



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:41 PM EDT

PDB ID : 1MHL / pdb_00001mhl
Title : CRYSTAL STRUCTURE OF HUMAN MYELOPEROXIDASE ISOFORM C
CRYSTALLIZED IN SPACE GROUP P2(1) AT PH 5.5 AND 20 DEG C
Authors : Fenna, R.E.; Zeng, J.; Davey, C.
Deposited on : 1995-06-09
Resolution : 2.25 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

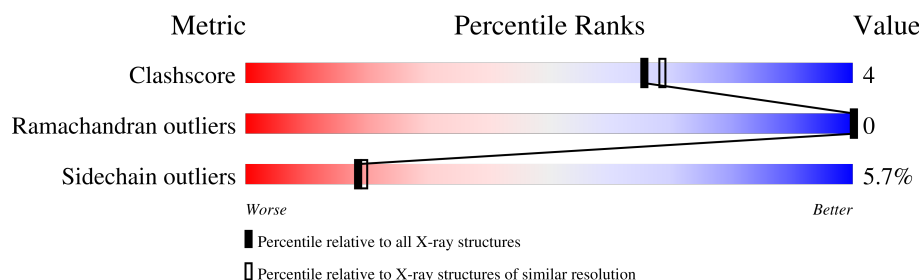
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	69% 22% 5% . .
1	B	108	68% 25% . . .
2	C	466	73% 22% . .
2	D	466	75% 22% .
3	E	6	17% 67% 17%
3	F	6	50% 50%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9847 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.

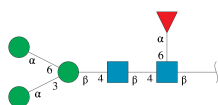
- Molecule 1 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	12	0	0
			837	529	148	155	5			
1	B	104	Total	C	N	O	S	7	0	0
			837	529	148	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

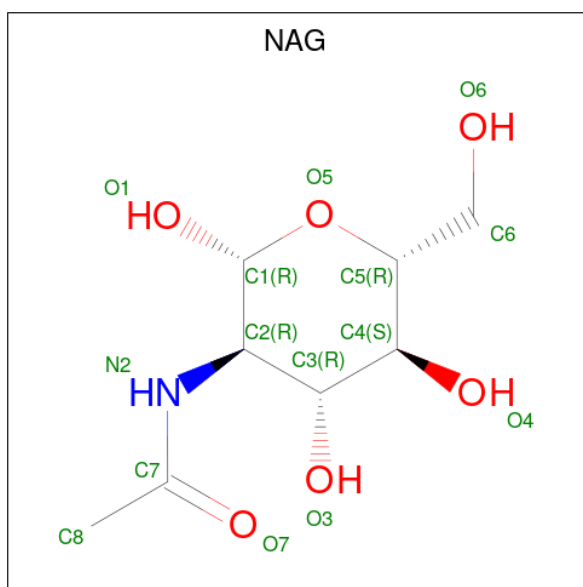
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	82	0	0
			3732	2351	687	667	27			
2	D	466	Total	C	N	O	S	109	0	0
			3732	2351	687	667	27			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			71	40	2	29			
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

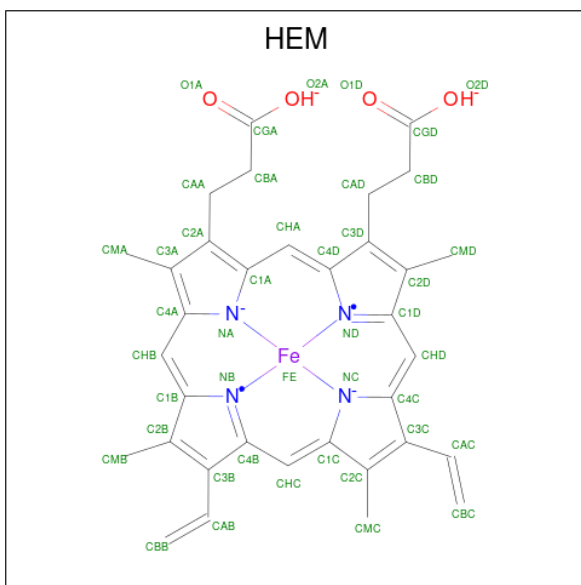
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	55	Total O 55 55	0	0
8	C	158	Total O 158 158	0	0
8	B	58	Total O 58 58	0	0
8	D	150	Total O 150 150	0	0

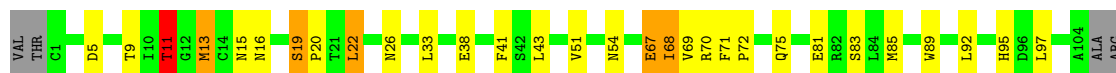
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: MYELOPEROXIDASE

Chain A: 



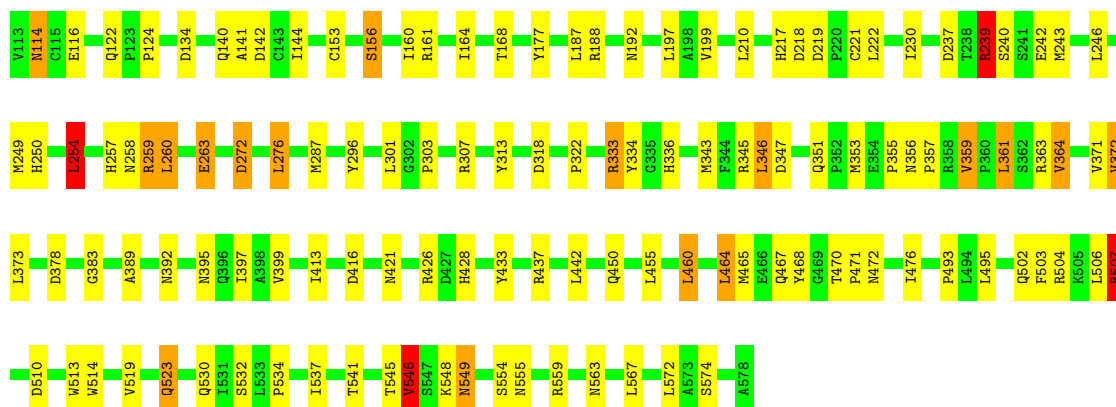
• Molecule 1: MYELOPEROXIDASE

Chain B: 



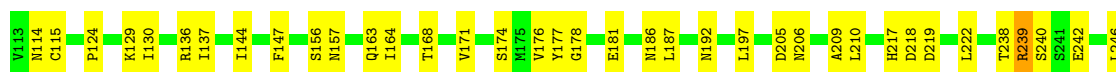
• Molecule 2: MYELOPEROXIDASE

Chain C: 



• Molecule 2: MYELOPEROXIDASE

Chain D: 





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

Chain E: 17% 67% 17%



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

Chain F: 50% 50%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.70Å 64.60Å 94.20Å 90.00° 97.90° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25	Depositor
% Data completeness (in resolution range)	92.6 (8.00-2.25)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9847	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, HEM, NAG, CA, CL, 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	0.99	2/862 (0.2%)	1.93	23/1174 (2.0%)
1	B	0.93	1/862 (0.1%)	1.88	25/1174 (2.1%)
2	C	0.98	5/3818 (0.1%)	1.78	85/5180 (1.6%)
2	D	0.94	7/3818 (0.2%)	1.79	79/5180 (1.5%)
All	All	0.96	15/9360 (0.2%)	1.81	212/12708 (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
2	C	0	1
2	D	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	HIS	CD2-NE2	-7.50	1.29	1.37
1	B	95	HIS	CD2-NE2	-7.12	1.30	1.37
2	C	476	ILE	CA-CB	6.80	1.62	1.54
2	D	217	HIS	CD2-NE2	-6.42	1.30	1.37
2	D	359	VAL	CA-CB	6.42	1.62	1.54
2	D	257	HIS	CD2-NE2	-6.25	1.30	1.37
2	C	217	HIS	CD2-NE2	-6.10	1.31	1.37
2	D	250	HIS	CD2-NE2	-6.05	1.31	1.37
2	C	257	HIS	CD2-NE2	-5.95	1.31	1.37
2	D	428	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	95	HIS	CG-ND1	-5.56	1.32	1.38
2	C	428	HIS	CD2-NE2	-5.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	336	HIS	CG-CD2	5.18	1.41	1.35
2	D	250	HIS	CG-ND1	-5.16	1.32	1.38
2	C	359	VAL	CA-CB	5.11	1.60	1.54

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	546	VAL	N-CA-CB	-11.45	96.49	112.52
1	A	11	THR	N-CA-CB	-10.31	93.28	110.39
1	A	15	ASN	N-CA-C	-9.91	100.56	111.36
2	D	356	ASN	CA-CB-CG	9.71	122.31	112.60
2	D	177	TYR	N-CA-C	9.20	124.64	113.23
1	A	68	ILE	N-CA-C	9.18	119.71	111.81
2	C	177	TYR	N-CA-C	9.08	124.49	113.23
2	D	549	ASN	CA-CB-CG	-8.77	103.83	112.60
2	D	507	ARG	NE-CZ-NH2	-8.63	111.44	119.20
2	C	114	ASN	OD1-CG-ND2	-8.55	114.05	122.60
2	C	347	ASP	CA-CB-CG	8.42	121.02	112.60
2	D	433	TYR	N-CA-C	8.32	121.17	111.02
2	D	468	TYR	N-CA-C	8.19	123.63	112.90
2	C	144	ILE	N-CA-C	-8.10	98.50	107.73
2	D	546	VAL	N-CA-CB	-8.01	98.98	112.44
2	D	240	SER	N-CA-C	8.01	120.01	111.28
2	D	157	ASN	N-CA-C	-8.00	103.54	113.38
1	B	11	THR	N-CA-CB	-7.97	97.41	110.40
2	C	523	GLN	OE1-CD-NE2	-7.73	114.87	122.60
1	B	5	ASP	CA-CB-CG	7.67	120.28	112.60
2	D	239	ARG	NE-CZ-NH1	7.63	129.13	121.50
2	C	548	LYS	N-CA-C	-7.63	100.25	110.55
2	C	343	MET	N-CA-C	-7.56	96.20	108.52
2	D	397	ILE	N-CA-C	7.55	118.14	110.82
1	B	96	ASP	N-CA-C	-7.50	104.28	113.50
2	D	209	ALA	N-CA-C	7.46	121.33	110.28
2	C	549	ASN	O-C-N	-7.44	114.55	122.96
2	C	246	LEU	N-CA-C	-7.42	102.56	111.69
2	C	519	VAL	N-CA-C	-7.31	103.73	110.82
1	B	9	THR	N-CA-C	-7.31	101.11	110.53
2	C	258	ASN	OD1-CG-ND2	-7.27	115.33	122.60
2	C	392	ASN	OD1-CG-ND2	-7.26	115.34	122.60
2	C	372	VAL	N-CA-C	7.22	117.31	110.53
2	C	240	SER	N-CA-C	7.17	119.95	111.71
2	C	502	GLN	OE1-CD-NE2	-7.04	115.56	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	514	TRP	N-CA-C	7.02	121.46	112.34
1	A	26	ASN	OD1-CG-ND2	-6.98	115.62	122.60
2	C	371	VAL	N-CA-C	-6.97	103.98	110.53
1	A	5	ASP	CA-CB-CG	6.95	119.55	112.60
2	C	399	VAL	N-CA-C	6.94	118.05	110.21
2	D	218	ASP	N-CA-C	-6.93	95.88	108.02
1	A	9	THR	N-CA-C	-6.88	101.66	110.53
2	D	347	ASP	CA-CB-CG	6.87	119.47	112.60
2	C	563	ASN	OD1-CG-ND2	-6.84	115.76	122.60
2	C	437	ARG	N-CA-C	-6.82	103.92	111.36
2	C	197	LEU	N-CA-C	-6.80	99.23	110.17
2	D	301	LEU	N-CA-C	6.76	120.75	112.23
2	D	507	ARG	NE-CZ-NH1	6.76	128.26	121.50
2	C	389	ALA	N-CA-C	-6.74	101.84	110.53
1	B	68	ILE	N-CA-C	6.71	117.76	112.12
2	C	472	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	13	MET	CA-CB-CG	6.70	127.49	114.10
2	D	246	LEU	N-CA-C	-6.66	103.95	111.14
2	C	545	THR	N-CA-C	-6.65	97.58	108.41
1	B	15	ASN	N-CA-C	-6.59	104.03	111.14
2	D	343	MET	N-CA-C	-6.58	97.80	108.52
2	C	549	ASN	CA-CB-CG	-6.56	106.04	112.60
2	D	295	ASP	N-CA-C	6.56	121.32	113.12
2	D	345	ARG	NE-CZ-NH2	-6.54	113.31	119.20
2	D	239	ARG	NE-CZ-NH2	-6.53	113.32	119.20
2	C	160	ILE	N-CA-C	-6.52	98.90	108.54
2	C	114	ASN	CB-CG-ND2	6.51	126.16	116.40
2	C	559	ARG	N-CA-C	6.50	118.90	111.11
2	C	239	ARG	NE-CZ-NH2	-6.47	113.38	119.20
2	D	164	ILE	N-CA-C	6.45	118.32	108.71
2	C	296	TYR	N-CA-C	6.45	119.56	111.24
1	B	16	ASN	N-CA-C	-6.43	98.25	108.73
2	C	546	VAL	CB-CA-C	6.39	120.27	110.82
2	C	442	LEU	CA-C-N	6.36	126.39	119.90
2	C	442	LEU	C-N-CA	6.36	126.39	119.90
2	D	168	THR	N-CA-C	-6.36	100.16	110.20
2	C	272	ASP	CA-CB-CG	6.32	118.92	112.60
2	D	549	ASN	CB-CG-ND2	-6.31	106.94	116.40
2	C	318	ASP	CA-CB-CG	6.30	118.90	112.60
2	C	395	ASN	N-CA-C	-6.28	104.93	112.59
2	D	321	ASP	CA-CB-CG	6.28	118.88	112.60
2	C	156	SER	CA-C-O	6.25	128.16	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	ARG	N-CA-C	-6.25	104.55	111.36
2	D	136	ARG	N-CA-C	6.21	120.67	112.72
2	C	122	GLN	OE1-CD-NE2	-6.20	116.40	122.60
2	D	197	LEU	N-CA-C	-6.18	99.62	109.76
2	D	324	ILE	N-CA-C	-6.18	100.73	108.89
2	D	555	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	D	163	GLN	OE1-CD-NE2	-6.15	116.45	122.60
2	D	314	ARG	N-CA-C	-6.13	102.20	111.34
2	D	219	ASP	CA-CB-CG	6.13	118.73	112.60
2	D	437	ARG	N-CA-C	-6.11	104.70	111.36
1	A	70	ARG	N-CA-C	6.10	118.85	110.24
1	A	71	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	97	LEU	N-CA-C	6.08	120.72	113.12
2	C	503	PHE	CA-CB-CG	-6.06	107.74	113.80
1	B	88	GLN	N-CA-C	6.06	117.89	111.28
2	C	397	ILE	N-CA-C	6.00	116.06	110.42
1	B	89	TRP	N-CA-C	-5.99	104.83	111.36
2	C	507	ARG	NE-CZ-NH2	-5.97	113.83	119.20
2	C	336	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	C	217	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	C	230	ILE	O-C-N	-5.95	117.62	121.37
1	B	97	LEU	N-CA-C	5.94	120.55	113.12
1	B	47	TRP	CG-CD2-CE3	5.91	139.81	133.90
2	C	507	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	A	11	THR	OG1-CB-CG2	5.87	121.04	109.30
1	A	16	ASN	N-CA-C	-5.87	99.16	108.73
1	A	9	THR	O-C-N	-5.85	115.45	122.65
2	D	178	GLY	N-CA-C	-5.85	105.74	112.29
2	D	176	VAL	N-CA-C	-5.84	106.01	111.45
2	C	514	TRP	N-CA-C	5.83	119.50	112.38
1	A	19	SER	CA-C-N	5.83	125.51	119.56
1	A	19	SER	C-N-CA	5.83	125.51	119.56
2	C	345	ARG	CB-CG-CD	-5.82	97.91	111.30
1	A	41	PHE	O-C-N	-5.80	115.78	121.93
2	D	450	GLN	OE1-CD-NE2	-5.79	116.81	122.60
2	D	144	ILE	N-CA-C	-5.78	101.23	108.05
2	C	504	ARG	N-CA-C	-5.76	105.08	111.36
2	D	205	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	69	VAL	N-CA-C	5.74	117.26	111.00
2	C	555	ASN	OD1-CG-ND2	-5.74	116.86	122.60
2	C	537	ILE	N-CA-C	-5.72	105.15	110.53
2	C	502	GLN	CG-CD-NE2	5.71	124.97	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	513	TRP	N-CA-C	-5.68	102.00	110.23
2	D	206	ASN	OD1-CG-ND2	-5.67	116.93	122.60
2	D	540	ASN	OD1-CG-ND2	-5.66	116.94	122.60
2	D	549	ASN	O-C-N	-5.65	116.58	122.96
2	D	336	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	A	81	GLU	N-CA-C	5.63	119.46	112.59
2	C	450	GLN	OE1-CD-NE2	-5.63	116.97	122.60
2	D	513	TRP	N-CA-C	-5.61	102.09	110.23
2	D	521	SER	N-CA-C	-5.61	103.29	110.53
2	D	171	VAL	N-CA-C	-5.60	98.42	106.55
2	D	399	VAL	N-CA-C	5.59	117.24	109.80
2	C	333	ARG	N-CA-C	-5.58	106.51	113.15
1	B	54	ASN	OD1-CG-ND2	-5.57	117.03	122.60
2	C	239	ARG	NE-CZ-NH1	5.55	127.05	121.50
2	D	434	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	B	4	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	26	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	B	99	PHE	N-CA-C	-5.52	99.09	108.26
2	D	181	GLU	N-CA-C	5.51	120.98	113.16
2	C	476	ILE	N-CA-C	5.50	116.89	110.62
1	A	89	TRP	N-CA-C	-5.50	105.37	111.36
2	C	243	MET	CG-SD-CE	5.49	112.98	100.90
2	D	333	ARG	N-CA-C	-5.48	106.63	113.15
2	C	468	TYR	N-CA-C	5.46	120.21	113.50
2	D	174	SER	CA-CB-OG	5.44	121.98	111.10
2	D	514	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	B	16	ASN	CA-CB-CG	-5.43	107.17	112.60
2	D	513	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	B	67	GLU	N-CA-C	5.42	119.06	112.23
2	C	493	PRO	N-CA-C	5.42	120.97	113.65
2	C	416	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	68	ILE	N-CA-CB	-5.40	101.41	110.86
2	D	250	HIS	CB-CG-CD2	-5.40	124.18	131.20
2	D	268	ASN	CA-CB-CG	5.39	117.99	112.60
2	D	375	GLY	N-CA-C	5.39	122.76	115.00
2	D	192	ASN	CA-CB-CG	5.39	117.99	112.60
1	A	67	GLU	N-CA-C	5.33	118.25	111.69
2	D	545	THR	N-CA-C	-5.33	100.21	108.90
2	D	442	LEU	CA-C-N	5.32	125.24	119.76
2	D	442	LEU	C-N-CA	5.32	125.24	119.76
1	B	16	ASN	O-C-N	-5.32	117.16	123.22
2	D	334	TYR	N-CA-C	-5.32	105.89	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	351	GLN	N-CA-C	-5.31	102.42	110.50
1	B	30	VAL	N-CA-C	-5.31	100.73	109.12
2	C	549	ASN	CB-CG-ND2	-5.31	108.44	116.40
2	C	140	GLN	OE1-CD-NE2	-5.30	117.30	122.60
2	D	372	VAL	N-CA-C	5.30	115.51	110.53
2	C	250	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	11	THR	CB-CA-C	5.28	121.34	110.31
2	C	218	ASP	N-CA-C	-5.28	97.08	107.69
2	D	186	ASN	OD1-CG-ND2	-5.26	117.34	122.60
2	C	254	LEU	N-CA-C	-5.26	105.46	111.14
1	B	64	VAL	O-C-N	-5.26	116.77	121.87
2	D	114	ASN	OD1-CG-ND2	-5.26	117.34	122.60
2	C	433	TYR	N-CA-C	5.26	119.99	111.37
2	C	168	THR	N-CA-C	-5.25	101.90	110.20
2	D	405	ARG	N-CA-C	5.24	118.98	112.59
2	C	219	ASP	CA-CB-CG	5.24	117.84	112.60
2	C	426	ARG	N-CA-C	-5.24	105.25	111.69
2	C	141	ALA	N-CA-C	-5.23	106.58	113.17
2	D	238	THR	N-CA-C	5.22	118.91	112.54
2	C	192	ASN	CA-CB-CG	5.22	117.82	112.60
2	D	130	ILE	CA-C-N	5.21	125.75	120.38
2	D	130	ILE	C-N-CA	5.21	125.75	120.38
2	D	339	ILE	N-CA-C	5.21	115.81	109.30
2	C	122	GLN	CG-CD-NE2	5.18	124.17	116.40
2	C	221	CYS	N-CA-C	5.18	117.83	111.82
2	C	188	ARG	N-CA-C	5.16	118.11	110.48
2	C	164	ILE	N-CA-C	5.14	116.71	108.89
1	A	85	MET	N-CA-C	-5.14	105.80	111.71
2	C	153	CYS	O-C-N	-5.14	116.74	121.37
2	D	555	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	71	PHE	O-C-N	-5.12	117.91	121.65
2	D	514	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	B	47	TRP	CB-CG-CD1	-5.11	119.24	126.90
2	C	134	ASP	N-CA-C	-5.11	103.60	109.93
2	D	268	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	B	71	PHE	CA-CB-CG	5.09	118.89	113.80
2	C	470	THR	CA-C-N	5.08	124.74	119.56
2	C	470	THR	C-N-CA	5.08	124.74	119.56
2	C	217	HIS	CB-CG-ND1	5.08	130.32	122.70
2	C	142	ASP	CA-CB-CG	5.07	117.67	112.60
2	D	129	LYS	CA-CB-CG	-5.05	104.00	114.10
2	D	563	ASN	OD1-CG-ND2	-5.05	117.55	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	156	SER	CA-C-O	5.05	126.67	120.92
2	D	254	LEU	N-CA-C	-5.05	105.86	111.36
1	B	46	GLY	N-CA-C	-5.04	107.74	115.00
1	B	3	GLU	CB-CG-CD	5.03	121.15	112.60
2	C	364	VAL	CB-CA-C	-5.02	105.20	110.62
2	C	287	MET	CG-SD-CE	-5.02	89.86	100.90
2	C	392	ASN	CB-CG-ND2	5.01	123.92	116.40
2	D	137	ILE	N-CA-CB	-5.00	105.95	111.66
2	D	389	ALA	N-CA-C	-5.00	104.08	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	334	TYR	Sidechain
2	D	334	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	837	0	798	12	0
1	B	837	0	798	7	0
2	C	3732	0	3725	32	0
2	D	3732	0	3725	26	0
3	E	71	0	61	1	0
3	F	71	0	61	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	43	0	30	2	0
7	B	43	0	30	1	0
8	A	55	0	0	0	0
8	B	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	158	0	0	0	0
8	D	150	0	0	0	0
All	All	9847	0	9280	70	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 (70) 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:19:SER:HB3	1:A:22:LEU:HD22	1.67	0.76
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.34	0.74
2:C:460:LEU:HD22	2:C:464:LEU:HD22	1.74	0.68
1:A:67:GLU:HG3	2:C:467:GLN:NE2	2.10	0.67
1:B:68:ILE:HD13	2:D:464:LEU:HD13	1.78	0.63
2:D:333:ARG:HH11	2:D:421:ASN:ND2	1.97	0.62
2:C:333:ARG:HH11	2:C:421:ASN:ND2	1.98	0.62
1:A:68:ILE:HD13	2:C:464:LEU:HD13	1.80	0.62
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.47	0.61
7:A:605:HEM:HMC2	7:A:605:HEM:HBC2	1.82	0.60
2:D:393:ARG:HH11	2:D:393:ARG:HG2	1.67	0.59
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.84	0.59
2:C:237:ASP:OD2	2:C:239:ARG:HD3	2.03	0.58
2:D:460:LEU:HD22	2:D:464:LEU:HD22	1.86	0.58
1:B:19:SER:HB3	1:B:22:LEU:HD22	1.86	0.57
7:B:605:HEM:HBB2	2:D:242:GLU:OE1	2.05	0.56
2:D:346:LEU:HD22	2:D:383:GLY:HA2	1.85	0.56
2:C:313:TYR:CD1	2:C:507:ARG:HD3	2.43	0.54
2:C:346:LEU:HD22	2:C:383:GLY:HA2	1.90	0.53
1:A:38:GLU:HG3	1:A:51:VAL:HG11	1.90	0.52
2:C:114:ASN:ND2	2:C:116:GLU:H	2.07	0.51
1:A:11:THR:HG22	1:A:13:MET:H	1.75	0.50
2:C:313:TYR:HD1	2:C:507:ARG:HD3	1.76	0.49
2:D:313:TYR:HD1	2:D:507:ARG:HD3	1.76	0.49
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.94	0.48
2:D:298:PRO:HG3	2:D:306:MET:HE2	1.94	0.48
2:C:532:SER:HB2	2:C:549:ASN:HD21	1.79	0.48
1:A:54:ASN:HD21	1:B:18:ARG:HG2	1.80	0.47
2:D:486:LYS:HD3	2:D:493:PRO:HD3	1.97	0.47
1:B:83:SER:HB3	2:D:554:SER:O	2.15	0.46
2:D:308:LYS:HE3	3:E:4:MAN:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:ARG:NH1	2:D:260:LEU:HD13	2.30	0.46
2:D:393:ARG:HD3	2:D:396:GLN:OE1	2.15	0.46
2:C:259:ARG:NH1	2:C:260:LEU:HD13	2.30	0.46
7:A:605:HEM:HBB2	2:C:242:GLU:OE1	2.16	0.45
1:A:83:SER:HB3	2:C:554:SER:O	2.16	0.45
2:D:265:LYS:HD3	2:D:276:LEU:HD21	1.99	0.45
1:A:38:GLU:CG	1:A:51:VAL:HG11	2.46	0.45
1:A:20:PRO:HD2	1:B:40:GLY:HA2	1.99	0.45
2:C:263:GLU:HB3	2:C:572:LEU:HD12	1.99	0.44
2:C:378:ASP:OD1	2:C:541:THR:HB	2.17	0.44
1:B:11:THR:HG22	1:B:13:MET:H	1.82	0.44
1:A:72:PRO:HB2	1:A:75:GLN:HG2	1.99	0.44
2:C:460:LEU:HD22	2:C:464:LEU:CD2	2.47	0.43
2:D:313:TYR:CD1	2:D:507:ARG:HD3	2.53	0.43
2:D:115:CYS:HB2	2:D:147:PHE:CE1	2.54	0.43
2:C:361:LEU:HA	2:C:364:VAL:HG22	2.01	0.42
2:C:363:ARG:HD3	2:C:363:ARG:HA	1.66	0.42
2:D:359:VAL:HA	2:D:360:PRO:HD3	1.83	0.42
2:D:370:ARG:O	2:D:374:GLU:HB2	2.18	0.42
2:C:272:ASP:O	2:C:276:LEU:HD22	2.20	0.42
2:C:534:PRO:HB3	2:C:546:VAL:HG13	2.00	0.42
2:C:506:LEU:O	2:C:510:ASP:HB2	2.19	0.42
2:D:363:ARG:HD3	2:D:363:ARG:HA	1.81	0.42
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.34	0.42
2:C:355:PRO:O	2:C:356:ASN:HB2	2.20	0.42
2:C:413:ILE:HD13	2:C:413:ILE:HG21	1.75	0.42
2:C:303:PRO:O	2:C:307:ARG:HG3	2.20	0.41
2:D:378:ASP:OD1	2:D:541:THR:HB	2.20	0.41
1:B:48:THR:HA	1:B:49:PRO:HD3	1.86	0.41
1:A:92:LEU:HD22	2:C:249:MET:HB3	2.02	0.41
2:C:353:MET:O	2:C:357:PRO:HB3	2.19	0.41
2:C:372:VAL:HG12	2:C:373:LEU:HD23	2.03	0.41
2:D:458:LEU:O	2:D:462:ARG:HG3	2.21	0.41
2:D:398:ALA:HB1	2:D:402:ILE:HD11	2.03	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.95	0.41
2:C:465:MET:HE1	2:C:471:PRO:HD3	2.03	0.41
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.56	0.41
2:D:361:LEU:HA	2:D:364:VAL:HG22	2.03	0.40
2:C:161:ARG:HH11	2:C:161:ARG:HD2	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	102/108 (94%)	99 (97%)	3 (3%)	0	100	100
1	B	102/108 (94%)	98 (96%)	4 (4%)	0	100	100
2	C	464/466 (100%)	450 (97%)	14 (3%)	0	100	100
2	D	464/466 (100%)	455 (98%)	9 (2%)	0	100	100
All	All	1132/1148 (99%)	1102 (97%)	30 (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	90/93 (97%)	87 (97%)	3 (3%)	33	42
1	B	90/93 (97%)	86 (96%)	4 (4%)	25	29
2	C	411/411 (100%)	385 (94%)	26 (6%)	16	16
2	D	411/411 (100%)	387 (94%)	24 (6%)	18	19
All	All	1002/1008 (99%)	945 (94%)	57 (6%)	18	19

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

Mol	Chain	Res	Type
1	A	11	THR
1	A	22	LEU

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Mol	Chain	Res	Type
1	A	43	LEU
2	C	124	PRO
2	C	156	SER
2	C	187	LEU
2	C	210	LEU
2	C	222	LEU
2	C	239	ARG
2	C	254	LEU
2	C	259	ARG
2	C	260	LEU
2	C	263	GLU
2	C	276	LEU
2	C	301	LEU
2	C	322	PRO
2	C	346	LEU
2	C	359	VAL
2	C	361	LEU
2	C	455	LEU
2	C	460	LEU
2	C	464	LEU
2	C	495	LEU
2	C	507	ARG
2	C	523	GLN
2	C	530	GLN
2	C	546	VAL
2	C	567	LEU
2	C	574	SER
1	B	11	THR
1	B	13	MET
1	B	22	LEU
1	B	43	LEU
2	D	124	PRO
2	D	187	LEU
2	D	210	LEU
2	D	222	LEU
2	D	239	ARG
2	D	254	LEU
2	D	260	LEU
2	D	276	LEU
2	D	301	LEU
2	D	346	LEU
2	D	355	PRO

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Mol	Chain	Res	Type
2	D	356	ASN
2	D	359	VAL
2	D	455	LEU
2	D	460	LEU
2	D	464	LEU
2	D	485	LEU
2	D	486	LYS
2	D	495	LEU
2	D	507	ARG
2	D	546	VAL
2	D	547	SER
2	D	567	LEU
2	D	574	SER

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	54	ASN
2	C	114	ASN
2	C	121	GLN
2	C	163	GLN
2	C	326	ASN
2	C	421	ASN
2	C	467	GLN
2	C	540	ASN
2	C	549	ASN
1	B	54	ASN
2	D	121	GLN
2	D	409	GLN
2	D	421	ASN
2	D	540	ASN
2	D	549	ASN
2	D	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
3	NAG	E	1	2,3	14,14,15	0.56	0	17,19,21	1.16	1 (5%)
3	NAG	E	2	3	14,14,15	0.91	0	17,19,21	1.04	2 (11%)
3	BMA	E	3	3	11,11,12	0.71	0	15,15,17	0.77	0
3	MAN	E	4	3	11,11,12	0.54	0	15,15,17	1.05	1 (6%)
3	MAN	E	5	3	11,11,12	0.61	0	15,15,17	0.99	1 (6%)
3	FUC	E	6	3	10,10,11	0.66	0	14,14,16	1.23	2 (14%)
3	NAG	F	1	2,3	14,14,15	0.70	0	17,19,21	1.54	2 (11%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	0.74	0
3	BMA	F	3	3	11,11,12	0.37	0	15,15,17	0.87	0
3	MAN	F	4	3	11,11,12	0.94	0	15,15,17	1.39	4 (26%)
3	MAN	F	5	3	11,11,12	0.75	0	15,15,17	1.50	2 (13%)
3	FUC	F	6	3	10,10,11	0.51	0	14,14,16	1.06	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	E	6	3	-	-	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	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	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	MAN	C1-O5-C5	4.54	118.27	112.19
3	F	1	NAG	C1-C2-N2	4.43	117.41	110.43
3	F	4	MAN	O2-C2-C1	3.08	116.28	109.22
3	E	5	MAN	C1-O5-C5	2.84	115.99	112.19
3	E	4	MAN	O2-C2-C1	2.64	115.27	109.22
3	E	6	FUC	C6-C5-C4	-2.51	108.48	113.08
3	F	5	MAN	C6-C5-C4	-2.51	106.84	113.02
3	E	2	NAG	C1-C2-N2	-2.36	106.72	110.43
3	F	4	MAN	C6-C5-C4	2.32	118.72	113.02
3	E	2	NAG	C4-C3-C2	-2.23	107.74	111.02
3	F	4	MAN	O5-C5-C4	-2.17	105.54	110.83
3	E	1	NAG	C3-C4-C5	2.10	114.05	110.23
3	F	1	NAG	C8-C7-N2	-2.04	112.73	116.12
3	E	6	FUC	O3-C3-C4	-2.04	105.58	110.38
3	F	4	MAN	C3-C4-C5	-2.02	106.56	110.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

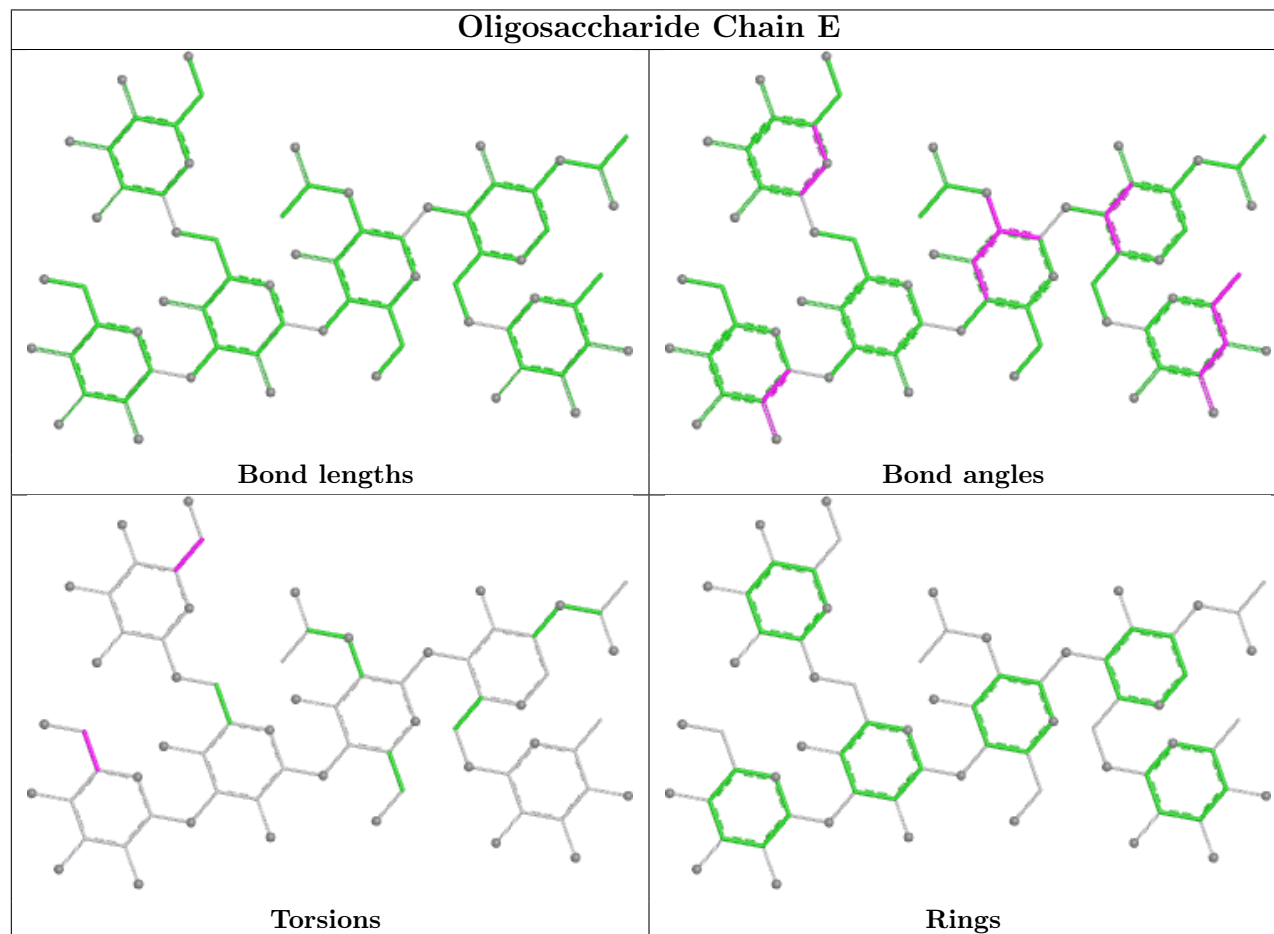
Mol	Chain	Res	Type	Atoms
3	E	4	MAN	O5-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6
3	E	5	MAN	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6

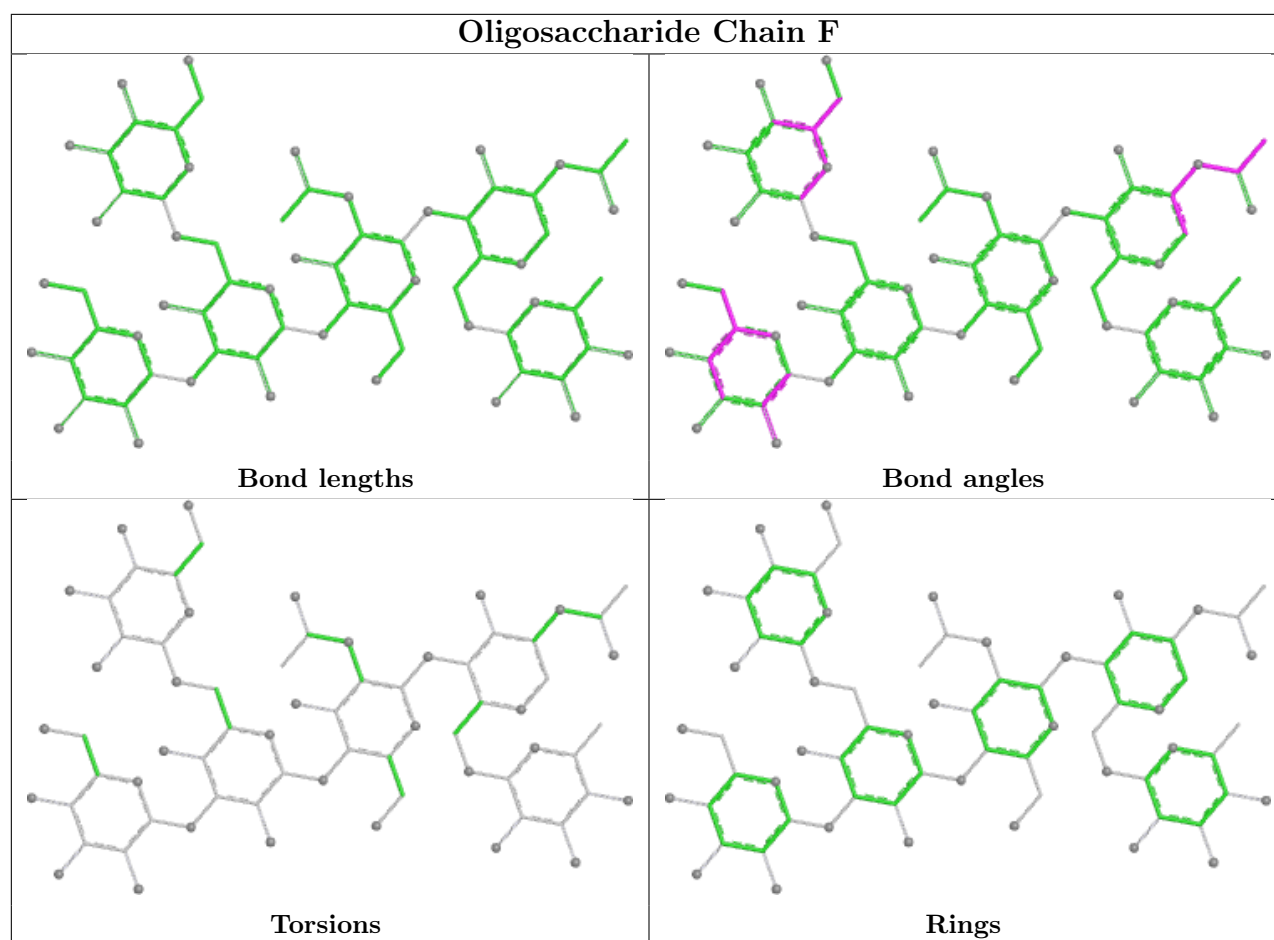
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4	MAN	1	0

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





5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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
7	HEM	A	605	2	50,50,50	1.27	6 (12%)	67,82,82	0.95	1 (1%)
4	NAG	B	630	2	14,14,15	1.10	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	A	630	2	14,14,15	1.23	2 (14%)	17,19,21	2.01	5 (29%)
7	HEM	B	605	1,2	50,50,50	1.39	9 (18%)	67,82,82	0.97	1 (1%)
4	NAG	B	620	2	14,14,15	0.98	1 (7%)	17,19,21	1.45	2 (11%)
4	NAG	A	620	2	14,14,15	0.83	1 (7%)	17,19,21	0.86	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
7	HEM	A	605	2	-	6/14/54/54	-
4	NAG	B	630	2	-	0/6/23/26	0/1/1/1
4	NAG	A	630	2	-	0/6/23/26	0/1/1/1
7	HEM	B	605	1,2	-	5/14/54/54	-
4	NAG	B	620	2	-	1/6/23/26	0/1/1/1
4	NAG	A	620	2	-	2/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	605	HEM	FE-NB	3.72	2.06	1.94
4	A	630	NAG	C1-C2	-3.64	1.47	1.52
7	A	605	HEM	CBC-CAC	3.40	1.46	1.30
7	B	605	HEM	CBC-CAC	3.19	1.45	1.30
7	B	605	HEM	CBB-CAB	3.15	1.45	1.30
7	B	605	HEM	FE-NC	3.15	2.05	1.95
4	B	630	NAG	C1-C2	-3.04	1.48	1.52
7	A	605	HEM	CBB-CAB	3.01	1.44	1.30
7	A	605	HEM	CAB-C3B	-2.70	1.40	1.47
7	A	605	HEM	FE-NA	2.69	2.04	1.95
7	B	605	HEM	O2A-CGA	-2.57	1.22	1.30
7	B	605	HEM	CAB-C3B	-2.48	1.40	1.47
7	A	605	HEM	O2A-CGA	-2.47	1.22	1.30
7	B	605	HEM	FE-ND	-2.44	1.87	1.94
4	A	620	NAG	C1-C2	2.27	1.55	1.52
7	A	605	HEM	O2D-CGD	-2.26	1.23	1.30
7	B	605	HEM	O2D-CGD	-2.17	1.23	1.30
4	B	620	NAG	C1-C2	-2.13	1.49	1.52
7	B	605	HEM	CAC-C3C	-2.03	1.42	1.47
4	A	630	NAG	O5-C1	-2.00	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	620	NAG	C1-O5-C5	4.49	118.20	112.19
4	A	630	NAG	C1-C2-N2	-3.73	104.55	110.43
4	A	630	NAG	C6-C5-C4	3.50	121.60	113.02
4	A	630	NAG	C3-C4-C5	-3.45	103.98	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	605	HEM	C3B-C4B-NB	3.34	111.87	109.47
4	A	630	NAG	O4-C4-C3	-2.91	103.52	110.38
4	A	630	NAG	O4-C4-C5	2.90	116.45	109.32
7	A	605	HEM	C3B-C4B-NB	2.84	111.51	109.47
4	B	630	NAG	C2-N2-C7	-2.76	119.20	122.90
4	A	620	NAG	C1-O5-C5	2.35	115.33	112.19
4	B	620	NAG	C2-N2-C7	-2.27	119.85	122.90
4	B	630	NAG	C3-C4-C5	-2.22	106.22	110.23
4	B	630	NAG	C6-C5-C4	2.13	118.26	113.02

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605	HEM	C2B-C3B-CAB-CBB
4	A	620	NAG	C4-C5-C6-O6
4	A	620	NAG	O5-C5-C6-O6
4	B	620	NAG	O5-C5-C6-O6
7	B	605	HEM	CAD-CBD-CGD-O2D
7	B	605	HEM	CAA-CBA-CGA-O1A
7	B	605	HEM	CAD-CBD-CGD-O1D
7	B	605	HEM	CAA-CBA-CGA-O2A
7	A	605	HEM	CAD-CBD-CGD-O2D
7	A	605	HEM	CAD-CBD-CGD-O1D
7	A	605	HEM	CAA-CBA-CGA-O1A
7	A	605	HEM	C4B-C3B-CAB-CBB
7	A	605	HEM	CAA-CBA-CGA-O2A
7	B	605	HEM	C2B-C3B-CAB-CBB

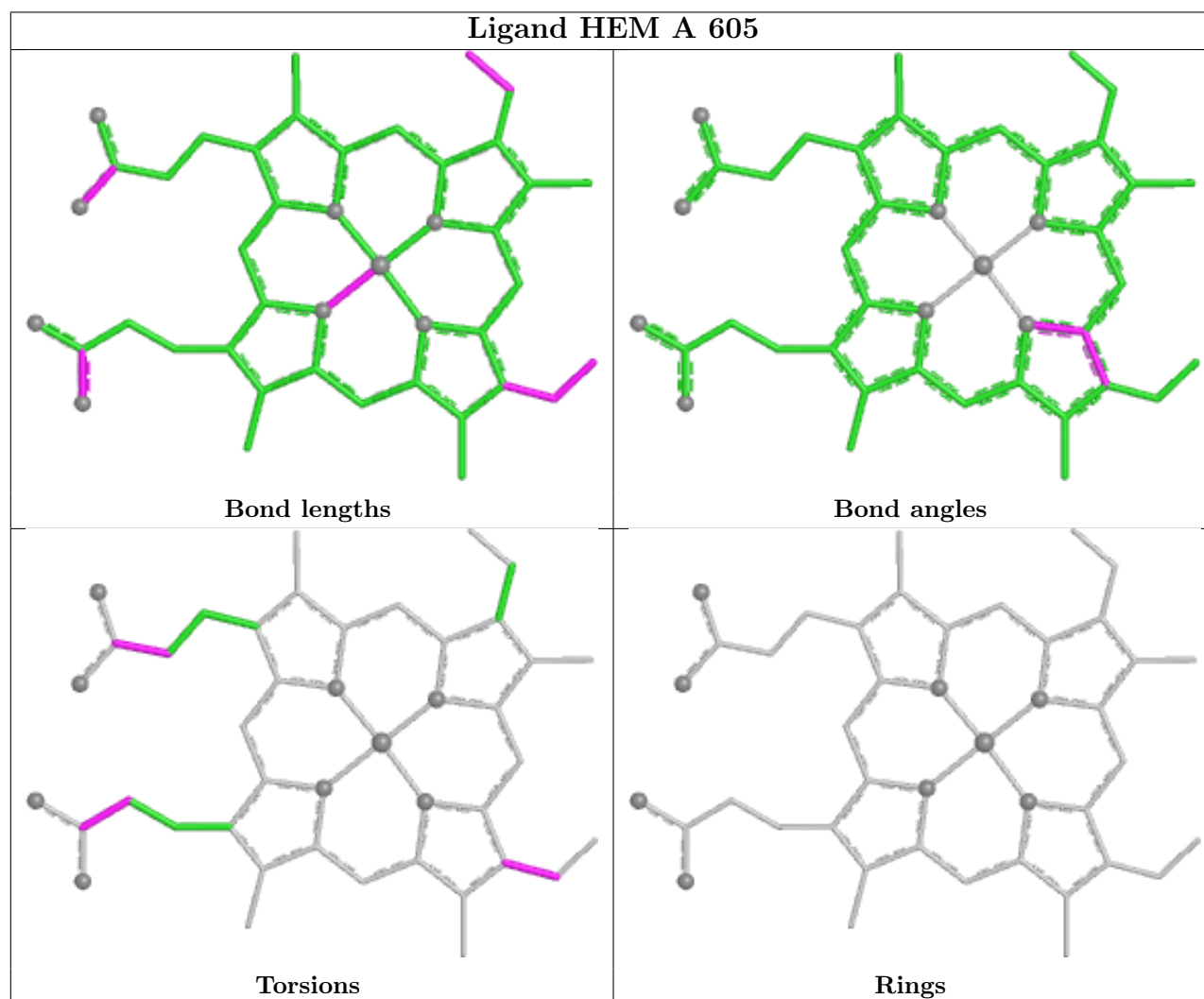
There are no ring outliers.

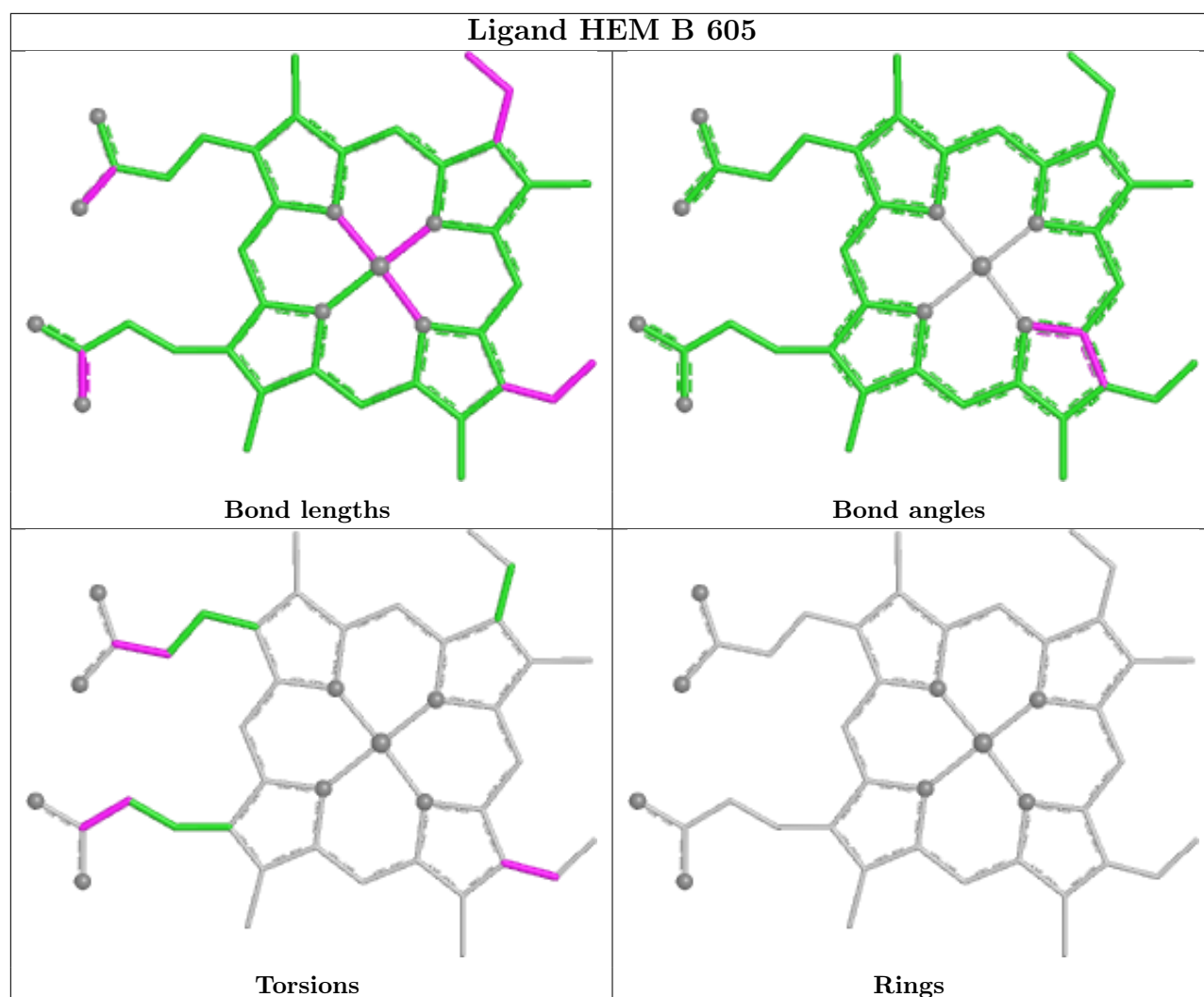
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	605	HEM	2	0
7	B	605	HEM	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.