
1	C	288	ARG
1	C	303	VAL
1	C	305	ARG
1	C	324	GLU
1	C	331	VAL
1	C	346	ASP
1	C	360	LYS
1	C	364	GLN
1	C	367	ARG
1	C	380	ILE
1	C	383	GLN
1	C	389	ARG
1	C	412	GLN
1	C	433	ASP
1	C	442	GLN
1	C	451	VAL
1	C	477	VAL
1	C	487	VAL
1	C	492	GLN
1	C	493	GLU
1	C	494	ASP
1	C	496	ASP
1	C	497	ARG
1	C	503	VAL
1	C	506	ASP
1	C	514	VAL
1	C	519	VAL
1	C	525	GLU
1	C	528	LEU
1	C	536	THR
1	C	538	VAL
1	C	539	LEU
1	C	547	ILE
1	C	553	VAL
1	C	572	VAL
1	C	575	THR
1	C	578	ASN
1	C	580	VAL
1	C	588	VAL
1	C	591	VAL

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Mol	Chain	Res	Type
1	C	593	ASP
1	C	616	GLN
1	C	617	MET
1	C	625	ASN
1	C	665	ARG
1	C	666	LEU
1	C	667	LEU
1	C	672	ARG
1	C	686	LEU
1	C	692	VAL
1	C	696	ARG
1	C	697	VAL
1	C	711	VAL
1	C	713	LEU
1	C	717	MET
1	C	730	GLU
1	C	737	LEU
1	C	745	ILE

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	240	HIS
1	A	300	GLN
1	A	364	GLN
1	A	395	GLN
1	A	436	GLN
1	A	550	ASN
1	A	555	ASN
1	A	623	GLN
1	A	663	GLN
1	A	731	ASN
1	B	300	GLN
1	B	383	GLN
1	B	392	ASN
1	B	436	GLN
1	B	442	GLN
1	B	483	ASN
1	B	489	ASN
1	B	535	GLN
1	B	546	GLN
1	B	562	GLN

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Mol	Chain	Res	Type
1	B	587	HIS
1	B	663	GLN
1	B	691	GLN
1	B	731	ASN
1	B	752	HIS
1	B	753	GLN
1	B	756	GLN
1	C	223	ASN
1	C	240	HIS
1	C	300	GLN
1	C	364	GLN
1	C	412	GLN
1	C	418	GLN
1	C	423	HIS
1	C	436	GLN
1	C	474	ASN
1	C	565	ASN
1	C	589	ASN
1	C	623	GLN
1	C	663	GLN
1	C	673	ASN
1	C	687	GLN
1	C	688	HIS
1	C	756	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 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	D	1	1,2	14,14,15	0.60	0	17,19,21	1.99	6 (35%)
2	NAG	D	2	2	14,14,15	0.76	0	17,19,21	1.42	2 (11%)
2	MAN	D	3	2	11,11,12	0.97	0	15,15,17	1.28	1 (6%)
2	MAN	D	4	2	11,11,12	0.77	0	15,15,17	1.33	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.85	0	17,19,21	1.56	3 (17%)
3	NAG	E	2	3	14,14,15	0.81	1 (7%)	17,19,21	2.29	5 (29%)
3	MAN	E	3	3	11,11,12	0.64	0	15,15,17	1.55	2 (13%)
4	NAG	F	1	1,4	14,14,15	0.61	0	17,19,21	1.58	3 (17%)
4	NAG	F	2	4	14,14,15	0.93	1 (7%)	17,19,21	1.79	4 (23%)
4	MAN	F	3	4	11,11,12	0.60	0	15,15,17	1.45	3 (20%)
4	MAN	F	4	4	11,11,12	0.79	0	15,15,17	1.82	4 (26%)
4	MAN	F	5	4	11,11,12	0.51	0	15,15,17	1.40	1 (6%)

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	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	1/1/4/5	1/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	MAN	E	3	3	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	MAN	F	3	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	MAN	F	5	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O5-C1	-2.13	1.40	1.43
4	F	2	NAG	O5-C5	-2.06	1.39	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	O5-C1-C2	-5.73	102.42	111.29
4	F	2	NAG	C2-N2-C7	-5.05	116.13	122.90
4	F	1	NAG	O5-C1-C2	-4.84	103.80	111.29
2	D	1	NAG	C1-O5-C5	4.49	118.20	112.19
4	F	5	MAN	C1-O5-C5	4.27	117.91	112.19
4	F	4	MAN	C1-O5-C5	4.25	117.89	112.19
3	E	2	NAG	C8-C7-N2	3.91	122.61	116.12
3	E	1	NAG	C1-C2-N2	-3.88	104.32	110.43
3	E	1	NAG	C4-C3-C2	3.78	116.56	111.02
3	E	3	MAN	C3-C4-C5	3.64	116.84	110.23
3	E	2	NAG	C4-C3-C2	-3.64	105.69	111.02
4	F	3	MAN	C3-C4-C5	3.58	116.72	110.23
2	D	1	NAG	C8-C7-N2	3.49	121.90	116.12
2	D	4	MAN	C1-C2-C3	3.44	114.65	109.64
3	E	3	MAN	C1-O5-C5	3.39	116.73	112.19
2	D	3	MAN	C2-C3-C4	3.37	116.79	110.86
4	F	3	MAN	C1-O5-C5	3.28	116.58	112.19
4	F	4	MAN	C3-C4-C5	3.17	115.98	110.23
4	F	2	NAG	O4-C4-C3	-2.84	103.67	110.38
2	D	2	NAG	O4-C4-C3	-2.83	103.70	110.38
4	F	2	NAG	C1-C2-N2	2.68	114.65	110.43
3	E	2	NAG	O7-C7-C8	-2.50	117.60	122.05
4	F	4	MAN	C2-C3-C4	2.44	115.16	110.86
2	D	1	NAG	C2-N2-C7	2.43	126.16	122.90
2	D	2	NAG	O5-C5-C6	-2.37	103.05	107.66
3	E	2	NAG	C1-O5-C5	-2.34	109.05	112.19
4	F	2	NAG	O6-C6-C5	-2.30	103.52	111.33
4	F	4	MAN	O2-C2-C3	2.22	114.75	110.15
4	F	1	NAG	C4-C3-C2	2.15	114.17	111.02
2	D	1	NAG	C1-C2-N2	-2.15	107.05	110.43
4	F	1	NAG	O3-C3-C4	-2.12	105.38	110.38
3	E	1	NAG	O4-C4-C3	-2.11	105.40	110.38
2	D	1	NAG	O4-C4-C3	-2.08	105.48	110.38
2	D	1	NAG	O7-C7-C8	-2.06	118.39	122.05
4	F	3	MAN	O4-C4-C3	-2.01	105.63	110.38

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3	MAN	C1
3	E	1	NAG	C1
3	E	3	MAN	C1
4	F	3	MAN	C1

All (20) torsion outliers are listed below:

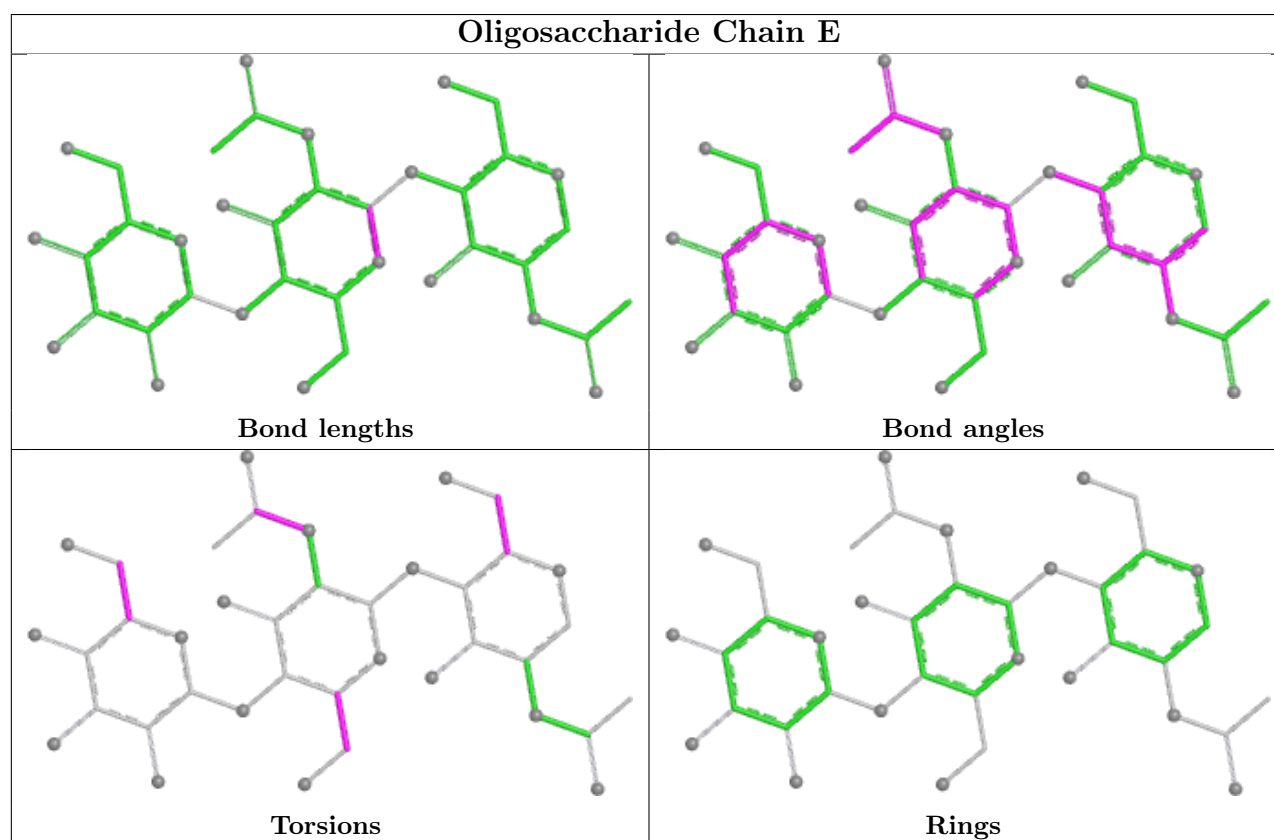
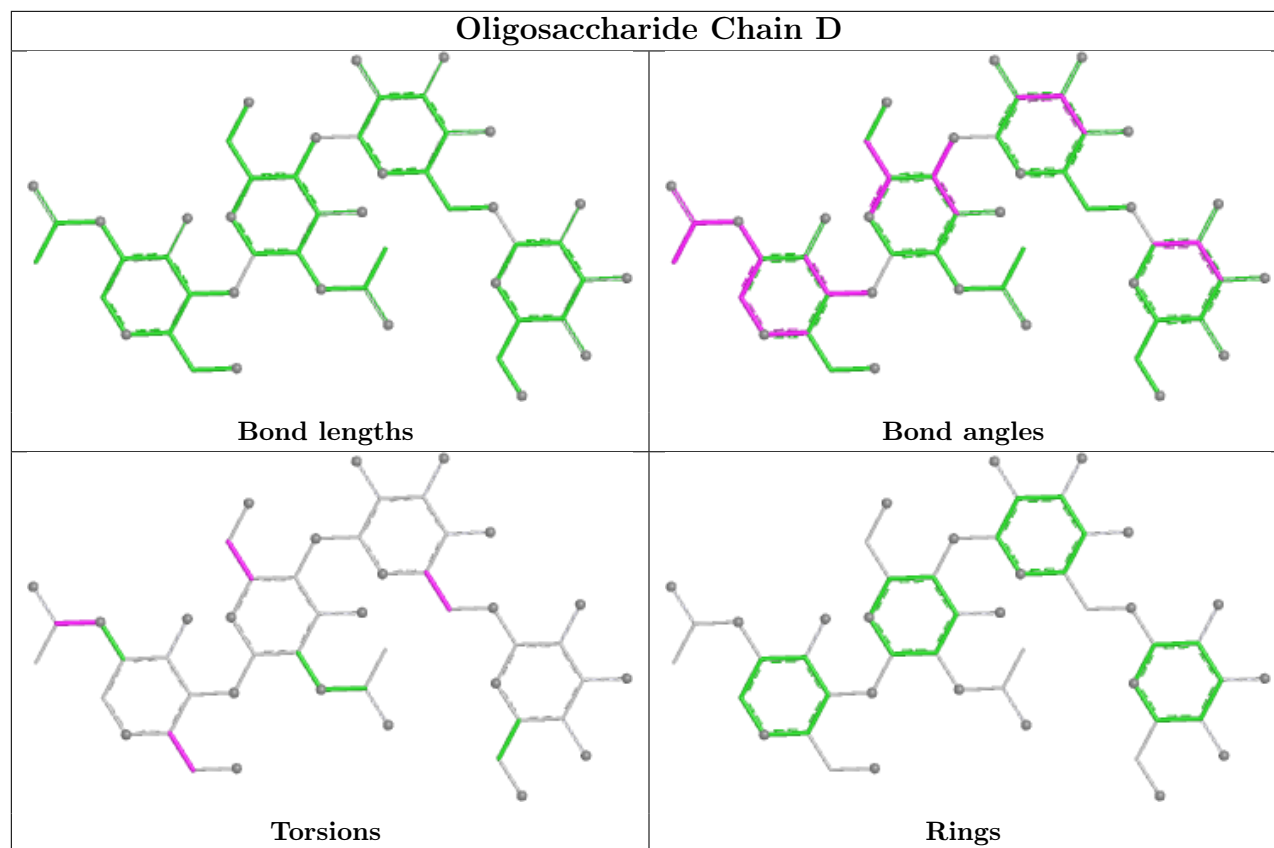
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
4	F	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

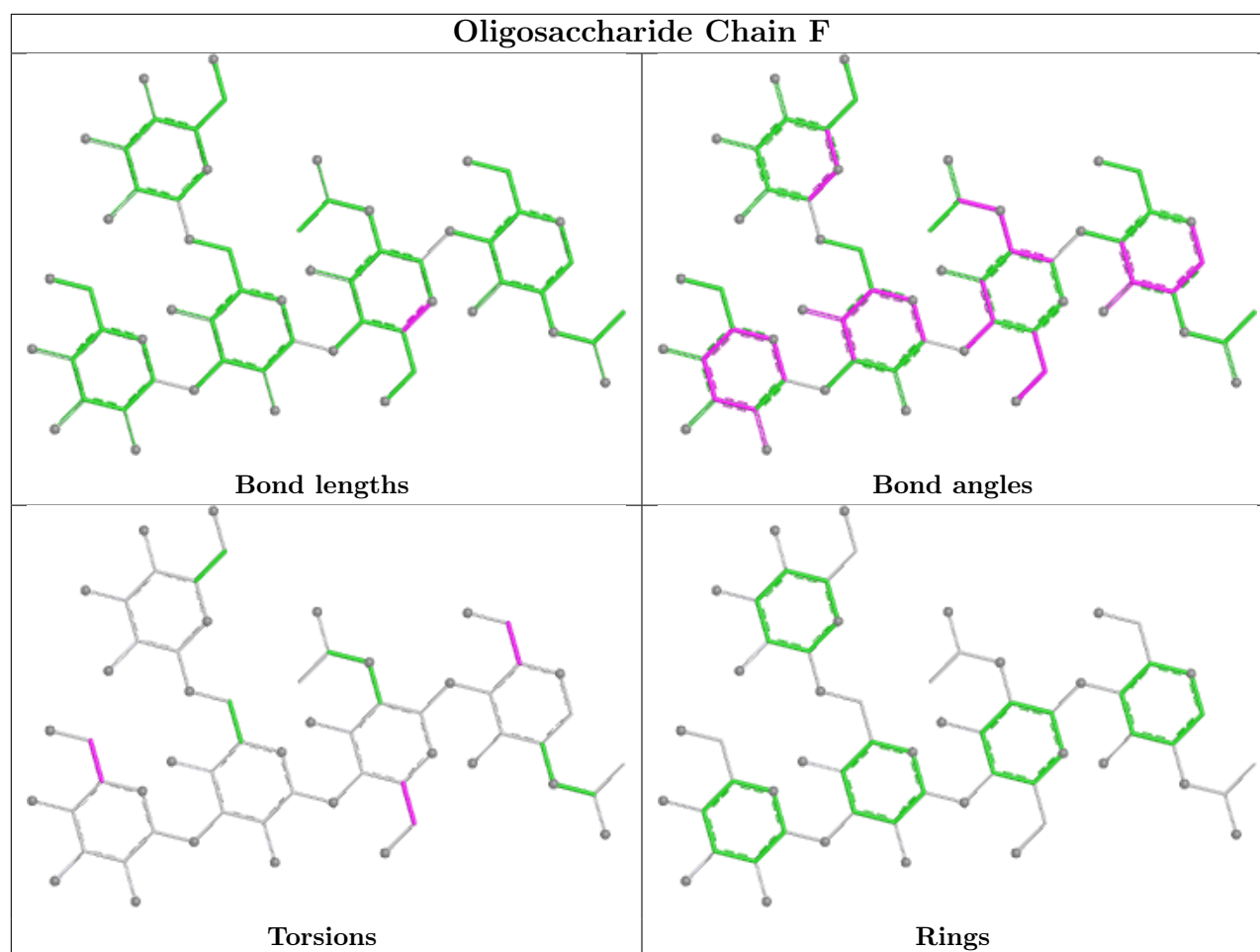
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	D	1	NAG	2	0

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





5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 88 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	A	1002	-	4,4,4	0.25	0	6,6,6	0.51	0
6	SO4	B	1001	-	4,4,4	0.31	0	6,6,6	0.45	0
6	SO4	C	1002	-	4,4,4	0.28	0	6,6,6	0.16	0
6	SO4	C	1003	-	4,4,4	0.26	0	6,6,6	0.37	0
6	SO4	A	1001	-	4,4,4	0.20	0	6,6,6	0.32	0
6	SO4	B	1002	-	4,4,4	0.19	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	C	1001	-	4,4,4	0.27	0	6,6,6	0.23	0
6	SO4	A	1004	-	4,4,4	0.29	0	6,6,6	0.19	0
6	SO4	A	1005	-	4,4,4	0.36	0	6,6,6	0.13	0
6	SO4	A	1003	-	4,4,4	0.27	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1003	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	535/551 (97%)	-0.09	7 (1%) 75 55	33, 49, 76, 90	0
1	B	535/551 (97%)	0.55	29 (5%) 31 18	24, 54, 70, 82	0
1	C	535/551 (97%)	0.23	15 (2%) 55 34	38, 54, 77, 85	0
All	All	1605/1653 (97%)	0.23	51 (3%) 50 30	24, 52, 75, 90	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	757	ALA	4.4
1	B	578	ASN	4.3
1	C	429	ALA	3.7
1	C	406	ALA	3.6
1	B	293	VAL	3.6
1	A	503	VAL	3.4
1	B	503	VAL	3.1
1	B	260	ALA	3.0
1	A	757	ALA	3.0
1	B	544	ASP	2.9
1	C	754	LEU	2.9
1	A	490	PRO	2.9
1	C	405	ASP	2.8
1	B	470	ASP	2.8
1	B	322	PRO	2.7
1	C	403	ILE	2.7
1	B	336	GLN	2.7
1	B	754	LEU	2.6
1	C	404	GLY	2.5
1	B	327	ASN	2.5
1	C	411	PRO	2.5
1	C	227	ARG	2.5
1	C	386	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	506	ASP	2.3
1	B	345	GLY	2.3
1	C	425	PHE	2.3
1	C	383	GLN	2.3
1	B	478	PRO	2.2
1	B	227	ARG	2.2
1	B	347	ALA	2.2
1	B	406	ALA	2.2
1	B	476	GLY	2.2
1	B	428	ASP	2.2
1	B	436	GLN	2.1
1	B	479	ASP	2.1
1	A	480	SER	2.1
1	A	495	ALA	2.1
1	C	228	PHE	2.1
1	B	379	ARG	2.1
1	B	522	GLU	2.1
1	B	308	ILE	2.1
1	B	339	THR	2.1
1	B	286	GLN	2.1
1	B	445	ARG	2.0
1	B	266	CYS	2.0
1	B	467	ALA	2.0
1	B	236	GLU	2.0
1	A	485	ARG	2.0
1	C	489	ASN	2.0
1	C	289	LYS	2.0
1	B	718	ARG	2.0

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

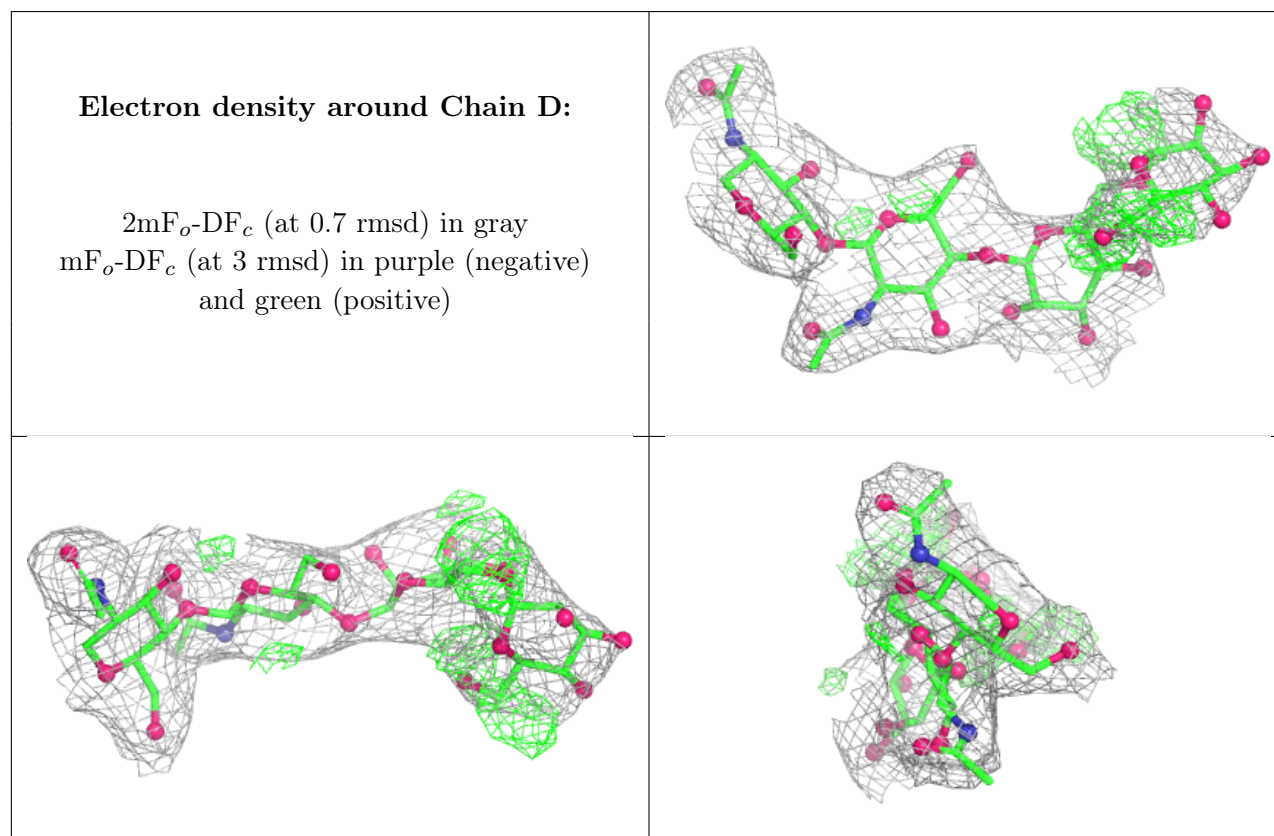
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

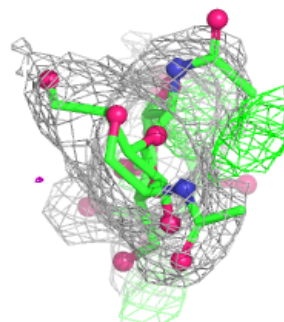
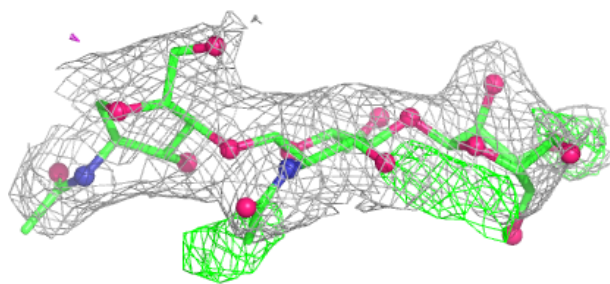
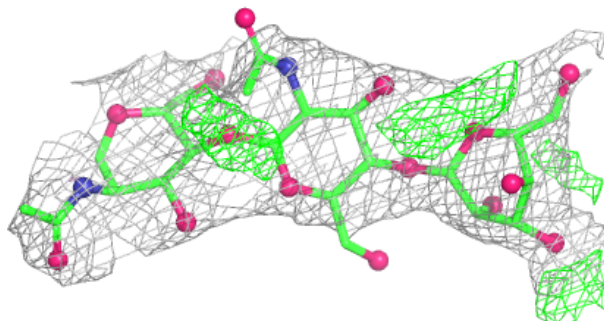
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	D	4	11/12	0.67	0.30	97,99,100,100	11
3	MAN	E	3	11/12	0.69	0.23	85,89,90,90	11
4	MAN	F	5	11/12	0.69	0.22	84,88,90,90	11
2	MAN	D	3	11/12	0.70	0.16	96,98,101,101	11
4	MAN	F	4	11/12	0.75	0.35	87,91,93,95	11
3	NAG	E	2	14/15	0.76	0.25	84,86,90,93	14
4	MAN	F	3	11/12	0.78	0.12	91,93,95,95	11
3	NAG	E	1	14/15	0.87	0.15	78,84,86,87	0
4	NAG	F	2	14/15	0.89	0.12	79,82,85,90	0
2	NAG	D	2	14/15	0.91	0.12	70,81,90,91	0
2	NAG	D	1	14/15	0.93	0.10	61,67,71,74	0
4	NAG	F	1	14/15	0.94	0.17	64,69,72,77	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.

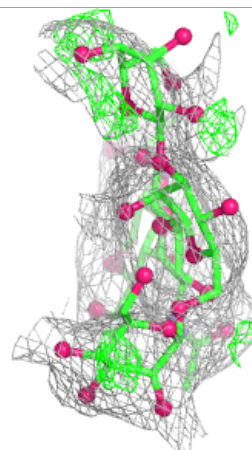
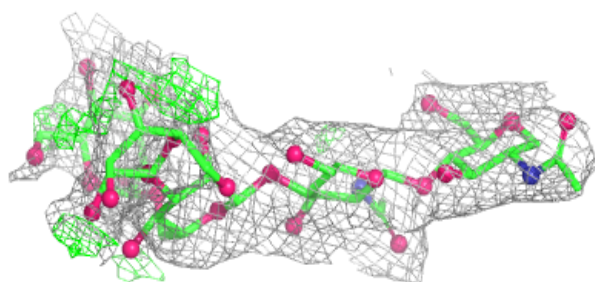
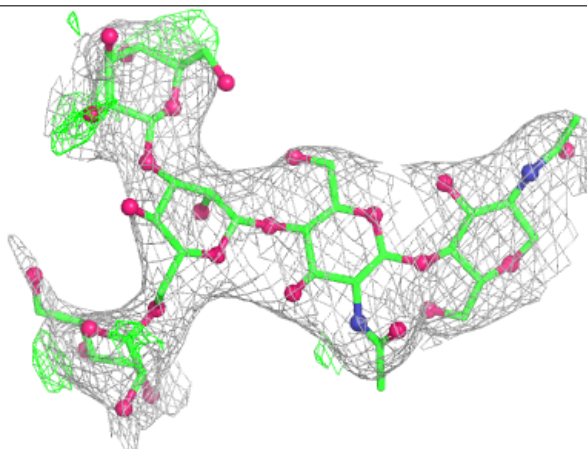


Electron density around Chain E:

$2mF_o - DF_c$ (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 ⓘ

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
6	SO4	A	1004	5/5	0.49	0.14	105,106,106,106	5
5	CA	C	810	1/1	0.57	0.16	174,174,174,174	0
5	CA	B	822	1/1	0.71	0.14	114,114,114,114	0
6	SO4	B	1002	5/5	0.73	0.17	94,94,95,97	5
6	SO4	C	1003	5/5	0.74	0.16	97,97,98,98	5
5	CA	B	811	1/1	0.76	0.14	123,123,123,123	0
6	SO4	A	1005	5/5	0.76	0.16	108,108,108,108	5
6	SO4	A	1003	5/5	0.77	0.15	106,107,107,107	5
6	SO4	A	1001	5/5	0.80	0.11	104,105,106,106	5
5	CA	C	809	1/1	0.81	0.12	108,108,108,108	0
6	SO4	C	1001	5/5	0.81	0.12	88,89,89,89	5
5	CA	A	824	1/1	0.81	0.09	160,160,160,160	0
6	SO4	C	1002	5/5	0.82	0.16	96,96,97,97	5
5	CA	B	816	1/1	0.84	0.15	111,111,111,111	0
5	CA	B	819	1/1	0.86	0.10	114,114,114,114	0
6	SO4	A	1002	5/5	0.86	0.20	94,94,97,97	5
5	CA	B	824	1/1	0.86	0.09	140,140,140,140	0
5	CA	A	816	1/1	0.87	0.12	114,114,114,114	0
5	CA	B	815	1/1	0.87	0.16	103,103,103,103	0
5	CA	C	822	1/1	0.87	0.11	118,118,118,118	0
5	CA	C	811	1/1	0.88	0.11	117,117,117,117	0
5	CA	C	816	1/1	0.88	0.09	123,123,123,123	0
5	CA	B	820	1/1	0.88	0.17	118,118,118,118	0
5	CA	C	819	1/1	0.89	0.10	118,118,118,118	0
5	CA	B	821	1/1	0.90	0.10	125,125,125,125	0
5	CA	B	817	1/1	0.90	0.11	127,127,127,127	0
5	CA	B	823	1/1	0.91	0.10	131,131,131,131	0
5	CA	A	820	1/1	0.92	0.09	119,119,119,119	0
5	CA	C	821	1/1	0.92	0.11	95,95,95,95	0
5	CA	A	821	1/1	0.92	0.12	104,104,104,104	0
5	CA	A	822	1/1	0.92	0.11	107,107,107,107	0
6	SO4	B	1001	5/5	0.93	0.08	82,82,85,85	0
5	CA	B	825	1/1	0.93	0.10	111,111,111,111	0
5	CA	C	813	1/1	0.93	0.07	119,119,119,119	0
5	CA	C	815	1/1	0.93	0.06	125,125,125,125	0
5	CA	B	829	1/1	0.93	0.08	89,89,89,89	0
5	CA	A	829	1/1	0.95	0.06	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	C	829	1/1	0.95	0.08	109,109,109,109	0
5	CA	B	818	1/1	0.95	0.07	106,106,106,106	0
5	CA	A	800	1/1	0.95	0.06	65,65,65,65	0
5	CA	C	820	1/1	0.96	0.09	125,125,125,125	0
5	CA	B	810	1/1	0.96	0.07	109,109,109,109	0
5	CA	A	819	1/1	0.96	0.07	119,119,119,119	0
5	CA	C	804	1/1	0.96	0.06	74,74,74,74	0
5	CA	A	805	1/1	0.96	0.05	60,60,60,60	0
5	CA	C	818	1/1	0.96	0.05	94,94,94,94	0
5	CA	B	804	1/1	0.96	0.06	83,83,83,83	0
5	CA	B	801	1/1	0.97	0.04	70,70,70,70	0
5	CA	C	824	1/1	0.97	0.09	115,115,115,115	0
5	CA	C	825	1/1	0.97	0.04	85,85,85,85	0
5	CA	A	801	1/1	0.97	0.04	56,56,56,56	0
5	CA	A	815	1/1	0.97	0.04	115,115,115,115	0
5	CA	C	812	1/1	0.97	0.07	117,117,117,117	0
5	CA	A	828	1/1	0.97	0.05	54,54,54,54	0
5	CA	B	814	1/1	0.97	0.05	121,121,121,121	0
5	CA	C	801	1/1	0.97	0.06	52,52,52,52	0
5	CA	C	817	1/1	0.97	0.07	105,105,105,105	0
5	CA	C	803	1/1	0.97	0.04	71,71,71,71	0
5	CA	A	804	1/1	0.97	0.04	78,78,78,78	0
5	CA	C	805	1/1	0.97	0.08	75,75,75,75	0
5	CA	C	807	1/1	0.97	0.09	65,65,65,65	0
5	CA	A	810	1/1	0.98	0.05	104,104,104,104	0
5	CA	A	811	1/1	0.98	0.05	75,75,75,75	0
5	CA	A	803	1/1	0.98	0.07	76,76,76,76	0
5	CA	A	807	1/1	0.98	0.04	61,61,61,61	0
5	CA	C	827	1/1	0.98	0.04	47,47,47,47	0
5	CA	C	828	1/1	0.98	0.04	58,58,58,58	0
5	CA	B	805	1/1	0.98	0.03	55,55,55,55	0
5	CA	B	806	1/1	0.98	0.05	54,54,54,54	0
5	CA	B	809	1/1	0.98	0.04	85,85,85,85	0
5	CA	A	823	1/1	0.98	0.05	103,103,103,103	0
5	CA	C	814	1/1	0.98	0.04	119,119,119,119	0
5	CA	A	817	1/1	0.98	0.06	81,81,81,81	0
5	CA	B	812	1/1	0.98	0.05	87,87,87,87	0
5	CA	B	828	1/1	0.98	0.05	69,69,69,69	0
5	CA	B	813	1/1	0.98	0.04	111,111,111,111	0
5	CA	A	825	1/1	0.98	0.04	93,93,93,93	0
5	CA	A	827	1/1	0.98	0.03	64,64,64,64	0
5	CA	C	823	1/1	0.99	0.02	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	C	808	1/1	0.99	0.03	64,64,64,64	0
5	CA	A	809	1/1	0.99	0.04	65,65,65,65	0
5	CA	C	826	1/1	0.99	0.03	85,85,85,85	0
5	CA	A	812	1/1	0.99	0.02	70,70,70,70	0
5	CA	B	802	1/1	0.99	0.04	53,53,53,53	0
5	CA	B	803	1/1	0.99	0.03	65,65,65,65	0
5	CA	B	826	1/1	0.99	0.04	86,86,86,86	0
5	CA	B	827	1/1	0.99	0.02	62,62,62,62	0
5	CA	A	818	1/1	0.99	0.03	85,85,85,85	0
5	CA	A	813	1/1	0.99	0.04	81,81,81,81	0
5	CA	A	826	1/1	0.99	0.03	86,86,86,86	0
5	CA	B	807	1/1	0.99	0.03	56,56,56,56	0
5	CA	B	808	1/1	0.99	0.05	56,56,56,56	0
5	CA	A	814	1/1	0.99	0.03	101,101,101,101	0
5	CA	C	806	1/1	0.99	0.03	72,72,72,72	0
5	CA	A	808	1/1	0.99	0.04	56,56,56,56	0
5	CA	A	802	1/1	1.00	0.01	58,58,58,58	0
5	CA	C	802	1/1	1.00	0.03	50,50,50,50	0
5	CA	A	806	1/1	1.00	0.03	54,54,54,54	0

6.5 Other polymers

There are no such residues in this entry.