



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:08 PM UTC

PDB ID : 1GXS / pdb_00001gxs
Title : Crystal Structure of Hydroxynitrile Lyase from Sorghum bicolor in Complex with Inhibitor Benzoic Acid: a novel cyanogenic enzyme
Authors : Lauble, H.; Miehlisch, B.; Foerster, S.; Wajant, H.; Effenberger, F.
Deposited on : 2002-04-11
Resolution : 2.30 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:

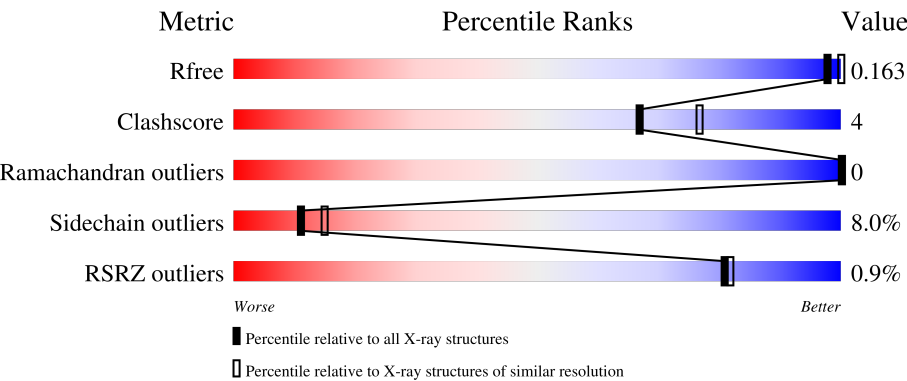
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	270	% 76%19%..
1	C	270	% 74%19%..
2	B	158	70%25%..
2	D	158	68%25%6%.
3	E	3	33%33%33%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 33% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7225 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 P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2120	1347	356	406	11			
1	C	267	Total	C	N	O	S	0	0	0
			2120	1347	356	406	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	LEU	PRO	variant	UNP Q8W4X3
A	79	ALA	PRO	variant	UNP Q8W4X3
A	112	GLY	VAL	variant	UNP Q8W4X3
A	203	SER	LEU	variant	UNP Q8W4X3
C	11	LEU	PRO	variant	UNP Q8W4X3
C	79	ALA	PRO	variant	UNP Q8W4X3
C	112	GLY	VAL	variant	UNP Q8W4X3
C	203	SER	LEU	variant	UNP Q8W4X3

- Molecule 2 is a protein called P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	158	Total	C	N	O	S	0	0	0
			1254	815	206	229	4			
2	D	158	Total	C	N	O	S	0	0	0
			1254	815	206	229	4			

There are 6 discrepancies between the modelled and reference sequences:

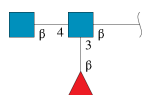
Chain	Residue	Modelled	Actual	Comment	Reference
B	408	THR	SER	variant	UNP Q8W4X3
B	409	VAL	PRO	variant	UNP Q8W4X3
B	410	ARG	SER	variant	UNP Q8W4X3
D	408	THR	SER	variant	UNP Q8W4X3

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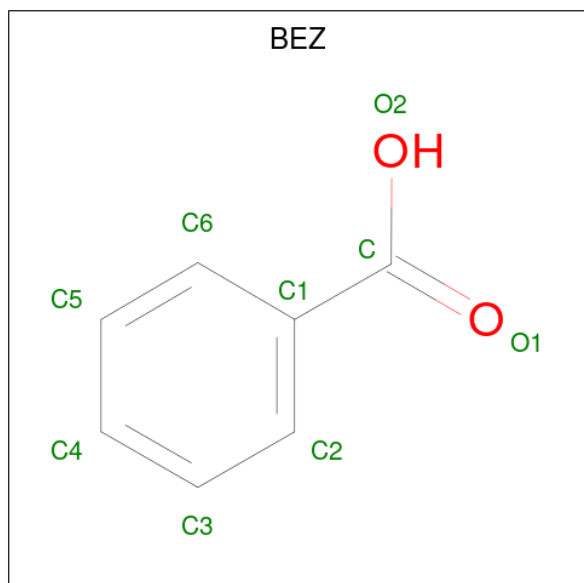
Chain	Residue	Modelled	Actual	Comment	Reference
D	409	VAL	PRO	variant	UNP Q8W4X3
D	410	ARG	SER	variant	UNP Q8W4X3

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



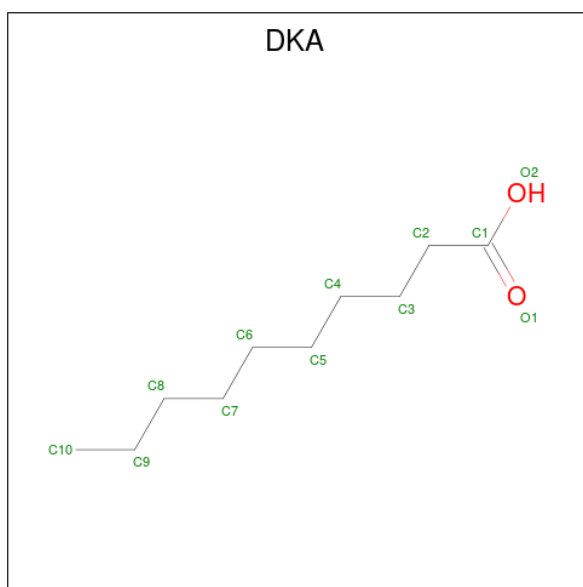
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is BENZOIC ACID (CCD ID: BEZ) (formula: C₇H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	7	2		
4	C	1	Total	C	O	0	0
			9	7	2		

- Molecule 5 is DECANOIC ACID (CCD ID: DKA) (formula: C₁₀H₂₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	10	2		
5	C	1	Total	C	O	0	0
			12	10	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

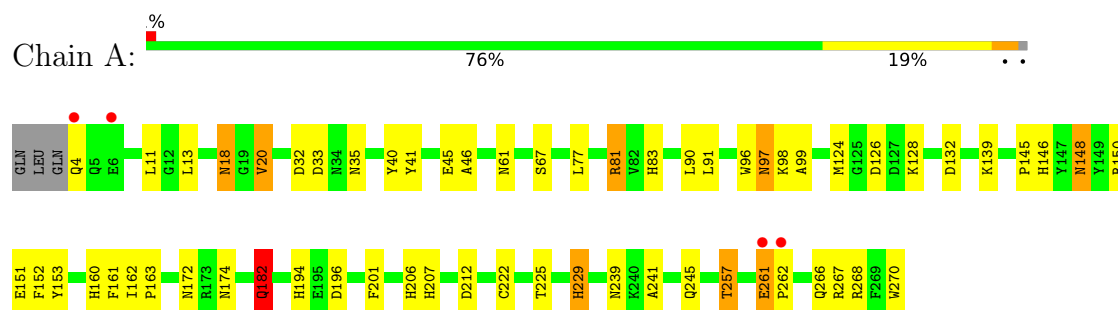
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total	O	0	0
			91	91		
7	B	73	Total	O	0	0
			73	73		
7	C	96	Total	O	0	0
			96	96		
7	D	71	Total	O	0	0
			71	71		

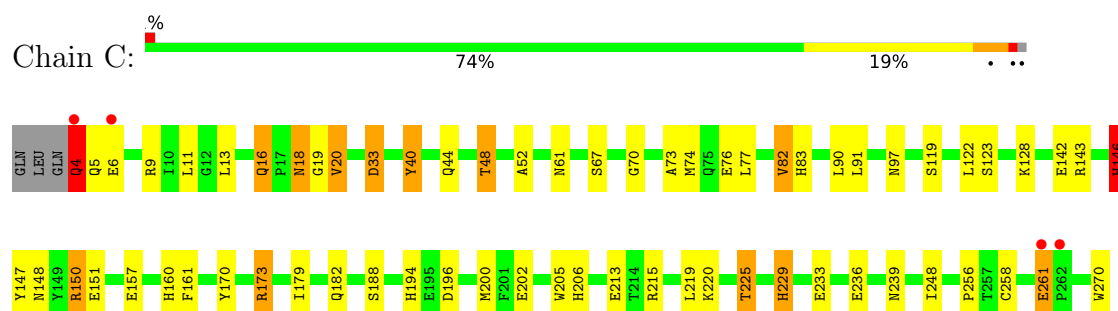
3 Residue-property plots [i](#)

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.

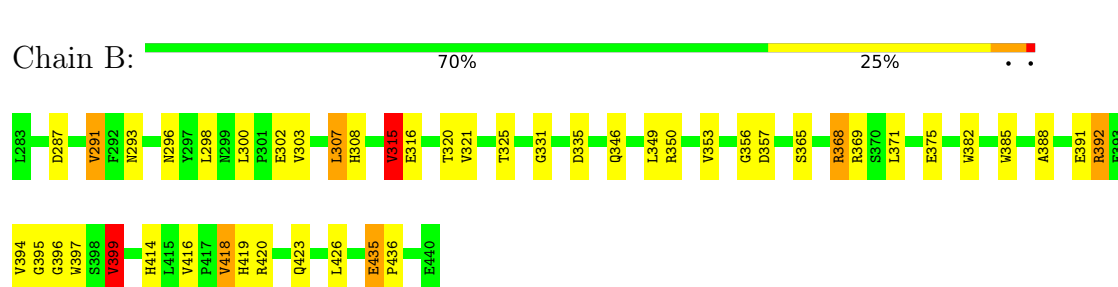
• Molecule 1: P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN A



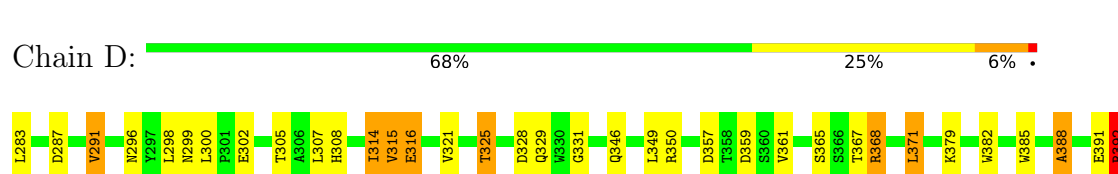
• Molecule 1: P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN A

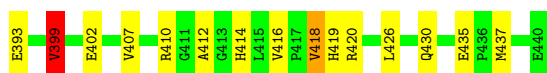


• Molecule 2: P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN B

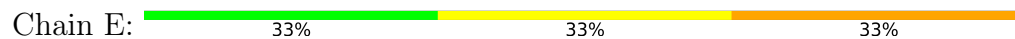


• Molecule 2: P-(S)-HYDROXYMANDELONITRILE LYASE CHAIN B

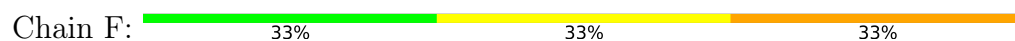




- Molecule 3: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-L-fucopyranose-(1-3)-[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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.70Å 103.70Å 90.60Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 8.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	85.2 (8.00-2.30) 86.0 (8.00-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.13 (at 2.32Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.165 , 0.222 0.164 , 0.163	Depositor DCC
R_{free} test set	2624 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.09	8/2187 (0.4%)	1.80	46/2978 (1.5%)
1	C	1.14	10/2187 (0.5%)	1.83	45/2978 (1.5%)
2	B	1.15	7/1296 (0.5%)	1.90	35/1781 (2.0%)
2	D	1.21	5/1296 (0.4%)	1.88	34/1781 (1.9%)
All	All	1.14	30/6966 (0.4%)	1.84	160/9518 (1.7%)

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	2
1	C	0	1
All	All	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	416	VAL	CA-CB	11.49	1.60	1.54
2	D	315	VAL	CA-CB	10.43	1.66	1.54
2	B	418	VAL	CA-CB	9.09	1.66	1.54
2	B	416	VAL	CA-CB	8.68	1.58	1.54
2	D	418	VAL	CA-CB	8.55	1.65	1.54
2	B	315	VAL	CA-CB	7.41	1.63	1.54
1	A	229	HIS	CD2-NE2	-7.18	1.29	1.37
1	C	20	VAL	CA-CB	7.17	1.62	1.54
1	C	179	ILE	CA-CB	7.02	1.61	1.53
1	A	20	VAL	CA-CB	6.71	1.63	1.54
2	D	419	HIS	CD2-NE2	-6.65	1.30	1.37
2	B	308	HIS	CD2-NE2	-6.58	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	321	VAL	CA-CB	6.45	1.62	1.54
1	C	146	HIS	CD2-NE2	-6.26	1.30	1.37
2	B	419	HIS	CD2-NE2	-6.19	1.31	1.37
1	C	82	VAL	CA-CB	6.18	1.62	1.54
1	A	83	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	207	HIS	CD2-NE2	-6.01	1.31	1.37
2	D	325	THR	CA-CB	5.98	1.62	1.53
1	A	194	HIS	CD2-NE2	-5.81	1.31	1.37
1	C	83	HIS	CD2-NE2	-5.73	1.31	1.37
1	C	229	HIS	CD2-NE2	-5.67	1.31	1.37
1	C	40	TYR	CA-CB	5.58	1.61	1.53
1	A	160	HIS	CD2-NE2	-5.52	1.31	1.37
2	B	414	HIS	CD2-NE2	-5.51	1.31	1.37
1	C	194	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	146	HIS	CD2-NE2	-5.31	1.32	1.37
1	C	248	ILE	CA-CB	5.14	1.61	1.54
1	C	160	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	83	HIS	CG-ND1	-5.08	1.32	1.38

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	GLN	N-CA-C	11.88	124.22	111.28
2	B	399	VAL	CB-CA-C	-11.47	92.83	110.50
1	A	18	ASN	N-CA-C	11.14	125.97	112.38
2	B	291	VAL	CB-CA-C	-11.06	97.55	112.04
2	D	399	VAL	CB-CA-C	-10.82	93.84	110.50
2	D	291	VAL	CB-CA-C	-10.05	94.80	111.29
1	A	212	ASP	CA-CB-CG	9.54	122.14	112.60
1	A	148	ASN	CA-CB-CG	9.46	122.06	112.60
1	A	161	PHE	CA-CB-CG	8.77	122.57	113.80
1	C	18	ASN	N-CA-C	8.42	120.53	111.36
2	B	291	VAL	N-CA-CB	8.35	120.90	110.47
1	A	148	ASN	OD1-CG-ND2	-8.23	114.37	122.60
1	C	97	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	C	48	THR	N-CA-CB	-8.16	98.67	111.56
1	A	225	THR	CA-CB-OG1	-7.97	97.64	109.60
2	B	399	VAL	N-CA-CB	7.92	124.43	111.44
2	D	399	VAL	N-CA-CB	7.62	123.93	111.44
1	C	148	ASN	OD1-CG-ND2	-7.35	115.25	122.60
2	D	419	HIS	CB-CG-CD2	-7.33	121.67	131.20
2	B	423	GLN	OE1-CD-NE2	-7.22	115.38	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	SER	N-CA-C	7.22	121.23	109.76
1	C	18	ASN	CA-CB-CG	-7.21	105.39	112.60
1	A	67	SER	N-CA-C	7.11	120.13	109.25
1	C	97	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	35	ASN	OD1-CG-ND2	-6.98	115.62	122.60
2	D	291	VAL	N-CA-CB	6.97	122.72	111.23
2	D	308	HIS	CA-CB-CG	6.96	120.75	113.80
1	C	73	ALA	N-CA-C	6.95	118.64	111.14
1	A	261	GLU	N-CA-C	6.92	123.08	113.45
1	C	261	GLU	N-CA-C	6.70	124.62	109.81
2	D	296	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	C	225	THR	N-CA-CB	-6.64	100.87	110.36
2	B	414	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	148	ASN	CB-CG-ND2	6.60	126.30	116.40
1	C	119	SER	N-CA-C	6.52	118.39	111.28
1	C	4	GLN	CB-CG-CD	6.49	123.63	112.60
1	A	207	HIS	CB-CG-CD2	-6.46	122.81	131.20
2	B	357	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	4	GLN	OE1-CD-NE2	-6.38	116.22	122.60
2	D	350	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	C	16	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	A	98	LYS	CA-CB-CG	-6.28	101.54	114.10
2	D	414	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	A	126	ASP	N-CA-C	6.26	117.77	111.07
1	A	45	GLU	CA-CB-CG	-6.23	101.64	114.10
1	C	147	TYR	N-CA-C	-6.21	105.35	113.17
2	D	316	GLU	CB-CG-CD	6.21	123.15	112.60
1	C	182	GLN	OE1-CD-NE2	-6.19	116.41	122.60
2	B	356	GLY	O-C-N	-6.19	117.04	123.48
2	D	407	VAL	O-C-N	-6.18	116.53	123.20
2	D	368	ARG	NE-CZ-NH2	-6.17	113.65	119.20
2	B	435	GLU	CA-C-N	6.17	126.13	120.03
2	B	435	GLU	C-N-CA	6.17	126.13	120.03
1	A	196	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	32	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	132	ASP	CA-CB-CG	6.04	118.64	112.60
2	B	419	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	266	GLN	OE1-CD-NE2	-6.01	116.59	122.60
2	B	385	TRP	CG-CD2-CE3	6.00	139.90	133.90
2	B	293	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	33	ASP	N-CA-C	5.94	117.84	111.36
2	B	296	ASN	OD1-CG-ND2	-5.92	116.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	416	VAL	N-CA-CB	-5.89	106.57	110.52
2	D	314	ILE	O-C-N	-5.88	115.96	121.90
2	D	321	VAL	CB-CA-C	-5.86	104.14	112.22
2	B	396	GLY	CA-C-O	-5.84	115.70	121.48
1	A	61	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	139	LYS	CA-CB-CG	5.84	125.78	114.10
2	B	397	TRP	CB-CG-CD1	-5.82	118.18	126.90
2	D	296	ASN	CB-CG-ND2	5.81	125.12	116.40
1	C	239	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	225	THR	CA-CB-CG2	5.80	120.36	110.50
2	B	397	TRP	CG-CD2-CE3	5.80	139.70	133.90
1	C	61	ASN	OD1-CG-ND2	-5.79	116.81	122.60
2	B	388	ALA	CA-C-N	5.79	125.46	119.56
2	B	388	ALA	C-N-CA	5.79	125.46	119.56
2	B	353	VAL	O-C-N	-5.78	116.92	123.10
1	C	194	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	229	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	C	148	ASN	CA-CB-CG	5.73	118.33	112.60
1	C	6	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	257	THR	N-CA-CB	-5.72	101.08	110.41
2	D	392	ARG	N-CA-C	5.72	120.40	112.45
1	A	194	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	A	182	GLN	N-CA-CB	-5.63	103.10	110.59
1	A	222	CYS	N-CA-C	5.63	122.25	109.81
1	A	33	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	152	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	97	ASN	CB-CG-ND2	5.59	124.78	116.40
1	A	172	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	C	44	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	C	205	TRP	CG-CD2-CE3	5.56	139.46	133.90
1	C	161	PHE	N-CA-C	5.52	117.30	111.28
2	D	437	MET	CG-SD-CE	5.50	112.99	100.90
2	D	357	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	205	TRP	CB-CG-CD1	-5.48	118.68	126.90
2	D	399	VAL	N-CA-C	-5.47	100.31	108.46
2	D	416	VAL	CA-C-O	-5.47	115.03	118.69
1	A	239	ASN	CA-CB-CG	5.46	118.06	112.60
1	A	146	HIS	CB-CG-CD2	-5.45	124.11	131.20
2	B	320	THR	CA-CB-OG1	-5.44	101.44	109.60
2	D	329	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	C	70	GLY	O-C-N	5.43	127.41	122.19
1	C	236	GLU	N-CA-CB	-5.43	102.14	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	388	ALA	O-C-N	-5.38	118.06	121.88
1	A	174	ASN	OD1-CG-ND2	-5.38	117.22	122.60
2	B	303	VAL	N-CA-C	-5.38	105.47	110.53
2	B	385	TRP	CB-CG-CD1	-5.38	118.83	126.90
2	B	399	VAL	N-CA-C	-5.38	100.45	108.46
1	C	215	ARG	NE-CZ-NH2	-5.36	114.37	119.20
2	D	299	ASN	OD1-CG-ND2	-5.36	117.24	122.60
2	D	305	THR	CA-CB-OG1	-5.35	101.58	109.60
2	D	359	ASP	CA-C-O	-5.34	114.61	120.69
1	C	157	GLU	N-CA-C	5.33	118.85	111.55
1	C	4	GLN	CG-CD-NE2	5.30	124.35	116.40
2	B	346	GLN	OE1-CD-NE2	-5.30	117.30	122.60
2	D	430	GLN	OE1-CD-NE2	-5.28	117.32	122.60
2	D	388	ALA	CA-C-N	5.26	125.07	119.28
2	D	388	ALA	C-N-CA	5.26	125.07	119.28
1	C	258	CYS	CA-C-O	5.25	126.59	120.49
2	B	335	ASP	CA-CB-CG	5.25	117.85	112.60
2	B	296	ASN	CB-CG-ND2	5.24	124.26	116.40
2	B	385	TRP	CE2-CD2-CG	-5.23	100.93	107.20
1	C	4	GLN	CA-C-O	-5.21	111.94	120.80
1	C	76	GLU	N-CA-C	5.20	118.92	111.02
1	C	202	GLU	CA-CB-CG	-5.19	103.72	114.10
1	A	97	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	268	ARG	CB-CA-C	-5.18	103.95	112.03
2	D	346	GLN	OE1-CD-NE2	-5.17	117.43	122.60
2	D	385	TRP	CA-CB-CG	5.16	123.41	113.60
2	D	402	GLU	CA-CB-CG	5.15	124.40	114.10
1	C	33	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	222	CYS	O-C-N	-5.14	115.41	121.32
2	D	328	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	270	TRP	CE2-CD2-CG	-5.13	101.05	107.20
2	B	397	TRP	CE2-CD2-CG	-5.12	101.05	107.20
2	D	392	ARG	CB-CG-CD	5.12	123.08	111.30
1	A	201	PHE	CA-CB-CG	-5.12	108.68	113.80
2	B	395	GLY	N-CA-C	-5.12	108.32	114.66
1	C	233	GLU	CB-CG-CD	5.12	121.30	112.60
2	D	287	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	196	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	19	GLY	CA-C-N	-5.10	116.50	122.93
1	C	19	GLY	C-N-CA	-5.10	116.50	122.93
2	B	394	VAL	O-C-N	-5.10	117.47	122.67
2	B	350	ARG	NE-CZ-NH1	5.09	126.59	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	CA-C-O	-5.08	115.69	121.58
2	B	368	ARG	NE-CZ-NH2	-5.07	114.63	119.20
1	A	96	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	A	150	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	A	222	CYS	CA-C-N	5.04	125.28	119.83
1	A	222	CYS	C-N-CA	5.04	125.28	119.83
1	C	270	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	270	TRP	CG-CD2-CE3	5.03	138.93	133.90
2	B	287	ASP	CA-C-O	-5.02	115.68	119.59
1	C	151	GLU	CA-CB-CG	5.01	124.13	114.10
1	C	256	PRO	CA-C-N	5.01	128.81	120.94
1	C	256	PRO	C-N-CA	5.01	128.81	120.94
1	A	81	ARG	N-CA-C	-5.01	101.76	109.52
1	A	99	ALA	O-C-N	-5.01	116.19	122.35

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	TYR	Sidechain
1	A	41	TYR	Sidechain
1	C	40	TYR	Sidechain

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	2120	0	1951	15	0
1	C	2120	0	1951	13	0
2	B	1254	0	1213	10	0
2	D	1254	0	1213	14	0
3	E	38	0	34	1	0
3	F	38	0	34	2	0
4	A	9	0	5	0	0
4	C	9	0	5	0	0
5	A	12	0	19	0	0
5	C	12	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	1	0
6	D	14	0	13	0	0
7	A	91	0	0	4	0
7	B	73	0	0	1	0
7	C	96	0	0	5	0
7	D	71	0	0	0	0
All	All	7225	0	6470	49	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 4.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLN:HG3	1:C:143:ARG:HG3	1.63	0.80
2:D:392:ARG:HE	2:D:393:GLU:H	1.41	0.69
2:B:392:ARG:HE	2:B:392:ARG:H	1.42	0.67
3:E:2:FUL:H5	3:E:3:NAG:H2	1.79	0.64
1:A:229:HIS:HE1	2:B:331:GLY:O	1.80	0.63
1:C:229:HIS:HE1	2:D:331:GLY:O	1.84	0.60
1:A:206:HIS:HD2	2:D:365:SER:OG	1.88	0.57
1:C:142:GLU:HG3	7:C:2048:HOH:O	2.05	0.56
1:C:206:HIS:HE1	7:C:2065:HOH:O	1.87	0.56
2:D:388:ALA:HB3	2:D:391:GLU:HG2	1.87	0.55
1:A:261:GLU:HG3	1:A:262:PRO:HD3	1.88	0.55
1:A:124:MET:HE1	1:A:128:LYS:HZ2	1.73	0.54
3:F:2:FUL:H5	3:F:3:NAG:H2	1.89	0.54
1:A:13:LEU:HD21	2:B:307:LEU:HD13	1.90	0.54
1:A:124:MET:HE1	1:A:128:LYS:NZ	2.22	0.54
2:D:382:TRP:CE3	2:D:399:VAL:HG22	2.43	0.53
1:C:146:HIS:HB3	7:C:2049:HOH:O	2.07	0.53
2:D:412:ALA:HB2	2:D:420:ARG:HG3	1.92	0.51
2:B:391:GLU:HA	2:B:392:ARG:HH21	1.76	0.51
1:A:145:PRO:HA	1:A:148:ASN:ND2	2.26	0.51
1:A:153:TYR:CE1	1:A:182:GLN:HB3	2.47	0.50
7:A:2062:HOH:O	2:D:368:ARG:HD2	2.12	0.49
2:D:392:ARG:HE	2:D:393:GLU:N	2.11	0.48
1:C:74:MET:HE2	1:C:82:VAL:CG2	2.44	0.48
2:B:325:THR:HG23	7:B:2023:HOH:O	2.13	0.48
2:B:368:ARG:HD2	7:C:2068:HOH:O	2.13	0.48
1:A:151:GLU:HG2	1:A:182:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:TYR:O	1:C:173:ARG:HG3	2.15	0.47
2:D:382:TRP:HE3	2:D:399:VAL:HG22	1.80	0.46
1:C:13:LEU:H	1:C:16:GLN:NE2	2.13	0.46
1:A:229:HIS:HD2	7:A:2071:HOH:O	1.99	0.46
1:A:162:ILE:HB	1:A:163:PRO:HD3	1.98	0.45
2:B:315:VAL:HG22	6:B:1310:NAG:HN2	1.83	0.44
1:C:52:ALA:HA	1:C:150:ARG:NH2	2.33	0.44
1:C:225:THR:HG22	7:C:2073:HOH:O	2.18	0.44
1:A:241:ALA:O	1:A:245:GLN:HG3	2.18	0.43
2:B:382:TRP:CE3	2:B:399:VAL:HG22	2.53	0.43
2:B:435:GLU:HA	2:B:436:PRO:HD3	1.85	0.43
2:D:410:ARG:O	2:D:420:ARG:HD2	2.18	0.43
2:D:314:ILE:HD11	3:F:3:NAG:H83	2.01	0.43
1:A:11:LEU:HD11	7:A:2002:HOH:O	2.19	0.42
1:C:200:MET:HE2	2:D:361:VAL:O	2.19	0.42
1:A:81:ARG:HD3	7:A:2023:HOH:O	2.20	0.41
2:D:283:LEU:HD12	2:D:283:LEU:HA	1.89	0.41
1:C:9:ARG:HH21	1:C:11:LEU:HA	1.86	0.41
1:C:220:LYS:HB3	1:C:220:LYS:HE2	1.85	0.41
1:A:46:ALA:HA	1:A:97:ASN:O	2.21	0.41
2:B:365:SER:O	2:B:369:ARG:HG3	2.20	0.41
2:D:367:THR:HG22	2:D:371:LEU:HD22	2.02	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	265/270 (98%)	251 (95%)	14 (5%)	0	100	100
1	C	265/270 (98%)	251 (95%)	14 (5%)	0	100	100
2	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	156/158 (99%)	156 (100%)	0	0	100	100
All	All	842/856 (98%)	813 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	223/226 (99%)	215 (96%)	8 (4%)	31	47
1	C	223/226 (99%)	205 (92%)	18 (8%)	11	14
2	B	135/135 (100%)	120 (89%)	15 (11%)	6	7
2	D	135/135 (100%)	119 (88%)	16 (12%)	5	6
All	All	716/722 (99%)	659 (92%)	57 (8%)	11	15

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	18	ASN
1	A	20	VAL
1	A	77	LEU
1	A	90	LEU
1	A	91	LEU
1	A	182	GLN
1	A	257	THR
2	B	291	VAL
2	B	298	LEU
2	B	300	LEU
2	B	302	GLU
2	B	307	LEU
2	B	315	VAL
2	B	316	GLU
2	B	349	LEU

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Mol	Chain	Res	Type
2	B	371	LEU
2	B	375	GLU
2	B	392	ARG
2	B	399	VAL
2	B	418	VAL
2	B	420	ARG
2	B	426	LEU
1	C	4	GLN
1	C	18	ASN
1	C	20	VAL
1	C	33	ASP
1	C	48	THR
1	C	77	LEU
1	C	90	LEU
1	C	91	LEU
1	C	122	LEU
1	C	123	SER
1	C	128	LYS
1	C	146	HIS
1	C	150	ARG
1	C	173	ARG
1	C	188	SER
1	C	213	GLU
1	C	219	LEU
1	C	261	GLU
2	D	291	VAL
2	D	298	LEU
2	D	300	LEU
2	D	302	GLU
2	D	307	LEU
2	D	315	VAL
2	D	316	GLU
2	D	325	THR
2	D	349	LEU
2	D	371	LEU
2	D	379	LYS
2	D	392	ARG
2	D	399	VAL
2	D	418	VAL
2	D	426	LEU
2	D	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	131	GLN
1	A	148	ASN
1	A	167	GLN
1	A	180	ASN
1	A	206	HIS
1	A	229	HIS
1	A	245	GLN
2	B	400	GLN
2	B	430	GLN
1	C	16	GLN
1	C	83	HIS
1	C	97	ASN
1	C	131	GLN
1	C	164	GLN
1	C	206	HIS
1	C	229	HIS
2	D	430	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](#)

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	0.70	0
3	FUL	E	2	3	10,10,11	0.45	0	14,14,16	0.50	0
3	NAG	E	3	3	14,14,15	0.36	0	17,19,21	0.81	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.45	0	17,19,21	0.69	0
3	FUL	F	2	3	10,10,11	0.41	0	14,14,16	0.35	0
3	NAG	F	3	3	14,14,15	0.41	0	17,19,21	0.82	1 (5%)

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	E	1	1,3	-	0/6/23/26	0/1/1/1
3	FUL	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	FUL	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	NAG	C4-C3-C2	-2.13	107.89	111.02
3	F	3	NAG	C4-C3-C2	-2.11	107.92	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

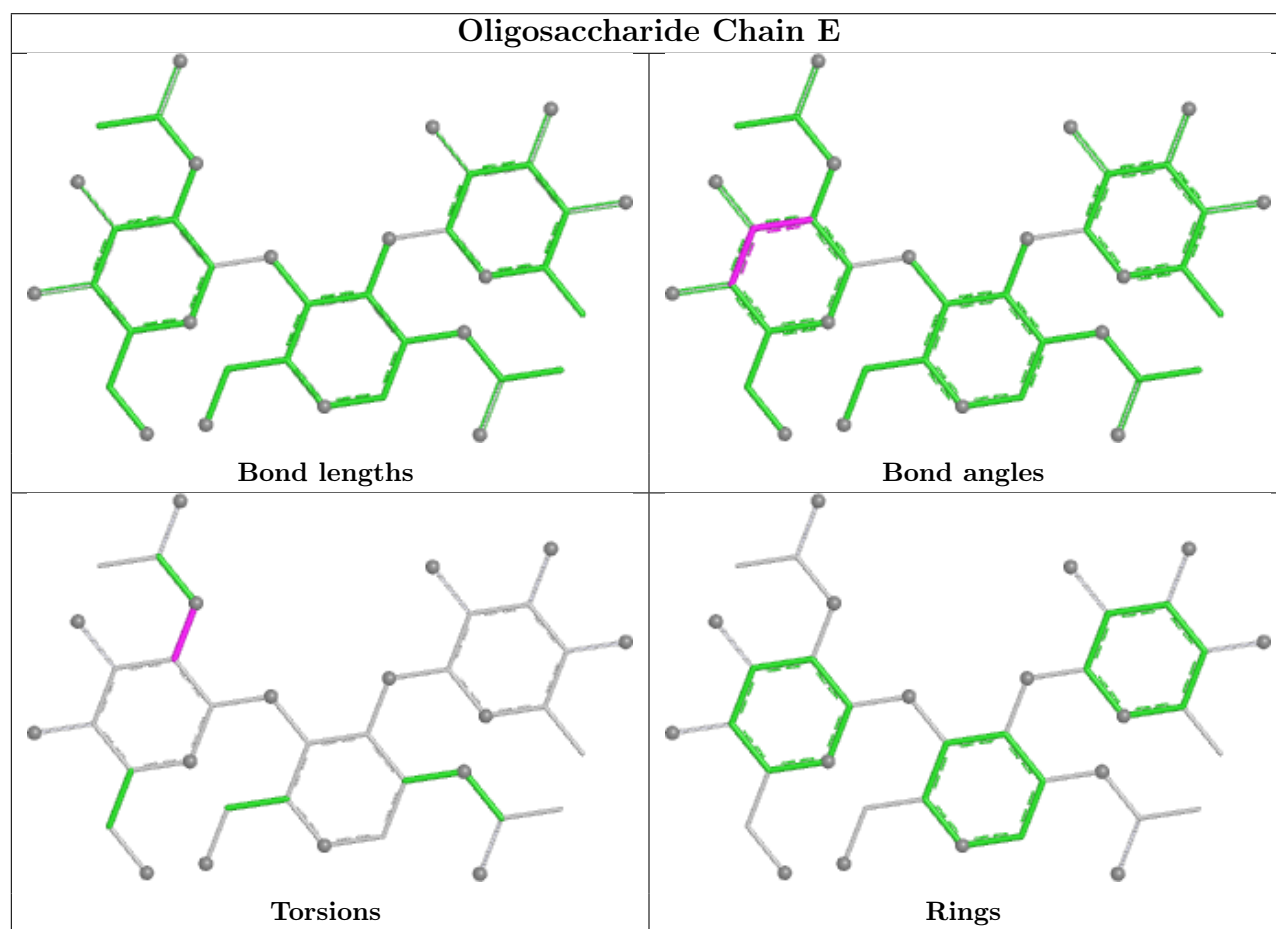
Mol	Chain	Res	Type	Atoms
3	F	3	NAG	C1-C2-N2-C7
3	E	3	NAG	C3-C2-N2-C7
3	F	3	NAG	C3-C2-N2-C7
3	E	3	NAG	C1-C2-N2-C7
3	F	3	NAG	C4-C5-C6-O6

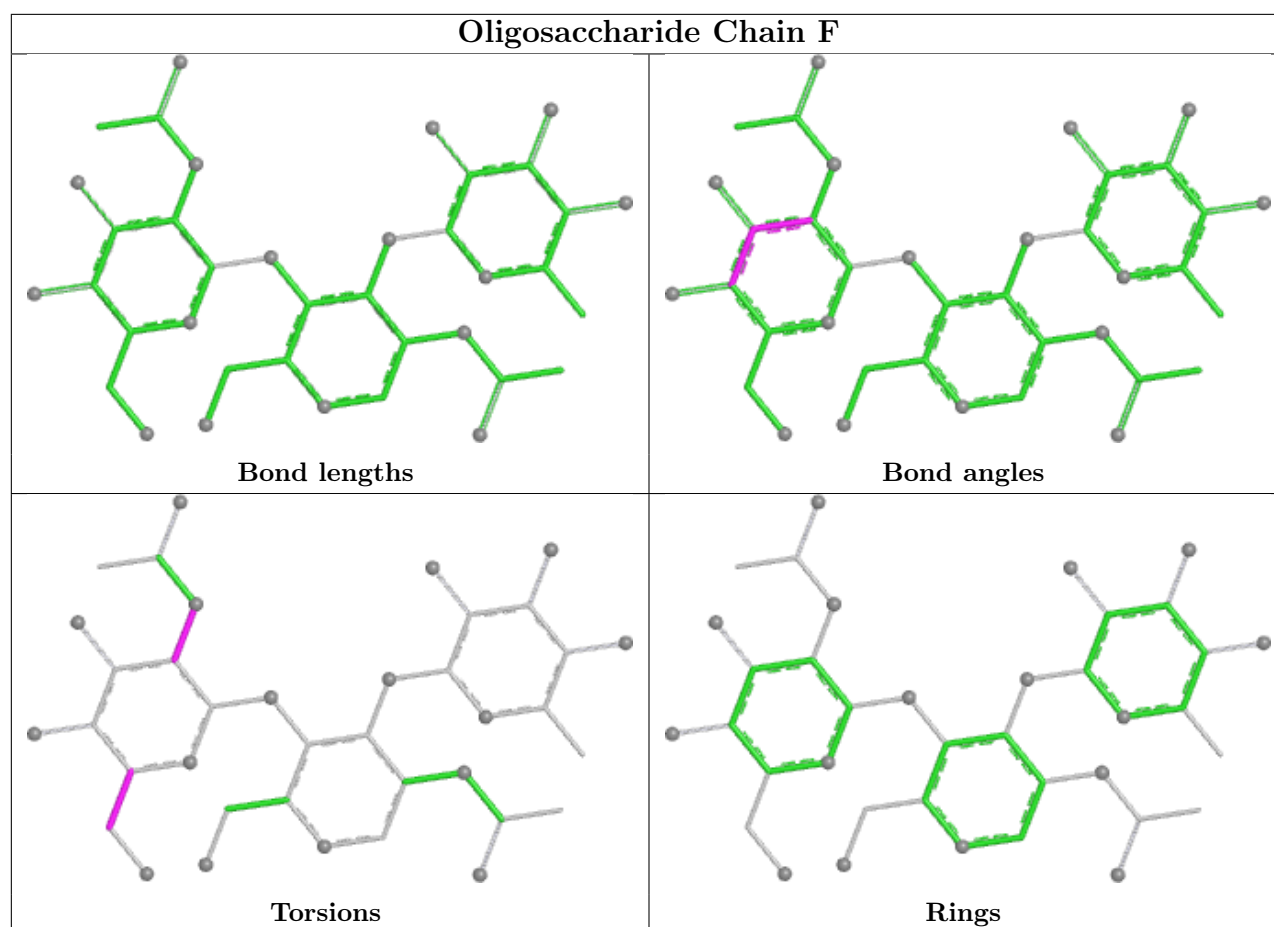
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	FUL	1	0
3	F	2	FUL	1	0
3	E	3	NAG	1	0
3	F	3	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](#)

6 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	$\# Z > 2$
6	NAG	D	1310	2	14,14,15	0.49	0	17,19,21	0.96	0
5	DKA	A	701	-	11,11,11	0.62	0	11,11,11	1.26	1 (9%)
5	DKA	C	702	-	11,11,11	0.67	0	11,11,11	1.30	1 (9%)
4	BEZ	C	602	-	9,9,9	1.38	1 (11%)	11,11,11	1.16	1 (9%)
6	NAG	B	1310	2	14,14,15	0.51	0	17,19,21	1.04	1 (5%)
4	BEZ	A	601	-	9,9,9	1.05	0	11,11,11	1.34	2 (18%)

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
6	NAG	D	1310	2	-	0/6/23/26	0/1/1/1
5	DKA	A	701	-	-	5/9/9/9	-
5	DKA	C	702	-	-	4/9/9/9	-
4	BEZ	C	602	-	-	0/4/4/4	0/1/1/1
6	NAG	B	1310	2	-	1/6/23/26	0/1/1/1
4	BEZ	A	601	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	BEZ	O2-C	-2.72	1.22	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	BEZ	O2-C-C1	3.08	122.75	114.84
4	A	601	BEZ	O2-C-O1	-2.76	117.42	123.35
4	C	602	BEZ	O2-C-O1	-2.74	117.46	123.35
5	A	701	DKA	C5-C4-C3	-2.55	101.46	114.37
5	C	702	DKA	C5-C4-C3	-2.43	102.09	114.37
6	B	1310	NAG	O7-C7-C8	-2.22	118.09	122.05

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	DKA	C4-C5-C6-C7
5	C	702	DKA	C4-C5-C6-C7
5	A	701	DKA	C2-C3-C4-C5
5	A	701	DKA	C3-C4-C5-C6
6	B	1310	NAG	O5-C5-C6-O6
5	C	702	DKA	O2-C1-C2-C3
5	C	702	DKA	O1-C1-C2-C3
5	A	701	DKA	O1-C1-C2-C3
5	A	701	DKA	O2-C1-C2-C3
5	C	702	DKA	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1310	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	267/270 (98%)	-0.81	4 (1%) 72 73	5, 16, 40, 85	0
1	C	267/270 (98%)	-0.84	4 (1%) 72 73	4, 15, 38, 79	0
2	B	158/158 (100%)	-0.89	0 100 100	5, 14, 35, 52	0
2	D	158/158 (100%)	-0.86	0 100 100	5, 14, 35, 53	0
All	All	850/856 (99%)	-0.84	8 (0%) 81 82	4, 15, 38, 85	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	GLU	3.5
1	A	261	GLU	3.2
1	C	262	PRO	3.0
1	C	6	GLU	2.6
1	A	262	PRO	2.2
1	C	4	GLN	2.2
1	C	261	GLU	2.1
1	A	4	GLN	2.0

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

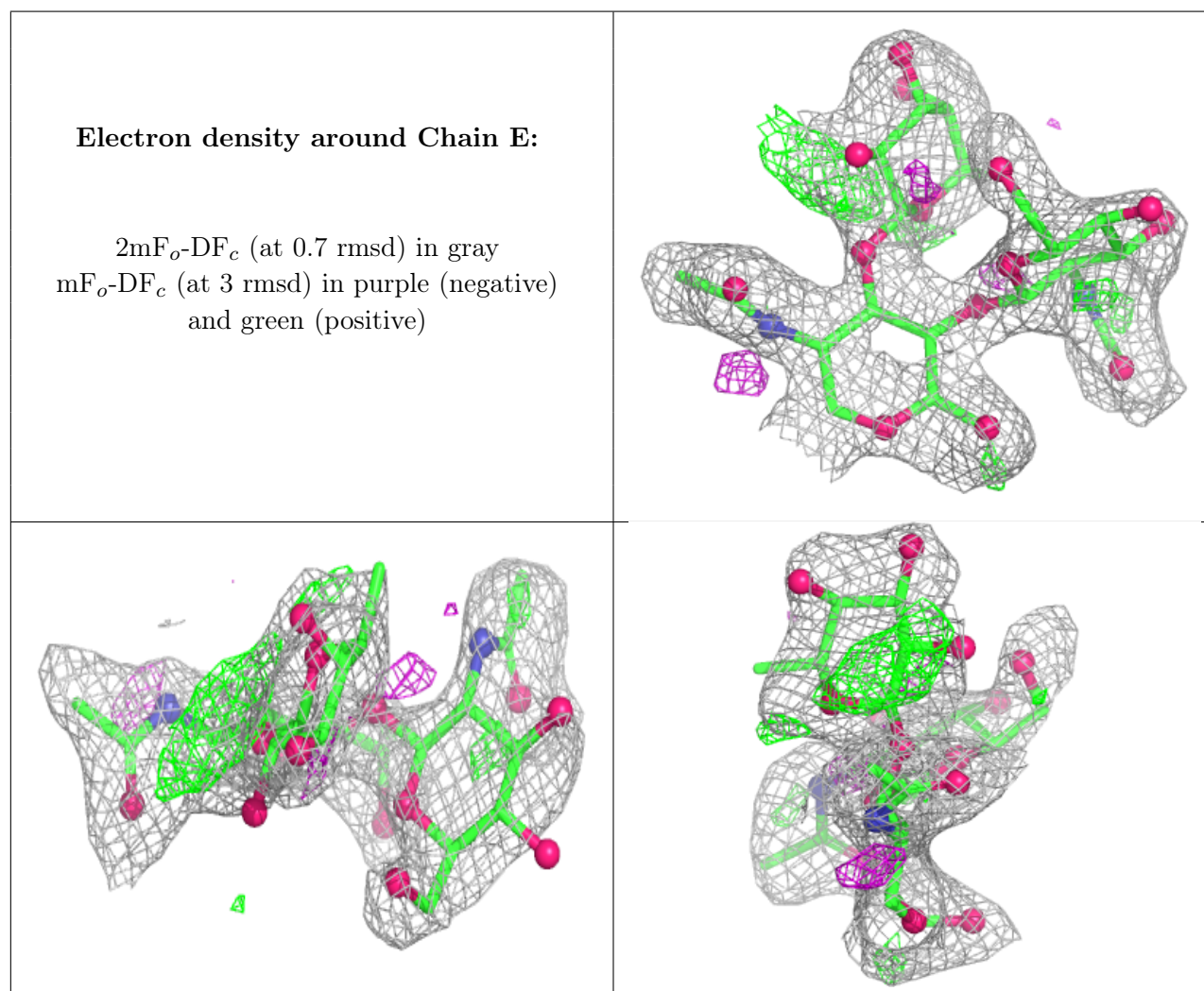
There are no non-standard protein/DNA/RNA residues in this entry.

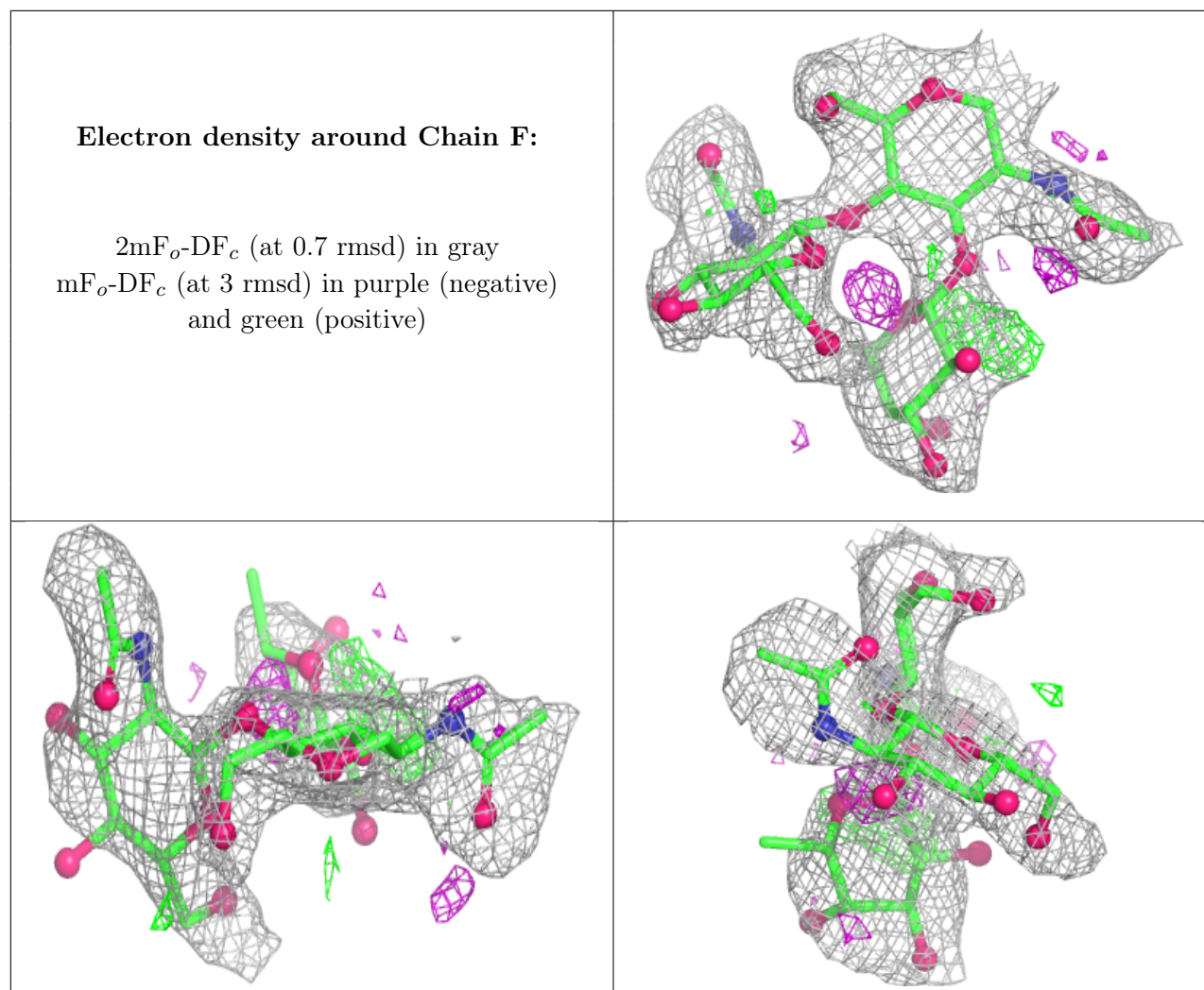
6.3 Carbohydrates [i](#)

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
3	FUL	E	2	10/11	0.69	0.17	56,61,67,71	0
3	FUL	F	2	10/11	0.77	0.19	57,59,65,72	0
3	NAG	F	3	14/15	0.77	0.14	64,70,75,81	0
3	NAG	E	3	14/15	0.83	0.13	55,61,66,67	0
3	NAG	E	1	14/15	0.85	0.10	35,41,53,55	0
3	NAG	F	1	14/15	0.87	0.10	37,44,53,59	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.





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	BEZ	C	602	9/9	0.89	0.08	18,22,27,32	0
4	BEZ	A	601	9/9	0.92	0.07	23,29,34,37	0
6	NAG	B	1310	14/15	0.92	0.07	7,24,31,40	0
5	DKA	A	701	12/12	0.93	0.06	17,27,36,40	0
5	DKA	C	702	12/12	0.94	0.06	19,22,27,29	0
6	NAG	D	1310	14/15	0.95	0.06	11,22,29,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.