



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:24 PM UTC

PDB ID : 2IWG / pdb_00002iwg
Title : COMPLEX BETWEEN THE PRYSPRY DOMAIN OF TRIM21 AND IGG FC
Authors : James, L.C.; Keeble, A.H.; Rhodes, D.A.; Trowsdale, J.
Deposited on : 2006-06-30
Resolution : 2.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

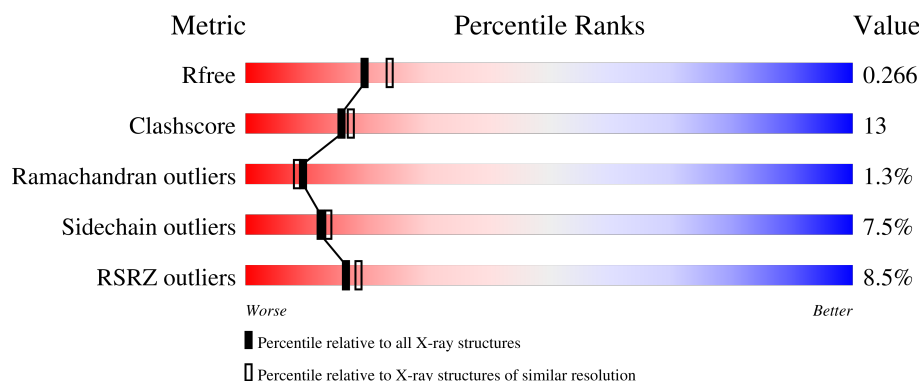
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	207	16% 57% 35% 8%
1	D	207	12% 58% 33% 8%
2	B	181	3% 54% 36% 10%
2	E	181	2% 52% 40% 7%
3	C	7	43% 57%

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Mol	Chain	Length	Quality of chain
3	F	7	 43% 57%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6590 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.

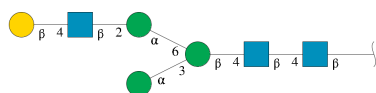
- Molecule 1 is a protein called IG GAMMA-1 CHAIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1658	1056	279	317	6			
1	D	207	Total	C	N	O	S	0	0	0
			1658	1056	279	317	6			

- Molecule 2 is a protein called 52 KDA RO PROTEIN.

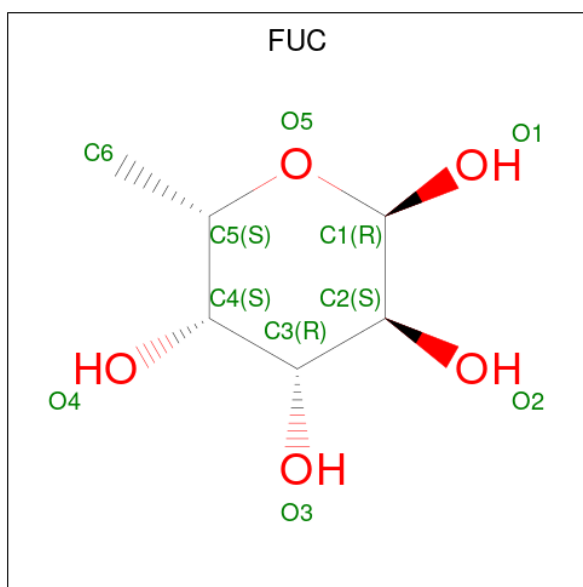
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1455	936	248	264	7			
2	E	181	Total	C	N	O	S	0	0	0
			1455	936	248	264	7			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-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	C	7	Total	C	N	O	0	0	0
			86	48	3	35			
3	F	7	Total	C	N	O	0	0	0
			86	48	3	35			

- Molecule 4 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

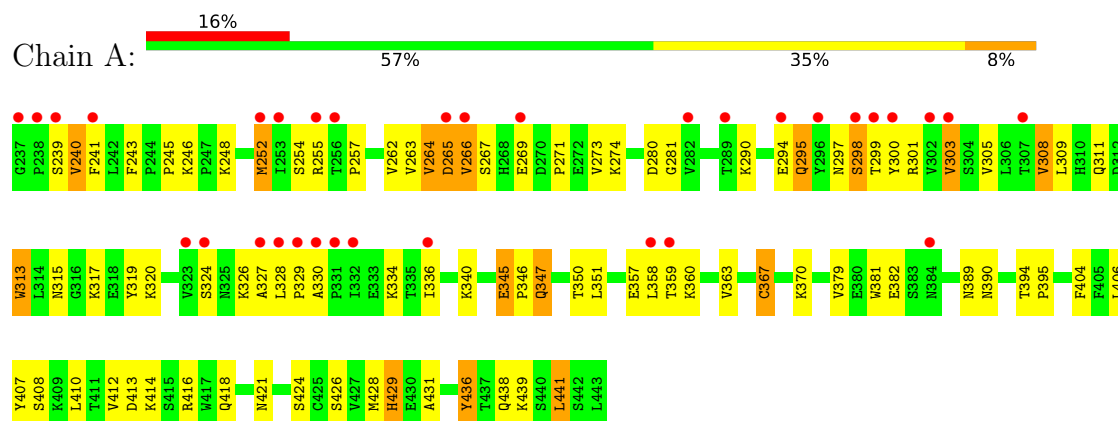
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	31	Total	O	0	0
			31	31		
5	D	42	Total	O	0	0
			42	42		
5	E	51	Total	O	0	0
			51	51		

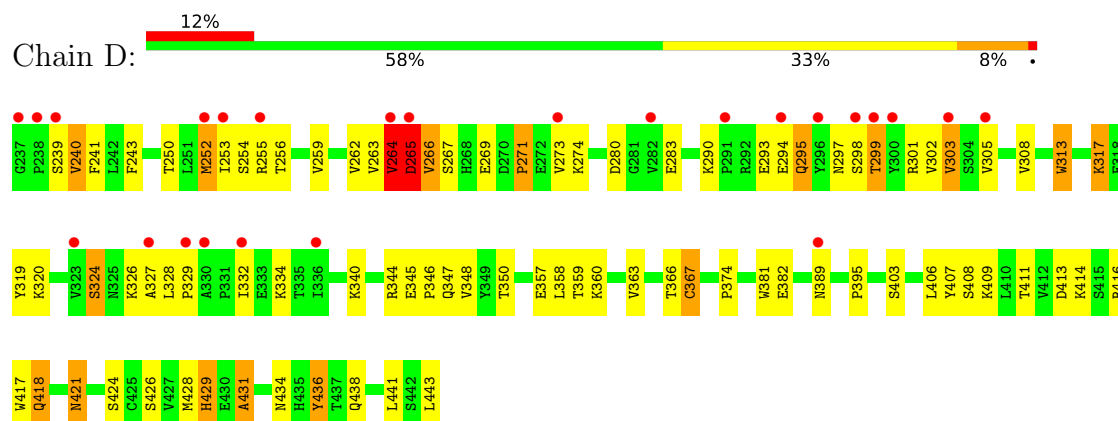
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

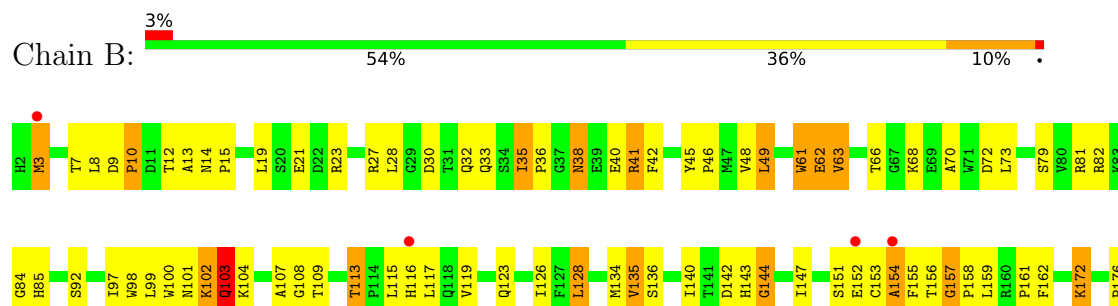
• Molecule 1: IG GAMMA-1 CHAIN C



• Molecule 1: IG GAMMA-1 CHAIN C



• Molecule 2: 52 KDA RO PROTEIN





• Molecule 2: 52 KDA RO PROTEIN



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	112.49Å 112.49Å 194.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	97.59 – 2.35 97.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	86.1 (97.59-2.35) 86.1 (97.59-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.253 (Not available) , 0.266	Depositor DCC
R_{free} test set	2533 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6590	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: GAL, BMA, NAG, MAN, FUC

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	1.86	30/1704 (1.8%)	1.48	25/2322 (1.1%)
1	D	1.86	28/1704 (1.6%)	1.49	17/2322 (0.7%)
2	B	2.02	36/1505 (2.4%)	1.70	28/2050 (1.4%)
2	E	1.97	34/1505 (2.3%)	1.70	34/2050 (1.7%)
All	All	1.93	128/6418 (2.0%)	1.59	104/8744 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	126	ILE	CA-CB	11.05	1.68	1.54
2	E	126	ILE	CA-CB	10.32	1.67	1.54
2	B	98	TRP	N-CA	-9.69	1.33	1.45
1	A	252	MET	N-CA	9.39	1.58	1.46
2	B	103	GLN	N-CA	9.24	1.58	1.46
2	E	98	TRP	N-CA	-8.59	1.35	1.45
1	A	410	LEU	N-CA	8.19	1.56	1.46
1	D	429	HIS	C-O	-7.99	1.14	1.23
2	B	3	MET	CG-SD	7.97	2.00	1.80
1	D	367	CYS	N-CA	-7.89	1.36	1.46
2	E	103	GLN	N-CA	7.65	1.56	1.46
1	D	263	VAL	CA-CB	-7.33	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	VAL	CA-C	7.13	1.61	1.52
2	B	61	TRP	C-O	-7.12	1.15	1.23
2	B	108	GLY	N-CA	7.11	1.55	1.45
1	A	263	VAL	CA-CB	-7.11	1.45	1.54
1	A	407	TYR	CA-C	7.01	1.61	1.52
1	D	259	VAL	CA-C	6.97	1.61	1.52
1	A	351	LEU	C-O	-6.95	1.16	1.24
2	E	3	MET	CG-SD	6.92	1.98	1.80
2	E	63	VAL	N-CA	-6.85	1.38	1.46
1	D	436	TYR	C-O	-6.83	1.15	1.23
2	B	63	VAL	N-CA	-6.82	1.38	1.46
1	A	429	HIS	CA-C	6.78	1.61	1.52
2	B	162	PHE	C-O	-6.78	1.15	1.24
2	E	163	PHE	C-O	6.76	1.32	1.23
2	B	3	MET	SD-CE	6.64	1.96	1.79
2	B	73	LEU	CA-C	-6.62	1.44	1.52
2	B	9	ASP	C-O	-6.55	1.15	1.24
1	D	252	MET	N-CA	6.55	1.54	1.46
2	B	3	MET	C-O	6.53	1.32	1.23
1	D	347	GLN	CG-CD	6.50	1.68	1.52
2	B	48	VAL	C-O	6.48	1.31	1.23
1	D	431	ALA	CA-CB	6.48	1.62	1.53
1	A	412	VAL	CA-CB	6.43	1.64	1.54
2	B	62	GLU	CA-C	-6.37	1.44	1.52
2	E	9	ASP	CA-C	-6.34	1.46	1.52
2	B	172	LYS	C-O	6.32	1.33	1.23
1	D	409	LYS	C-O	6.30	1.31	1.24
2	B	128	LEU	N-CA	6.28	1.53	1.46
1	A	394	THR	N-CA	6.21	1.54	1.45
2	E	113	THR	CA-C	6.18	1.59	1.52
1	A	367	CYS	N-CA	-6.17	1.38	1.46
2	B	45	TYR	CA-C	-6.17	1.46	1.52
1	D	271	PRO	CA-C	6.14	1.60	1.52
2	E	163	PHE	CG-CD2	6.12	1.51	1.38
1	A	301	ARG	CA-C	6.09	1.60	1.52
2	E	107	ALA	CA-CB	-6.03	1.44	1.53
2	E	9	ASP	C-O	-6.03	1.16	1.24
1	D	406	LEU	C-O	-5.98	1.16	1.23
1	A	308	VAL	CA-CB	5.94	1.63	1.54
1	D	407	TYR	CA-C	5.92	1.59	1.52
1	A	298	SER	C-O	5.87	1.31	1.23
2	E	172	LYS	C-O	5.87	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	GLU	CA-C	5.83	1.59	1.52
2	B	48	VAL	CA-CB	5.83	1.61	1.55
2	E	135	VAL	CB-CG1	-5.82	1.33	1.52
1	D	301	ARG	CA-C	5.81	1.60	1.52
2	B	113	THR	CA-C	5.80	1.59	1.52
2	B	136	SER	N-CA	5.77	1.52	1.45
2	B	100	TRP	C-O	-5.76	1.16	1.23
2	B	116	HIS	C-O	-5.76	1.17	1.24
1	D	256	THR	CA-CB	5.74	1.60	1.53
1	D	417	TRP	CA-C	-5.72	1.45	1.52
2	E	40	GLU	C-O	-5.68	1.16	1.24
2	E	92	SER	CA-C	5.67	1.60	1.52
2	B	156	THR	CA-CB	5.66	1.63	1.54
2	E	99	LEU	C-O	-5.66	1.17	1.24
2	E	68	LYS	CE-NZ	-5.65	1.32	1.49
1	A	436	TYR	C-O	-5.63	1.17	1.23
2	B	41	ARG	CZ-NH2	-5.63	1.26	1.33
2	B	135	VAL	CB-CG1	-5.62	1.33	1.52
2	E	42	PHE	CA-C	-5.62	1.45	1.52
2	B	116	HIS	CA-C	-5.58	1.46	1.52
2	E	41	ARG	CZ-NH2	-5.57	1.26	1.33
2	E	77	ARG	CA-C	-5.57	1.45	1.52
1	D	305	VAL	CA-C	5.56	1.59	1.52
2	B	79	SER	CA-C	-5.56	1.45	1.52
1	A	266	VAL	CA-CB	5.52	1.61	1.54
1	D	347	GLN	C-O	-5.50	1.17	1.24
1	D	299	THR	N-CA	5.49	1.52	1.45
2	E	3	MET	N-CA	5.49	1.53	1.45
2	B	92	SER	CA-C	5.48	1.59	1.52
1	A	439	LYS	CA-C	-5.47	1.45	1.52
2	E	24	ARG	CA-C	5.47	1.59	1.52
2	E	45	TYR	CA-C	-5.46	1.47	1.52
2	B	40	GLU	C-O	-5.45	1.16	1.24
2	E	127	PHE	C-O	-5.44	1.17	1.24
2	E	124	VAL	CA-CB	5.44	1.61	1.54
2	B	10	PRO	C-O	-5.40	1.17	1.24
1	A	404	PHE	CA-C	-5.38	1.46	1.52
1	A	257	PRO	CA-C	5.37	1.58	1.52
1	A	295	GLN	CA-C	5.35	1.59	1.52
2	B	119	VAL	CA-C	5.34	1.58	1.52
2	B	48	VAL	CA-C	-5.33	1.46	1.52
1	D	313	TRP	C-O	-5.32	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	LYS	CE-NZ	-5.32	1.33	1.49
1	D	348	VAL	C-O	-5.32	1.18	1.24
1	A	252	MET	C-O	5.28	1.30	1.24
2	E	3	MET	C-O	5.27	1.31	1.23
1	A	429	HIS	C-O	-5.25	1.17	1.23
1	A	294	GLU	N-CA	5.24	1.52	1.46
1	D	407	TYR	CG-CD1	5.24	1.50	1.39
1	D	253	ILE	CA-C	5.24	1.59	1.52
1	A	441	LEU	N-CA	-5.21	1.40	1.46
1	D	295	GLN	CA-C	5.20	1.59	1.52
2	E	156	THR	CA-CB	5.20	1.62	1.54
2	E	119	VAL	CA-C	5.20	1.58	1.52
1	D	324	SER	N-CA	5.20	1.52	1.46
2	E	108	GLY	N-CA	5.19	1.52	1.45
1	A	347	GLN	CG-CD	5.19	1.65	1.52
2	E	137	PHE	CD1-CE1	5.15	1.54	1.38
1	A	379	VAL	CA-CB	5.13	1.62	1.54
1	A	309	LEU	C-O	5.10	1.30	1.23
2	E	116	HIS	CA-C	-5.09	1.46	1.52
1	D	434	ASN	N-CA	5.09	1.53	1.46
1	A	406	LEU	CA-C	-5.09	1.46	1.52
1	D	403	SER	C-O	-5.08	1.17	1.23
2	E	62	GLU	CA-C	-5.07	1.46	1.52
1	A	330	ALA	CA-CB	5.05	1.63	1.54
1	D	436	TYR	N-CA	-5.05	1.39	1.46
1	D	294	GLU	N-CA	5.04	1.52	1.46
2	E	48	VAL	CA-C	-5.04	1.46	1.52
2	B	66	THR	C-O	5.03	1.29	1.23
2	E	24	ARG	C-O	-5.03	1.17	1.24
1	A	330	ALA	C-N	5.03	1.39	1.33
2	B	162	PHE	CA-C	-5.02	1.46	1.52
2	B	3	MET	CA-C	5.01	1.59	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ASP	N-CA-C	9.71	125.01	110.64
1	A	266	VAL	N-CA-C	-8.85	95.70	108.53
1	A	265	ASP	CB-CA-C	8.17	119.85	109.80
2	E	9	ASP	CA-C-N	8.00	127.64	119.56
2	E	9	ASP	C-N-CA	8.00	127.64	119.56
2	B	134	MET	N-CA-C	7.41	121.61	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	GLY	N-CA-C	7.36	126.39	112.62
1	D	266	VAL	N-CA-C	-7.32	97.81	108.71
2	E	103	GLN	N-CA-C	7.28	126.30	110.80
2	E	72	ASP	OD1-CG-OD2	-7.27	105.45	122.90
2	B	49	LEU	N-CA-C	7.16	121.08	110.48
2	B	103	GLN	N-CA-C	7.16	126.05	110.80
2	E	157	GLY	CA-C-N	7.15	127.14	119.78
2	E	157	GLY	C-N-CA	7.15	127.14	119.78
2	E	84	GLY	N-CA-C	7.09	125.61	112.77
2	E	134	MET	N-CA-C	6.94	120.84	109.24
2	B	157	GLY	CA-C-N	6.92	126.88	119.76
2	B	157	GLY	C-N-CA	6.92	126.88	119.76
2	B	72	ASP	OD1-CG-OD2	-6.91	106.32	122.90
1	D	265	ASP	N-CA-C	6.86	125.42	110.80
2	B	104	LYS	N-CA-C	6.72	119.70	108.20
1	D	408	SER	CA-C-N	-6.59	113.71	123.00
1	D	408	SER	C-N-CA	-6.59	113.71	123.00
2	E	104	LYS	N-CA-C	6.59	119.47	108.20
2	E	109	THR	N-CA-C	-6.56	100.81	110.52
2	E	74	GLY	N-CA-C	6.50	119.61	110.38
2	B	147	ILE	N-CA-C	-6.48	106.24	111.81
2	B	109	THR	N-CA-C	-6.47	101.21	110.59
1	D	411	THR	CB-CA-C	-6.44	99.24	109.80
2	E	43	ASP	N-CA-C	6.41	121.10	113.28
1	A	421	ASN	N-CA-C	6.36	118.51	110.24
2	B	14	ASN	CA-C-N	6.33	126.03	119.82
2	B	14	ASN	C-N-CA	6.33	126.03	119.82
1	A	240	VAL	N-CA-C	6.29	117.36	108.17
1	A	243	PHE	N-CA-C	6.28	119.63	110.14
1	A	246	LYS	CA-C-N	6.25	125.75	119.24
1	A	246	LYS	C-N-CA	6.25	125.75	119.24
2	B	119	VAL	CA-C-N	6.25	126.82	120.38
2	B	119	VAL	C-N-CA	6.25	126.82	120.38
2	E	147	ILE	N-CA-C	-6.23	106.45	111.81
1	D	313	TRP	N-CA-C	-6.18	104.46	111.14
1	A	273	VAL	N-CA-C	6.12	116.74	108.17
2	E	13	ALA	N-CA-C	6.12	119.14	109.96
1	D	240	VAL	N-CA-C	6.12	116.92	108.12
1	D	243	PHE	N-CA-C	6.11	119.36	110.14
1	D	421	ASN	N-CA-C	6.02	118.07	110.24
1	A	408	SER	CA-C-N	-6.01	114.64	123.05
1	A	408	SER	C-N-CA	-6.01	114.64	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ASP	CA-C-O	6.00	126.52	120.88
2	B	13	ALA	N-CA-C	5.99	118.94	109.96
1	A	313	TRP	N-CA-C	-5.93	104.74	111.14
1	A	395	PRO	CA-C-N	-5.90	113.86	119.76
1	A	395	PRO	C-N-CA	-5.90	113.86	119.76
1	D	301	ARG	N-CA-C	5.90	118.37	107.99
1	A	301	ARG	N-CA-C	5.84	118.27	107.99
2	E	41	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	D	389	ASN	N-CA-C	5.81	120.07	112.92
2	B	144	GLY	N-CA-C	-5.81	106.95	115.72
2	B	103	GLN	CA-C-N	-5.75	115.36	122.84
2	B	103	GLN	C-N-CA	-5.75	115.36	122.84
2	E	149	SER	N-CA-C	5.69	117.68	108.34
2	E	135	VAL	CB-CA-C	5.65	118.05	110.42
2	B	41	ARG	NE-CZ-NH2	-5.59	114.17	119.20
2	E	91	LYS	N-CA-C	-5.58	106.52	113.38
1	D	395	PRO	CA-C-N	-5.56	114.20	119.76
1	D	395	PRO	C-N-CA	-5.56	114.20	119.76
2	E	14	ASN	CA-C-N	5.55	125.26	119.82
2	E	14	ASN	C-N-CA	5.55	125.26	119.82
2	E	143	HIS	N-CA-C	5.54	122.60	110.80
1	D	265	ASP	CB-CA-C	5.49	121.35	110.42
2	E	48	VAL	CA-CB-CG1	5.45	119.67	110.40
2	E	126	ILE	N-CA-C	-5.40	99.86	107.75
1	D	303	VAL	N-CA-C	5.37	116.32	108.53
1	A	281	GLY	CA-C-N	-5.36	115.98	123.10
1	A	281	GLY	C-N-CA	-5.36	115.98	123.10
2	B	79	SER	CB-CA-C	-5.36	99.29	109.95
1	A	243	PHE	CA-C-N	-5.35	114.87	120.38
1	A	243	PHE	C-N-CA	-5.35	114.87	120.38
1	A	336	ILE	N-CA-C	5.35	117.78	108.90
1	D	273	VAL	N-CA-C	5.33	115.63	108.17
2	B	68	LYS	CD-CE-NZ	-5.32	94.88	111.90
1	A	300	TYR	N-CA-C	5.29	117.38	108.96
2	B	126	ILE	N-CA-C	-5.26	100.75	108.11
2	E	181	PRO	CA-C-N	-5.24	112.26	121.70
2	E	181	PRO	C-N-CA	-5.24	112.26	121.70
2	E	99	LEU	CA-C-O	-5.21	114.54	120.32
2	E	24	ARG	N-CA-C	-5.17	106.93	114.12
2	B	180	CYS	CA-C-N	5.17	124.97	119.28
2	B	180	CYS	C-N-CA	5.17	124.97	119.28
2	E	49	LEU	N-CA-C	5.15	118.11	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	117	LEU	CD1-CG-CD2	-5.15	99.48	110.80
2	B	117	LEU	CD1-CG-CD2	-5.12	99.53	110.80
2	E	79	SER	CB-CA-C	-5.12	99.73	110.17
2	B	41	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	340	LYS	N-CA-C	5.11	117.27	110.53
1	D	348	VAL	N-CA-C	5.10	115.25	108.11
2	E	45	TYR	O-C-N	5.10	125.50	121.88
1	A	303	VAL	N-CA-C	5.09	115.92	108.53
2	E	29	GLY	N-CA-C	5.07	120.89	112.89
2	B	45	TYR	O-C-N	5.06	125.47	121.88
1	A	389	ASN	N-CA-C	5.06	119.14	112.92
2	B	23	ARG	CA-CB-CG	-5.05	104.00	114.10
2	E	73	LEU	CA-C-O	-5.04	115.35	120.99
2	E	135	VAL	N-CA-C	5.00	115.17	107.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	264	VAL	Peptide
1	D	264	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1658	0	1625	45	0
1	D	1658	0	1625	40	0
2	B	1455	0	1381	38	0
2	E	1455	0	1381	37	0
3	C	86	0	73	6	0
3	F	86	0	73	6	0
4	A	10	0	10	2	0
4	D	10	0	10	3	0
5	A	48	0	0	2	0
5	B	31	0	0	3	0
5	D	42	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	51	0	0	3	0
All	All	6590	0	6178	168	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 13.

All (168) 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:265:ASP:HB3	1:A:299:THR:HB	1.30	1.06
1:D:265:ASP:HB3	1:D:299:THR:HB	1.39	1.00
1:A:252:MET:HG2	1:A:428:MET:HE1	1.51	0.92
4:D:1451:FUC:H2	3:F:1:NAG:O6	1.71	0.88
1:A:265:ASP:HB3	1:A:299:THR:CB	2.06	0.85
1:D:252:MET:HG2	1:D:428:MET:HE1	1.57	0.84
2:B:101:ASN:O	2:B:102:LYS:O	1.96	0.83
4:A:1451:FUC:H2	3:C:1:NAG:O6	1.78	0.83
2:E:38:ASN:HD21	2:E:41:ARG:NH1	1.82	0.78
2:E:101:ASN:O	2:E:102:LYS:O	2.00	0.78
1:A:252:MET:HE3	1:A:255:ARG:HG3	1.66	0.77
1:D:265:ASP:HB3	1:D:299:THR:CB	2.15	0.77
1:A:239:SER:HB2	1:A:264:VAL:HG23	1.66	0.77
2:E:3:MET:CB	2:E:182:LEU:HD13	2.16	0.76
2:B:3:MET:CB	2:B:182:LEU:HD13	2.15	0.76
2:B:3:MET:HB2	2:B:182:LEU:HD13	1.67	0.75
1:D:239:SER:HB2	1:D:264:VAL:HG23	1.68	0.75
3:C:2:NAG:H83	3:C:4:MAN:O4	1.88	0.74
1:A:248:LYS:HB3	1:A:252:MET:HE2	1.70	0.73
1:D:290:LYS:HB2	1:D:303:VAL:HG23	1.72	0.71
2:B:153:CYS:O	2:B:154:ALA:HB3	1.89	0.71
2:E:3:MET:HB2	2:E:182:LEU:HD13	1.72	0.71
3:F:2:NAG:H83	3:F:4:MAN:O4	1.90	0.71
1:D:326:LYS:C	1:D:328:LEU:H	1.99	0.69
2:E:153:CYS:O	2:E:154:ALA:HB3	1.92	0.69
4:D:1451:FUC:C1	3:F:2:NAG:HN2	2.06	0.68
1:A:326:LYS:C	1:A:328:LEU:H	2.03	0.67
1:D:421:ASN:O	5:D:2032:HOH:O	2.11	0.67
4:A:1451:FUC:C1	3:C:2:NAG:HN2	2.08	0.66
2:E:12:THR:HG21	2:E:49:LEU:HB2	1.77	0.66
2:E:19:LEU:HD12	2:E:19:LEU:N	2.10	0.66
1:A:290:LYS:HB2	1:A:303:VAL:HG23	1.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ASN:HD21	2:B:41:ARG:NH1	1.95	0.65
1:D:252:MET:CG	1:D:428:MET:HE1	2.27	0.65
1:D:382:GLU:HG2	1:D:424:SER:HB2	1.76	0.65
1:A:382:GLU:HG2	1:A:424:SER:HB2	1.78	0.64
2:B:81:ARG:NH2	2:B:85:HIS:O	2.31	0.64
1:A:347:GLN:HG2	5:A:2024:HOH:O	1.97	0.64
2:B:35:ILE:HB	2:B:36:PRO:HD2	1.80	0.64
2:E:154:ALA:HB3	5:E:2035:HOH:O	1.98	0.64
2:B:101:ASN:C	2:B:102:LYS:O	2.38	0.64
1:A:350:THR:HB	1:A:441:LEU:HD22	1.81	0.63
1:D:350:THR:HB	1:D:441:LEU:HD22	1.79	0.63
1:A:241:PHE:CE1	3:C:3:BMA:H2	2.34	0.63
1:D:241:PHE:CE1	3:F:3:BMA:H2	2.33	0.62
2:B:12:THR:HG21	2:B:49:LEU:HB2	1.80	0.62
2:E:35:ILE:HB	2:E:36:PRO:HD2	1.80	0.62
2:E:38:ASN:ND2	2:E:38:ASN:H	1.98	0.62
1:D:274:LYS:HB3	1:D:324:SER:HB2	1.82	0.61
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.83	0.61
1:A:358:LEU:HD23	1:A:363:VAL:HG11	1.81	0.60
2:B:19:LEU:HD12	2:B:19:LEU:N	2.16	0.60
2:B:62:GLU:HB3	5:B:2013:HOH:O	2.00	0.60
2:B:38:ASN:HD22	2:B:38:ASN:H	1.50	0.59
2:E:3:MET:HB3	2:E:182:LEU:HD13	1.85	0.59
2:B:38:ASN:H	2:B:38:ASN:ND2	2.00	0.58
2:E:154:ALA:CB	5:E:2035:HOH:O	2.51	0.58
1:A:248:LYS:CB	1:A:252:MET:HE2	2.33	0.58
2:E:19:LEU:N	2:E:19:LEU:CD1	2.66	0.58
2:B:153:CYS:O	2:B:154:ALA:CB	2.52	0.57
2:E:101:ASN:C	2:E:102:LYS:O	2.46	0.57
2:E:38:ASN:H	2:E:38:ASN:HD22	1.51	0.57
1:D:254:SER:OG	1:D:255:ARG:NH1	2.38	0.56
2:B:154:ALA:O	2:B:155:PHE:HB2	2.05	0.56
1:A:347:GLN:CG	5:A:2024:HOH:O	2.51	0.56
1:A:241:PHE:CE2	3:C:2:NAG:H4	2.41	0.56
2:E:154:ALA:O	2:E:155:PHE:HB2	2.05	0.56
1:D:358:LEU:HD23	1:D:363:VAL:HG11	1.88	0.56
2:E:38:ASN:HD21	2:E:41:ARG:HH11	1.52	0.56
1:A:266:VAL:HG12	1:A:271:PRO:HA	1.88	0.56
1:D:326:LYS:C	1:D:328:LEU:N	2.64	0.56
1:D:280:ASP:OD2	1:D:317:LYS:HD2	2.06	0.55
1:A:320:LYS:HG3	1:A:334:LYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:HIS:HD2	1:D:431:ALA:H	1.55	0.55
1:D:429:HIS:CD2	1:D:431:ALA:H	2.25	0.55
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.42	0.54
1:D:436:TYR:OH	1:D:438:GLN:NE2	2.37	0.54
2:E:81:ARG:NH2	2:E:85:HIS:O	2.40	0.54
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.42	0.54
2:E:61:TRP:CZ2	2:E:161:PRO:HB3	2.43	0.54
2:E:22:ASP:N	5:E:2004:HOH:O	2.40	0.54
2:E:107:ALA:HB3	2:E:113:THR:HB	1.89	0.53
2:B:28:LEU:HD13	2:B:46:PRO:HB3	1.90	0.53
1:D:266:VAL:HG12	1:D:271:PRO:HA	1.90	0.53
1:A:254:SER:OG	1:A:255:ARG:NH1	2.41	0.53
1:D:252:MET:HA	1:D:428:MET:HE1	1.91	0.52
2:B:63:VAL:N	5:B:2013:HOH:O	2.42	0.52
1:A:436:TYR:OH	1:A:438:GLN:NE2	2.37	0.52
1:A:252:MET:HE3	1:A:255:ARG:CG	2.37	0.52
2:E:3:MET:HE3	2:E:182:LEU:HB3	1.91	0.52
1:A:429:HIS:CD2	1:A:431:ALA:H	2.28	0.52
1:D:240:VAL:HB	1:D:332:ILE:HD11	1.92	0.52
2:E:153:CYS:O	2:E:154:ALA:CB	2.56	0.52
1:A:280:ASP:OD2	1:A:317:LYS:HD2	2.11	0.51
2:B:3:MET:HB3	2:B:182:LEU:HD13	1.91	0.50
2:B:35:ILE:HD12	2:B:41:ARG:CZ	2.42	0.50
1:A:413:ASP:HB2	1:A:416:ARG:HG3	1.94	0.50
1:A:240:VAL:HG13	1:A:262:VAL:O	2.12	0.50
2:B:19:LEU:N	2:B:19:LEU:CD1	2.74	0.50
1:D:241:PHE:CE2	3:F:2:NAG:H4	2.47	0.49
2:B:128:LEU:HD21	2:B:159:LEU:HD12	1.94	0.49
1:A:429:HIS:HD2	1:A:431:ALA:H	1.61	0.49
1:A:308:VAL:HG12	1:A:319:TYR:CE2	2.48	0.49
2:E:28:LEU:HD13	2:E:46:PRO:HB3	1.93	0.49
2:B:3:MET:HB2	2:B:182:LEU:CD1	2.39	0.49
1:A:326:LYS:C	1:A:328:LEU:N	2.66	0.48
1:A:245:PRO:HD2	1:A:313:TRP:CH2	2.48	0.48
2:B:27:ARG:HB3	2:B:176:PRO:HB3	1.95	0.48
1:D:414:LYS:O	1:D:418:GLN:HB2	2.13	0.48
1:D:413:ASP:HB2	1:D:416:ARG:HG3	1.96	0.48
1:D:308:VAL:HG12	1:D:319:TYR:CE2	2.48	0.48
1:A:267:SER:C	1:A:269:GLU:N	2.71	0.48
2:B:99:LEU:HD11	2:B:103:GLN:N	2.29	0.48
2:E:38:ASN:ND2	2:E:41:ARG:HH11	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HG2	1:A:428:MET:CE	2.33	0.47
2:E:35:ILE:HD12	2:E:41:ARG:CZ	2.44	0.47
2:B:107:ALA:HB3	2:B:113:THR:HB	1.95	0.47
1:D:320:LYS:HG3	1:D:334:LYS:O	2.14	0.47
1:A:370:LYS:HB2	1:A:370:LYS:HE3	1.64	0.47
2:B:3:MET:HE3	2:B:182:LEU:HB3	1.97	0.47
1:A:252:MET:HA	1:A:428:MET:CE	2.45	0.46
1:D:252:MET:HA	1:D:428:MET:CE	2.44	0.46
2:E:38:ASN:ND2	2:E:41:ARG:NH1	2.58	0.46
2:B:61:TRP:CZ2	2:B:161:PRO:HB3	2.49	0.46
1:A:252:MET:HA	1:A:428:MET:HE1	1.98	0.46
2:E:3:MET:HB2	2:E:182:LEU:CD1	2.44	0.46
4:D:1451:FUC:H2	3:F:1:NAG:C6	2.46	0.45
2:E:27:ARG:HB3	2:E:176:PRO:HB3	1.98	0.45
1:A:265:ASP:CB	1:A:299:THR:CB	2.90	0.45
2:B:70:ALA:HA	2:B:99:LEU:O	2.16	0.45
1:D:267:SER:C	1:D:269:GLU:N	2.72	0.45
1:D:443:LEU:HB2	5:D:2040:HOH:O	2.15	0.45
2:E:15:PRO:HB2	2:E:32:GLN:HG3	1.99	0.45
2:B:181:PRO:O	2:B:182:LEU:C	2.59	0.44
2:E:10:PRO:O	2:E:41:ARG:NH2	2.51	0.44
1:D:250:THR:HG21	1:D:313:TRP:CD1	2.52	0.44
2:B:180:CYS:HA	2:B:181:PRO:HD3	1.78	0.44
1:D:240:VAL:HG13	1:D:262:VAL:O	2.18	0.44
1:D:295:GLN:O	1:D:298:SER:N	2.51	0.44
1:A:360:LYS:O	1:A:414:LYS:HD3	2.17	0.43
1:A:345:GLU:HA	1:A:346:PRO:HD2	1.86	0.43
2:E:19:LEU:CD1	2:E:19:LEU:H	2.32	0.43
1:D:345:GLU:HA	1:D:346:PRO:HD2	1.81	0.43
1:D:374:PRO:O	1:D:429:HIS:HE1	2.02	0.43
2:E:99:LEU:HD11	2:E:103:GLN:N	2.34	0.43
2:B:42:PHE:CE2	2:B:82:ARG:HD3	2.54	0.43
2:E:70:ALA:HA	2:E:99:LEU:O	2.18	0.43
2:B:15:PRO:HB2	2:B:32:GLN:HG3	2.01	0.42
2:E:35:ILE:HB	2:E:36:PRO:CD	2.48	0.42
2:B:142:ASP:O	2:B:144:GLY:N	2.52	0.42
1:A:357:GLU:C	1:A:359:THR:H	2.28	0.42
2:B:35:ILE:HB	2:B:36:PRO:CD	2.49	0.42
1:D:357:GLU:C	1:D:359:THR:H	2.28	0.42
1:A:295:GLN:O	1:A:298:SER:N	2.53	0.42
2:B:10:PRO:O	2:B:41:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:C	1:A:269:GLU:H	2.28	0.42
2:B:157:GLY:HA3	2:B:158:PRO:HD2	1.86	0.42
1:D:350:THR:HA	1:D:366:THR:O	2.19	0.42
2:E:128:LEU:HD21	2:E:159:LEU:HD12	2.02	0.42
2:E:47:MET:HG2	2:E:164:SER:HB2	2.01	0.41
1:D:252:MET:HG2	1:D:428:MET:CE	2.40	0.41
2:B:101:ASN:ND2	5:B:2018:HOH:O	2.54	0.41
1:A:311:GLN:HG3	1:A:315:ASN:ND2	2.36	0.41
1:A:317:LYS:H	1:A:317:LYS:HG2	1.70	0.40
1:D:360:LYS:O	1:D:414:LYS:HD3	2.21	0.40
1:A:295:GLN:C	1:A:297:ASN:N	2.77	0.40
2:B:97:ILE:HG22	2:B:107:ALA:HA	2.03	0.40
3:C:2:NAG:C8	3:C:4:MAN:O4	2.65	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	196/207 (95%)	184 (94%)	10 (5%)	2 (1%)	12	12
1	D	205/207 (99%)	194 (95%)	9 (4%)	2 (1%)	12	12
2	B	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	7	6
2	E	179/181 (99%)	164 (92%)	12 (7%)	3 (2%)	7	6
All	All	759/776 (98%)	705 (93%)	44 (6%)	10 (1%)	9	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	102	LYS
2	B	143	HIS

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Mol	Chain	Res	Type
2	E	102	LYS
2	E	143	HIS
2	B	154	ALA
2	E	154	ALA
1	A	327	ALA
1	D	327	ALA
1	D	329	PRO
1	A	329	PRO

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	62/193 (32%)	59 (95%)	3 (5%)	23	29
1	D	193/193 (100%)	182 (94%)	11 (6%)	18	23
2	B	158/158 (100%)	143 (90%)	15 (10%)	8	7
2	E	158/158 (100%)	144 (91%)	14 (9%)	9	10
All	All	571/702 (81%)	528 (92%)	43 (8%)	12	13

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

Mol	Chain	Res	Type
1	A	390	ASN
1	A	418	GLN
1	A	426	SER
2	B	7	THR
2	B	8	LEU
2	B	21	GLU
2	B	30	ASP
2	B	33	GLN
2	B	35	ILE
2	B	38	ASN
2	B	103	GLN
2	B	115	LEU
2	B	123	GLN

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Mol	Chain	Res	Type
2	B	135	VAL
2	B	140	ILE
2	B	151	SER
2	B	152	GLU
2	B	172	LYS
1	D	264	VAL
1	D	265	ASP
1	D	283	GLU
1	D	293	GLU
1	D	297	ASN
1	D	302	VAL
1	D	317	LYS
1	D	340	LYS
1	D	344	ARG
1	D	418	GLN
1	D	426	SER
2	E	8	LEU
2	E	19	LEU
2	E	21	GLU
2	E	33	GLN
2	E	38	ASN
2	E	83	LYS
2	E	103	GLN
2	E	115	LEU
2	E	123	GLN
2	E	135	VAL
2	E	140	ILE
2	E	151	SER
2	E	152	GLU
2	E	172	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	A	429	HIS
1	A	434	ASN
1	A	438	GLN
2	B	25	GLN
2	B	33	GLN
2	B	38	ASN
2	B	85	HIS

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Mol	Chain	Res	Type
1	D	342	GLN
1	D	390	ASN
1	D	429	HIS
1	D	434	ASN
1	D	438	GLN
2	E	33	GLN
2	E	38	ASN
2	E	53	HIS

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](#)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	1.31	2 (14%)	17,19,21	2.10	4 (23%)
3	NAG	C	2	3	14,14,15	0.89	0	17,19,21	1.57	4 (23%)
3	BMA	C	3	3	11,11,12	0.89	1 (9%)	15,15,17	1.97	5 (33%)
3	MAN	C	4	3	11,11,12	0.79	0	15,15,17	2.23	7 (46%)
3	NAG	C	5	3	14,14,15	0.70	0	17,19,21	1.57	1 (5%)
3	GAL	C	6	3	11,11,12	0.85	1 (9%)	15,15,17	1.89	4 (26%)
3	MAN	C	7	3	11,11,12	1.74	4 (36%)	15,15,17	2.13	6 (40%)
3	NAG	F	1	3,1	14,14,15	1.09	1 (7%)	17,19,21	2.13	4 (23%)
3	NAG	F	2	3	14,14,15	0.80	0	17,19,21	1.53	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	0.90	1 (9%)	15,15,17	1.75	5 (33%)
3	MAN	F	4	3	11,11,12	0.85	0	15,15,17	1.97	4 (26%)
3	NAG	F	5	3	14,14,15	0.67	0	17,19,21	1.61	2 (11%)
3	GAL	F	6	3	11,11,12	1.05	0	15,15,17	2.12	6 (40%)
3	MAN	F	7	3	11,11,12	1.41	2 (18%)	15,15,17	2.23	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	4/6/23/26	0/1/1/1
3	GAL	C	6	3	-	2/2/19/22	0/1/1/1
3	MAN	C	7	3	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	NAG	F	5	3	-	4/6/23/26	0/1/1/1
3	GAL	F	6	3	-	2/2/19/22	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7	MAN	C2-C3	3.02	1.57	1.52
3	C	7	MAN	C4-C5	2.73	1.58	1.53
3	C	1	NAG	C1-C2	2.62	1.55	1.52
3	F	7	MAN	C2-C3	2.57	1.56	1.52
3	C	7	MAN	C4-C3	2.32	1.58	1.52
3	F	7	MAN	C4-C3	2.30	1.58	1.52
3	C	6	GAL	C1-C2	2.24	1.57	1.52
3	C	3	BMA	O5-C1	2.21	1.47	1.43
3	F	1	NAG	C1-C2	2.13	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C8-C7	2.12	1.54	1.50
3	C	7	MAN	C1-C2	2.07	1.57	1.52
3	F	3	BMA	O5-C1	2.02	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	MAN	C1-O5-C5	5.46	119.51	112.19
3	F	5	NAG	C1-O5-C5	5.39	119.41	112.19
3	C	5	NAG	C1-O5-C5	5.04	118.94	112.19
3	C	6	GAL	O2-C2-C1	4.75	120.11	109.22
3	C	1	NAG	O4-C4-C5	-4.72	97.69	109.32
3	F	1	NAG	O4-C4-C5	-4.68	97.79	109.32
3	C	7	MAN	C1-O5-C5	4.65	118.42	112.19
3	C	1	NAG	O5-C5-C6	4.65	116.71	107.66
3	F	6	GAL	O2-C2-C1	4.54	119.61	109.22
3	F	1	NAG	O5-C5-C6	4.48	116.38	107.66
3	C	3	BMA	O3-C3-C4	-4.44	99.91	110.38
3	F	7	MAN	C1-C2-C3	-4.35	103.30	109.64
3	F	4	MAN	C2-C3-C4	4.11	118.09	110.86
3	C	7	MAN	C1-C2-C3	-4.04	103.76	109.64
3	C	4	MAN	O3-C3-C4	-3.82	101.36	110.38
3	C	2	NAG	C8-C7-N2	3.71	122.27	116.12
3	C	4	MAN	C2-C3-C4	3.70	117.36	110.86
3	F	3	BMA	O3-C3-C4	-3.59	101.91	110.38
3	F	6	GAL	O5-C5-C6	3.41	114.29	107.66
3	F	2	NAG	O7-C7-C8	-3.36	116.07	122.05
3	F	1	NAG	C1-C2-N2	3.35	115.71	110.43
3	F	2	NAG	C8-C7-N2	3.31	121.61	116.12
3	F	6	GAL	C2-C3-C4	3.26	116.60	110.86
3	C	4	MAN	C1-O5-C5	3.15	116.41	112.19
3	F	2	NAG	C4-C3-C2	3.08	115.54	111.02
3	C	3	BMA	O5-C5-C6	3.03	113.55	107.66
3	F	1	NAG	O3-C3-C4	3.01	117.47	110.38
3	C	2	NAG	O7-C7-C8	-3.00	116.71	122.05
3	C	2	NAG	C4-C3-C2	2.94	115.33	111.02
3	C	1	NAG	O3-C3-C4	2.91	117.24	110.38
3	C	7	MAN	O2-C2-C3	2.87	116.10	110.15
3	F	7	MAN	O2-C2-C3	2.84	116.03	110.15
3	F	4	MAN	O3-C3-C4	-2.81	103.75	110.38
3	C	3	BMA	O6-C6-C5	-2.80	101.81	111.33
3	C	1	NAG	C1-C2-N2	2.77	114.81	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	GAL	O6-C6-C5	-2.75	101.95	111.33
3	F	3	BMA	C1-C2-C3	2.71	113.58	109.64
3	F	6	GAL	O4-C4-C3	2.68	116.70	110.38
3	F	3	BMA	O5-C5-C6	2.68	112.88	107.66
3	F	4	MAN	C1-C2-C3	2.65	113.50	109.64
3	C	4	MAN	C1-C2-C3	2.62	113.46	109.64
3	C	6	GAL	O5-C5-C6	2.52	112.58	107.66
3	C	4	MAN	O6-C6-C5	-2.52	102.76	111.33
3	C	3	BMA	C3-C4-C5	2.49	114.75	110.23
3	F	3	BMA	O6-C6-C5	-2.47	102.93	111.33
3	C	6	GAL	O6-C6-C5	-2.42	103.09	111.33
3	C	4	MAN	O5-C1-C2	-2.42	105.02	110.79
3	C	7	MAN	O2-C2-C1	2.41	114.73	109.22
3	C	6	GAL	C2-C3-C4	2.34	114.98	110.86
3	F	6	GAL	C1-O5-C5	-2.33	109.06	112.19
3	F	4	MAN	O5-C1-C2	-2.32	105.24	110.79
3	C	3	BMA	C1-C2-C3	2.31	113.00	109.64
3	C	4	MAN	O5-C5-C4	2.29	116.41	110.83
3	F	7	MAN	C2-C3-C4	2.22	114.76	110.86
3	F	3	BMA	C3-C4-C5	2.18	114.18	110.23
3	C	2	NAG	C2-N2-C7	-2.10	120.08	122.90
3	C	7	MAN	O3-C3-C4	2.09	115.30	110.38
3	C	7	MAN	C2-C3-C4	2.09	114.53	110.86
3	F	5	NAG	C4-C3-C2	2.07	114.05	111.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	NAG	O7-C7-N2-C2
3	F	5	NAG	O7-C7-N2-C2
3	C	5	NAG	C8-C7-N2-C2
3	F	5	NAG	C8-C7-N2-C2
3	F	7	MAN	O5-C5-C6-O6
3	C	7	MAN	O5-C5-C6-O6
3	F	6	GAL	C4-C5-C6-O6
3	C	6	GAL	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	7	MAN	C4-C5-C6-O6
3	F	6	GAL	O5-C5-C6-O6
3	C	6	GAL	O5-C5-C6-O6
3	F	5	NAG	C4-C5-C6-O6
3	C	5	NAG	C4-C5-C6-O6
3	C	5	NAG	O5-C5-C6-O6
3	F	5	NAG	O5-C5-C6-O6

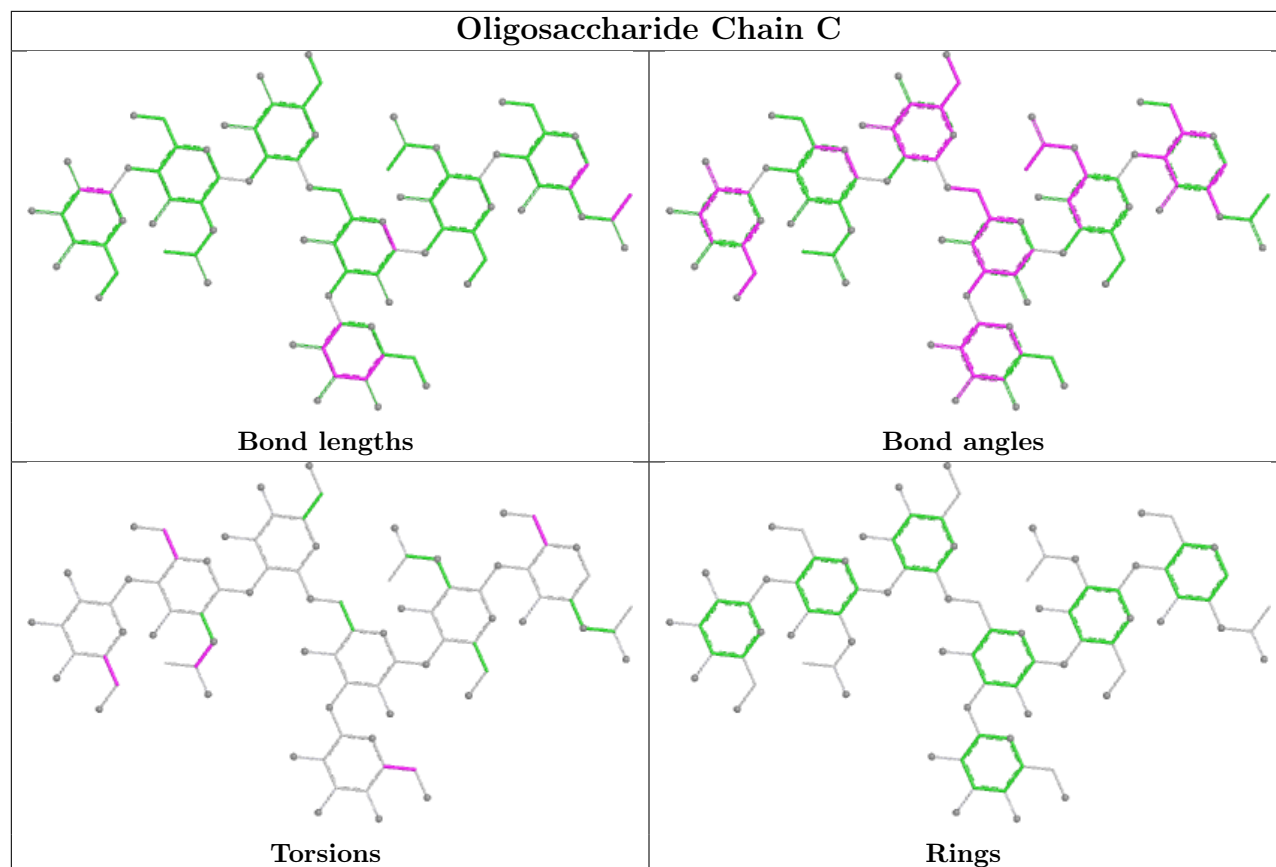
There are no ring outliers.

8 monomers are involved in 12 short contacts:

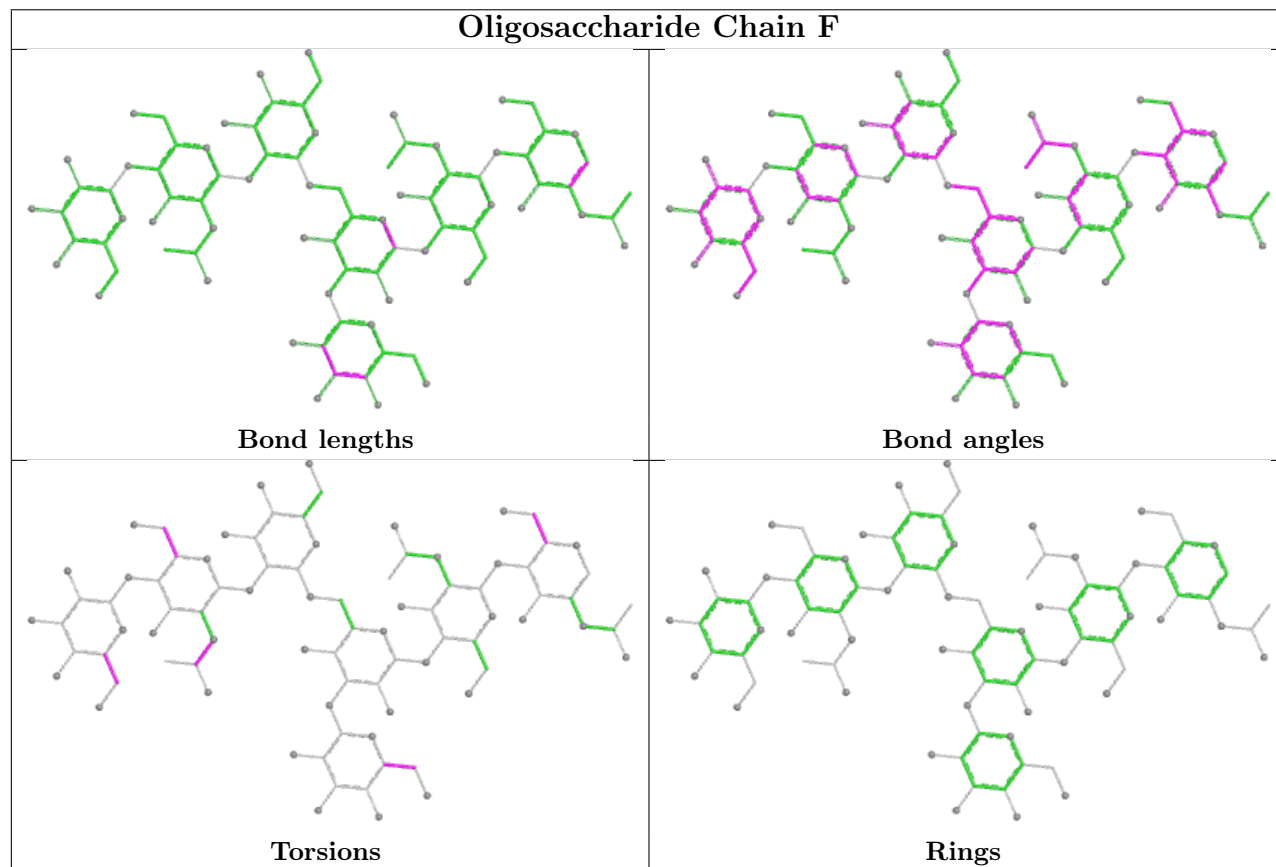
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	F	4	MAN	1	0
3	C	3	BMA	1	0
3	C	4	MAN	2	0
3	F	2	NAG	3	0
3	C	1	NAG	1	0
3	C	2	NAG	4	0
3	F	3	BMA	1	0

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

Oligosaccharide Chain C



Oligosaccharide Chain F



5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	D	1451	-	10,10,11	1.52	3 (30%)	14,14,16	2.36	7 (50%)
4	FUC	A	1451	-	10,10,11	1.77	4 (40%)	14,14,16	2.40	4 (28%)

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	FUC	D	1451	-	-	-	0/1/1/1
4	FUC	A	1451	-	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1451	FUC	C1-C2	2.58	1.58	1.52
4	A	1451	FUC	O5-C5	2.56	1.48	1.43
4	A	1451	FUC	C2-C3	2.52	1.56	1.52
4	A	1451	FUC	C6-C5	2.43	1.57	1.51
4	D	1451	FUC	O5-C5	2.29	1.48	1.43
4	D	1451	FUC	C2-C3	2.16	1.55	1.52
4	D	1451	FUC	C6-C5	2.14	1.56	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1451	FUC	C1-C2-C3	6.47	119.07	109.64
4	D	1451	FUC	C1-C2-C3	6.38	118.93	109.64
4	A	1451	FUC	O5-C5-C6	3.88	115.83	107.40
4	D	1451	FUC	O5-C5-C6	3.18	114.30	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1451	FUC	C6-C5-C4	2.45	117.56	113.08
4	D	1451	FUC	O4-C4-C5	2.24	114.68	109.74
4	D	1451	FUC	O3-C3-C2	-2.21	105.53	110.05
4	D	1451	FUC	C6-C5-C4	2.20	117.10	113.08
4	D	1451	FUC	O2-C2-C3	-2.16	105.67	110.15
4	A	1451	FUC	C3-C4-C5	-2.12	106.59	109.81
4	D	1451	FUC	C3-C4-C5	-2.10	106.62	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1451	FUC	3	0
4	A	1451	FUC	2	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	207/207 (100%)	0.89	33 (15%) 5 5	48, 78, 90, 90	0
1	D	207/207 (100%)	0.86	25 (12%) 8 10	48, 78, 90, 90	0
2	B	181/181 (100%)	0.41	5 (2%) 55 61	48, 64, 82, 89	0
2	E	181/181 (100%)	0.42	3 (1%) 69 74	49, 64, 82, 89	0
All	All	776/776 (100%)	0.66	66 (8%) 16 18	48, 70, 90, 90	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TYR	4.5
1	D	296	TYR	4.4
2	B	3	MET	4.2
1	A	253	ILE	3.9
1	D	253	ILE	3.5
1	D	282	VAL	3.3
1	A	298	SER	3.2
1	A	239	SER	3.2
1	D	323	VAL	3.1
1	A	336	ILE	3.1
2	E	3	MET	3.1
1	D	239	SER	3.1
2	E	152	GLU	3.0
2	E	182	LEU	2.9
1	A	282	VAL	2.9
1	D	299	THR	2.9
1	D	336	ILE	2.9
1	D	265	ASP	2.8
1	D	238	PRO	2.8
1	A	299	THR	2.8
1	A	252	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	330	ALA	2.7
1	A	329	PRO	2.6
1	A	238	PRO	2.6
1	D	330	ALA	2.6
1	A	323	VAL	2.6
2	B	182	LEU	2.5
1	A	327	ALA	2.5
1	D	291	PRO	2.5
1	D	300	TYR	2.5
1	D	327	ALA	2.4
1	D	298	SER	2.4
1	A	265	ASP	2.3
1	A	332	ILE	2.3
2	B	152	GLU	2.3
1	A	300	TYR	2.3
1	D	255	ARG	2.3
1	A	324	SER	2.3
1	D	294	GLU	2.3
1	A	266	VAL	2.3
1	A	303	VAL	2.2
1	A	359	THR	2.2
2	B	154	ALA	2.2
1	A	328	LEU	2.2
1	A	384	ASN	2.2
2	B	116	HIS	2.2
1	A	289	THR	2.2
1	D	305	VAL	2.2
1	A	331	PRO	2.2
1	D	329	PRO	2.2
1	A	307	THR	2.2
1	D	332	ILE	2.1
1	D	273	VAL	2.1
1	A	237	GLY	2.1
1	D	252	MET	2.1
1	D	303	VAL	2.1
1	A	358	LEU	2.1
1	A	241	PHE	2.1
1	A	256	THR	2.1
1	A	269	GLU	2.1
1	A	294	GLU	2.1
1	D	264	VAL	2.1
1	D	237	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	2.0
1	A	302	VAL	2.0
1	D	389	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

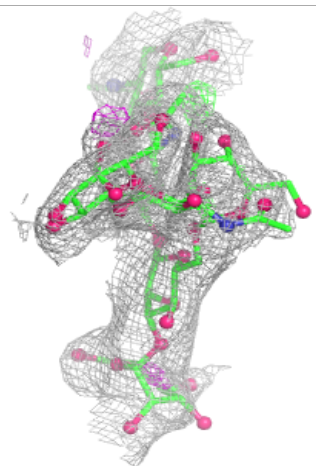
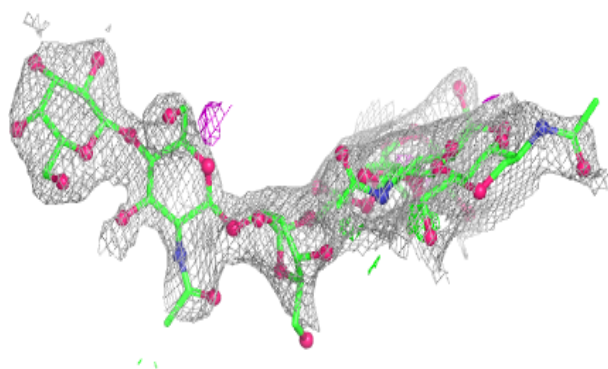
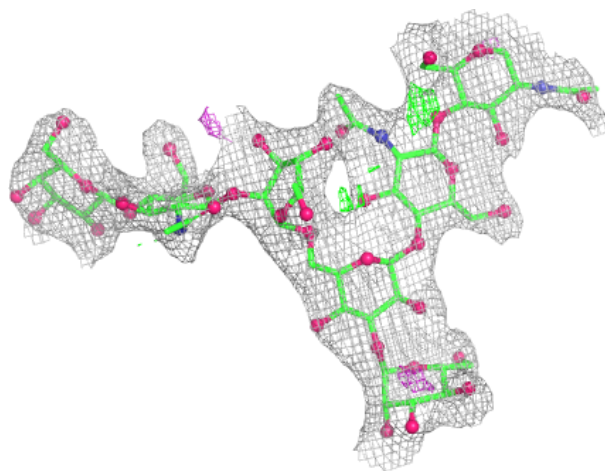
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

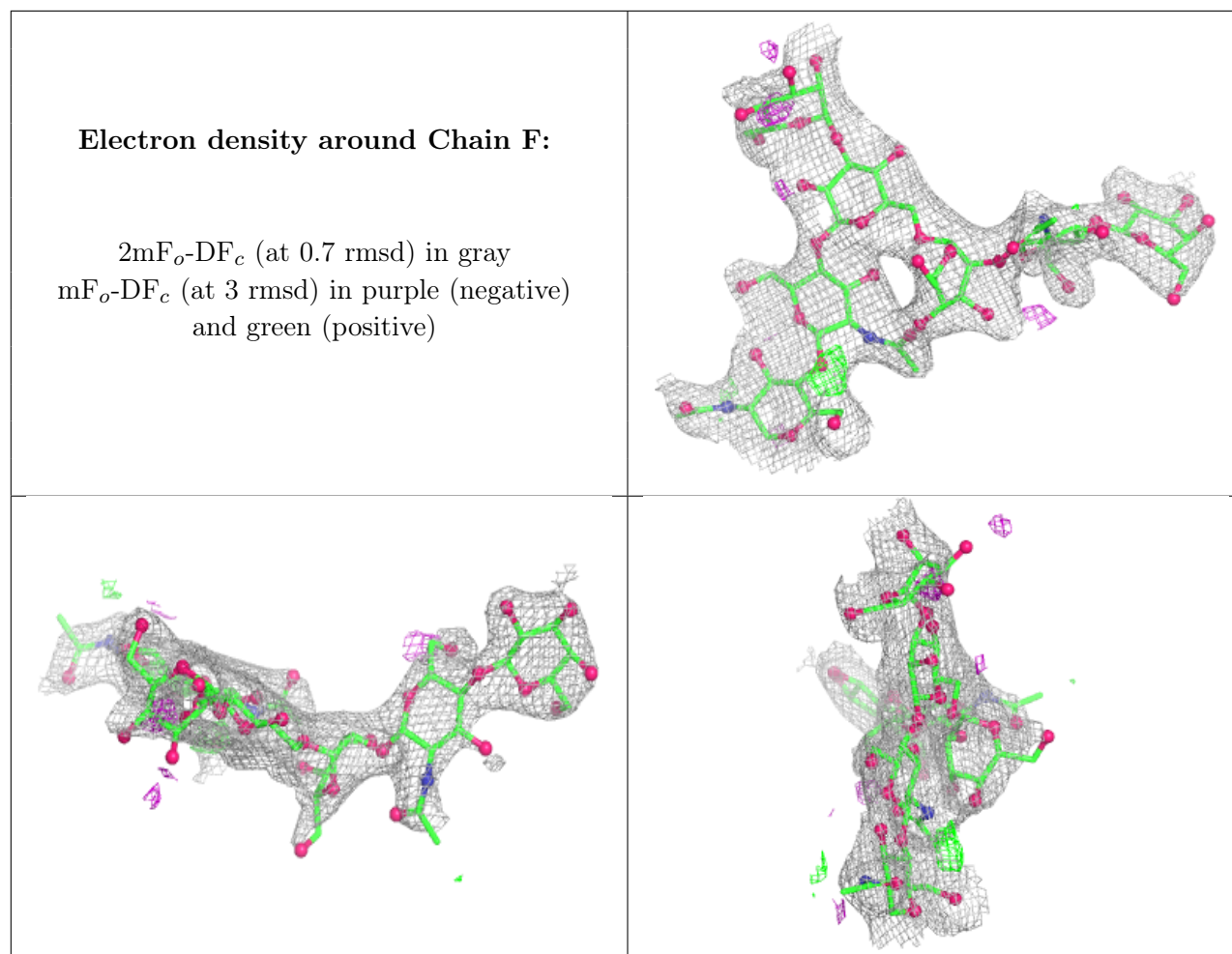
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	87,90,90,90	0
3	NAG	C	2	14/15	-	-	88,89,90,90	0
3	BMA	C	3	11/12	-	-	88,89,90,90	0
3	MAN	C	4	11/12	-	-	89,90,90,90	0
3	NAG	C	5	14/15	-	-	76,87,90,90	0
3	GAL	C	6	11/12	-	-	83,85,90,90	0
3	MAN	C	7	11/12	-	-	89,90,90,90	0
3	MAN	F	7	11/12	0.64	0.18	89,90,90,90	0
3	MAN	F	4	11/12	0.84	0.15	89,90,90,90	0
3	NAG	F	5	14/15	0.88	0.16	76,88,90,90	0
3	BMA	F	3	11/12	0.88	0.11	88,89,90,90	0
3	NAG	F	1	14/15	0.89	0.13	87,90,90,90	0
3	NAG	F	2	14/15	0.93	0.11	88,89,90,90	0
3	GAL	F	6	11/12	0.95	0.10	83,85,90,90	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 C:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
4	FUC	D	1451	10/11	0.81	0.17	89,90,90,90	0
4	FUC	A	1451	10/11	0.82	0.17	89,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.