Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 08:19 AM EDT

PDB ID	:	1MHL
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:

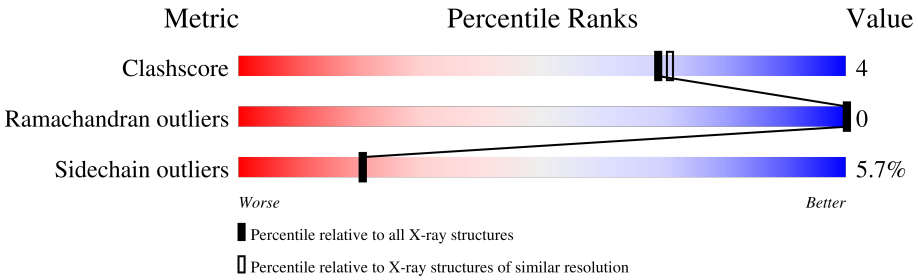
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	75% 19%
1	B	108	81% 13%
2	C	466	79% 18%
2	D	466	83% 14%
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.

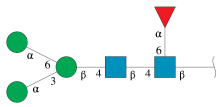
- Molecule 1 is a protein called MYELOPEROXIDASE.

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.

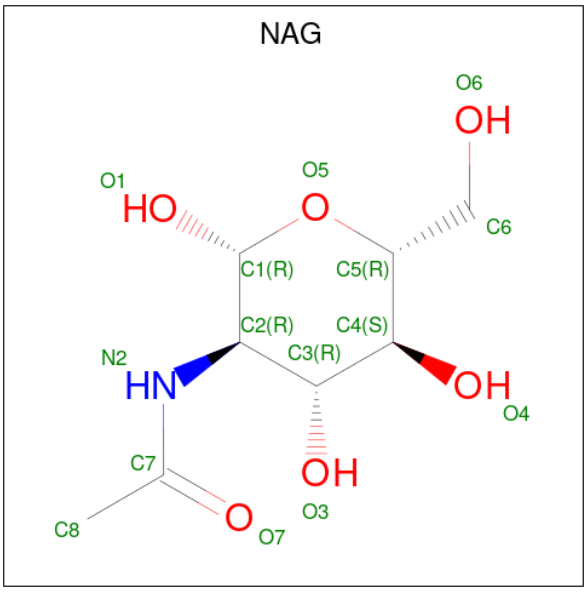
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	82	0	0
			3732	2351	687	667	27			
2	D	466	Total	C	N	O	S	109	0	0
			3732	2351	687	667	27			

- 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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

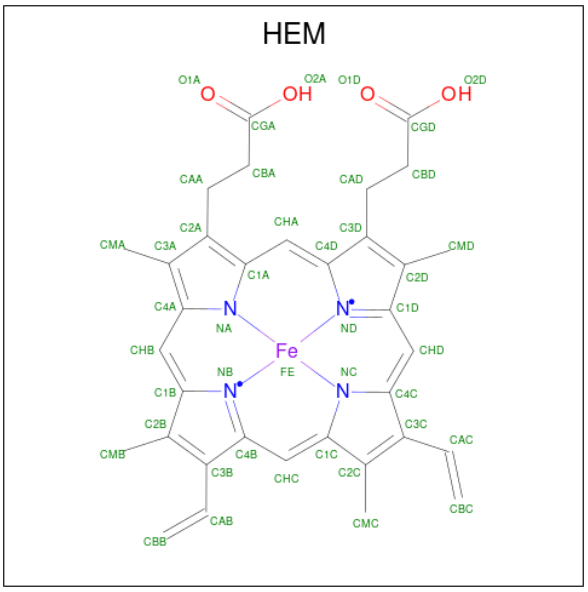
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 8 is water.

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

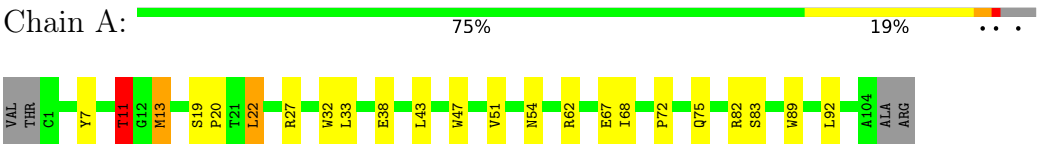
3 Residue-property plots (i)

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. 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.

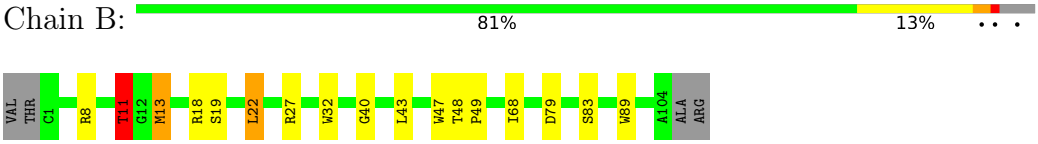
• Molecule 1: MYELOPEROXIDASE

Chain A:



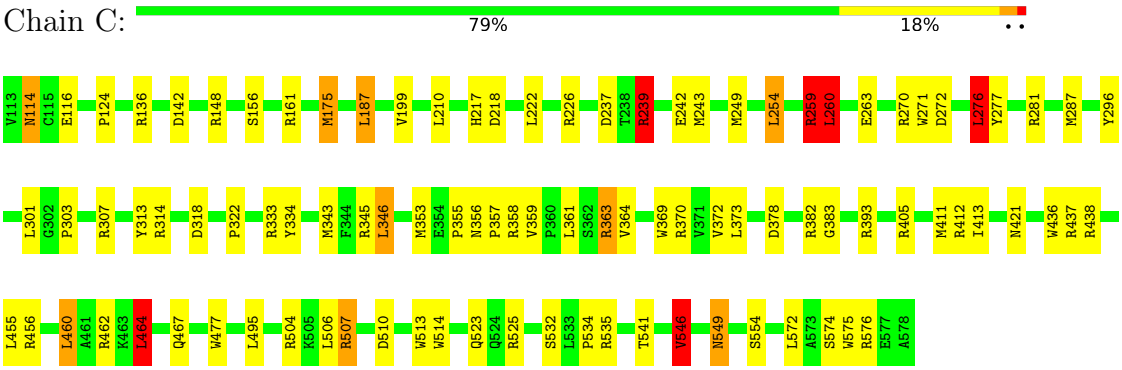
• Molecule 1: MYELOPEROXIDASE

Chain B:



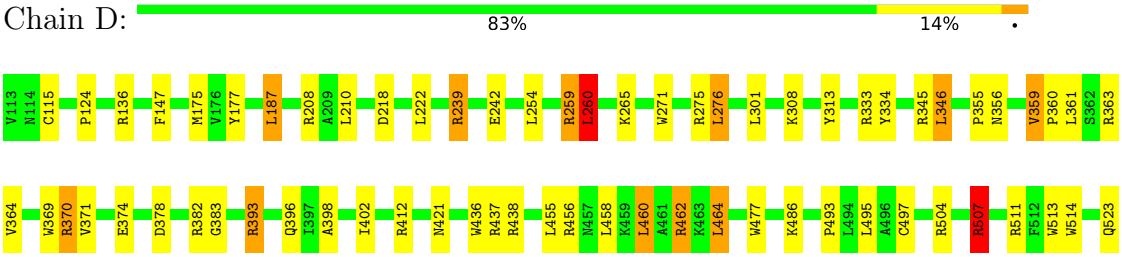
• Molecule 2: MYELOPEROXIDASE

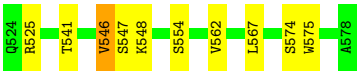
Chain C:



• Molecule 2: MYELOPEROXIDASE

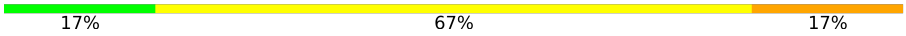
Chain D:





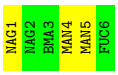
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• 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:



4 Data and refinement statistics (i)

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: NAG, BMA, CL, HEM, CA, FUC, 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	0.82	0/862	1.62	14/1174 (1.2%)
1	B	0.77	0/862	1.59	14/1174 (1.2%)
2	C	0.78	0/3818	1.58	76/5180 (1.5%)
2	D	0.75	0/3818	1.57	53/5180 (1.0%)
All	All	0.77	0/9360	1.58	157/12708 (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
2	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	507	ARG	NE-CZ-NH2	-17.73	111.44	120.30
2	D	239	ARG	NE-CZ-NH1	17.67	129.13	120.30
2	D	507	ARG	NE-CZ-NH1	15.93	128.26	120.30
2	C	507	ARG	NE-CZ-NH1	14.17	127.38	120.30
2	D	345	ARG	NE-CZ-NH2	-13.97	113.31	120.30
2	D	239	ARG	NE-CZ-NH2	-13.96	113.32	120.30
2	C	239	ARG	NE-CZ-NH2	-13.84	113.38	120.30
2	C	239	ARG	NE-CZ-NH1	13.51	127.05	120.30
2	C	507	ARG	NE-CZ-NH2	-12.95	113.83	120.30
2	D	345	ARG	NE-CZ-NH1	11.18	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	345	ARG	NE-CZ-NH2	-10.43	115.08	120.30
2	D	370	ARG	NE-CZ-NH2	-10.12	115.24	120.30
2	D	393	ARG	NE-CZ-NH1	9.86	125.23	120.30
2	C	370	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	C	382	ARG	NE-CZ-NH2	-9.79	115.41	120.30
2	D	370	ARG	NE-CZ-NH1	9.55	125.08	120.30
2	D	438	ARG	NE-CZ-NH1	9.50	125.05	120.30
2	C	370	ARG	NE-CZ-NH1	9.50	125.05	120.30
2	D	513	TRP	CD1-CG-CD2	9.47	113.87	106.30
2	C	405	ARG	NE-CZ-NH1	9.14	124.87	120.30
2	D	382	ARG	NE-CZ-NH2	-9.12	115.74	120.30
2	C	369	TRP	CD1-CG-CD2	8.98	113.48	106.30
1	A	11	THR	N-CA-CB	-8.96	93.28	110.30
2	D	514	TRP	CD1-CG-CD2	8.85	113.38	106.30
2	C	438	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	B	27	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	13	MET	CA-CB-CG	8.35	127.49	113.30
2	D	513	TRP	CE2-CD2-CG	-8.26	100.69	107.30
2	C	382	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	D	369	TRP	CD1-CG-CD2	8.16	112.83	106.30
2	D	438	ARG	NE-CZ-NH2	-8.13	116.23	120.30
2	C	438	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	C	437	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	D	393	ARG	NE-CZ-NH2	-8.03	116.28	120.30
2	C	243	MET	CG-SD-CE	7.99	112.98	100.20
2	C	514	TRP	CD1-CG-CD2	7.99	112.69	106.30
2	D	436	TRP	CD1-CG-CD2	7.86	112.59	106.30
2	D	382	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	D	514	TRP	CE2-CD2-CG	-7.80	101.06	107.30
2	D	504	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	47	TRP	CD1-CG-CD2	7.68	112.45	106.30
2	C	575	TRP	CD1-CG-CD2	7.67	112.44	106.30
2	C	504	ARG	NE-CZ-NH1	7.67	124.13	120.30
2	C	393	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	D	136	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	C	271	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	B	47	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	C	477	TRP	CD1-CG-CD2	7.38	112.20	106.30
2	C	513	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	D	369	TRP	CE2-CD2-CG	-7.32	101.45	107.30
2	C	436	TRP	CD1-CG-CD2	7.26	112.11	106.30
1	A	62	ARG	NE-CZ-NH1	7.22	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	314	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	C	369	TRP	CE2-CD2-CG	-7.18	101.55	107.30
2	D	575	TRP	CD1-CG-CD2	7.18	112.04	106.30
2	D	436	TRP	CE2-CD2-CG	-7.16	101.57	107.30
2	C	513	TRP	CD1-CG-CD2	7.15	112.02	106.30
2	D	575	TRP	CE2-CD2-CG	-7.13	101.59	107.30
2	C	514	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	47	TRP	CD1-CG-CD2	7.08	111.97	106.30
2	C	462	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	C	281	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	C	318	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	32	TRP	CE2-CD2-CG	-6.99	101.70	107.30
2	D	437	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	C	575	TRP	CE2-CD2-CG	-6.87	101.80	107.30
2	D	271	TRP	CD1-CG-CD2	6.84	111.77	106.30
2	C	314	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	C	546	VAL	N-CA-CB	-6.82	96.49	111.50
2	C	436	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	A	47	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	11	THR	N-CA-CB	-6.78	97.41	110.30
2	C	525	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	C	296	TYR	CB-CG-CD2	-6.76	116.94	121.00
2	C	412	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	C	259	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	32	TRP	CD1-CG-CD2	6.70	111.66	106.30
1	B	32	TRP	CD1-CG-CD2	6.69	111.65	106.30
2	C	148	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	D	275	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	C	271	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	B	32	TRP	CE2-CD2-CG	-6.62	102.01	107.30
2	D	462	ARG	NE-CZ-NH1	6.57	123.59	120.30
2	C	477	TRP	CE2-CD2-CG	-6.57	102.05	107.30
1	B	47	TRP	CG-CD2-CE3	6.56	139.81	133.90
2	D	271	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	B	8	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	D	437	ARG	NE-CZ-NH2	-6.49	117.06	120.30
2	C	287	MET	CG-SD-CE	-6.46	89.86	100.20
2	C	525	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	C	148	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	8	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	C	412	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	D	477	TRP	CD1-CG-CD2	6.27	111.32	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	89	TRP	CE2-CD2-CG	-6.26	102.29	107.30
2	C	243	MET	CA-CB-CG	6.20	123.84	113.30
1	A	89	TRP	CE2-CD2-CG	-6.19	102.35	107.30
2	C	363	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	C	369	TRP	CG-CD1-NE1	-6.14	103.96	110.10
2	C	276	LEU	CA-CB-CG	6.13	129.41	115.30
2	D	514	TRP	CG-CD2-CE3	6.04	139.34	133.90
2	C	345	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	89	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	B	47	TRP	CB-CG-CD1	-5.97	119.24	127.00
2	D	456	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	C	456	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	C	393	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	D	477	TRP	CE2-CD2-CG	-5.89	102.59	107.30
2	C	437	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	D	525	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	C	270	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	89	TRP	CD1-CG-CD2	5.76	110.91	106.30
2	D	546	VAL	N-CA-CB	-5.69	98.98	111.50
2	C	358	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	82	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	79	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	7	TYR	CB-CG-CD2	-5.67	117.60	121.00
2	C	535	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	D	513	TRP	CG-CD1-NE1	-5.65	104.45	110.10
2	D	525	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	D	218	ASP	N-CA-C	-5.60	95.88	111.00
1	A	27	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	D	511	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	C	343	MET	N-CA-C	-5.48	96.20	111.00
1	A	32	TRP	CG-CD2-CE3	5.48	138.83	133.90
2	C	277	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	D	513	TRP	CB-CG-CD1	-5.46	119.89	127.00
2	D	514	TRP	CB-CG-CD1	-5.44	119.93	127.00
2	C	462	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	D	514	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	C	464	LEU	CA-CB-CG	5.42	127.76	115.30
2	C	136	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	C	575	TRP	CG-CD1-NE1	-5.34	104.76	110.10
2	C	535	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	C	226	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	C	345	ARG	CB-CG-CD	-5.27	97.91	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	D	369	TRP	CG-CD1-NE1	-5.25	104.85	110.10
2	C	405	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	D	260	LEU	CA-CB-CG	5.23	127.34	115.30
2	C	576	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	C	260	LEU	CA-CB-CG	5.21	127.28	115.30
2	C	514	TRP	CG-CD2-CE3	5.19	138.57	133.90
2	D	187	LEU	CA-CB-CG	5.17	127.18	115.30
2	C	218	ASP	N-CA-C	-5.15	97.08	111.00
2	C	175	MET	CA-CB-CG	5.15	122.06	113.30
2	D	271	TRP	CG-CD2-CE3	5.13	138.52	133.90
2	D	208	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	C	549	ASN	O-C-N	-5.09	114.55	122.70
2	C	411	MET	CG-SD-CE	-5.08	92.06	100.20
2	D	412	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	C	187	LEU	CA-CB-CG	5.08	126.98	115.30
2	D	371	VAL	CG1-CB-CG2	-5.08	102.77	110.90
2	C	513	TRP	CB-CG-CD1	-5.07	120.41	127.00
2	C	142	ASP	CB-CG-OD1	5.07	122.86	118.30
2	D	177	TYR	N-CA-C	5.05	124.64	111.00
1	A	47	TRP	CG-CD1-NE1	-5.03	105.07	110.10

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	31	0
2	D	3732	0	3725	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
8	C	158	0	0	0	0
8	D	150	0	0	0	0
All	All	9847	0	9280	68	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 (68) 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
2:D:393:ARG:HH11	2:D:393:ARG:HG2	1.67	0.59
7:A:605:HEM:HMC1	7:A:605:HEM:HBC2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	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 (i)

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%)	38	46
1	B	90/93 (97%)	86 (96%)	4 (4%)	28	32
2	C	411/411 (100%)	387 (94%)	24 (6%)	20	20
2	D	411/411 (100%)	385 (94%)	26 (6%)	18	17
All	All	1002/1008 (99%)	945 (94%)	57 (6%)	20	20

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

Mol	Chain	Res	Type
1	A	11	THR
1	A	22	LEU
1	A	43	LEU
2	C	114	ASN
2	C	124	PRO
2	C	156	SER
2	C	175	MET
2	C	187	LEU
2	C	210	LEU
2	C	217	HIS
2	C	222	LEU
2	C	239	ARG
2	C	254	LEU
2	C	259	ARG
2	C	260	LEU
2	C	276	LEU
2	C	301	LEU
2	C	322	PRO
2	C	346	LEU
2	C	359	VAL
2	C	455	LEU
2	C	460	LEU
2	C	464	LEU
2	C	495	LEU
2	C	523	GLN
2	C	546	VAL
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	175	MET

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Mol	Chain	Res	Type
2	D	187	LEU
2	D	210	LEU
2	D	222	LEU
2	D	239	ARG
2	D	254	LEU
2	D	259	ARG
2	D	260	LEU
2	D	276	LEU
2	D	301	LEU
2	D	346	LEU
2	D	355	PRO
2	D	356	ASN
2	D	359	VAL
2	D	455	LEU
2	D	460	LEU
2	D	464	LEU
2	D	495	LEU
2	D	497	CYS
2	D	507	ARG
2	D	523	GLN
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	114	ASN
2	C	421	ASN
2	C	467	GLN
2	C	549	ASN
1	B	54	ASN
1	B	80	GLN
2	D	421	ASN
2	D	549	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
3	NAG	E	2	3	14,14,15	0.90	0	17,19,21	1.02	2 (11%)
3	BMA	E	3	3	11,11,12	0.73	0	15,15,17	0.85	0
3	MAN	E	4	3	11,11,12	0.56	0	15,15,17	1.14	1 (6%)
3	MAN	E	5	3	11,11,12	0.63	0	15,15,17	1.04	1 (6%)
3	FUC	E	6	3	10,10,11	0.68	0	14,14,16	1.27	2 (14%)
3	NAG	F	1	3,2	14,14,15	0.68	0	17,19,21	1.46	1 (5%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	0.75	0
3	BMA	F	3	3	11,11,12	0.38	0	15,15,17	1.00	0
3	MAN	F	4	3	11,11,12	0.97	0	15,15,17	1.53	4 (26%)
3	MAN	F	5	3	11,11,12	0.77	0	15,15,17	1.52	2 (13%)
3	FUC	F	6	3	10,10,11	0.53	0	14,14,16	1.14	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	3,2	-	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	3,2	-	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 (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5	MAN	C1-O5-C5	4.48	118.27	112.19
3	F	1	NAG	C1-C2-N2	4.05	117.41	110.49
3	F	4	MAN	O2-C2-C1	3.49	116.28	109.15
3	E	4	MAN	O2-C2-C1	2.99	115.27	109.15
3	E	5	MAN	C1-O5-C5	2.80	115.99	112.19
3	F	5	MAN	C6-C5-C4	-2.63	106.84	113.00
3	E	6	FUC	C6-C5-C4	-2.49	108.48	113.07
3	F	4	MAN	C6-C5-C4	2.44	118.72	113.00
3	E	2	NAG	C4-C3-C2	-2.23	107.74	111.02
3	E	2	NAG	C1-C2-N2	-2.21	106.72	110.49
3	F	4	MAN	O5-C5-C4	-2.17	105.54	110.83
3	E	1	NAG	C3-C4-C5	2.13	114.05	110.24
3	E	6	FUC	O3-C3-C4	-2.06	105.58	110.35
3	F	4	MAN	C3-C4-C5	-2.06	106.56	110.24

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

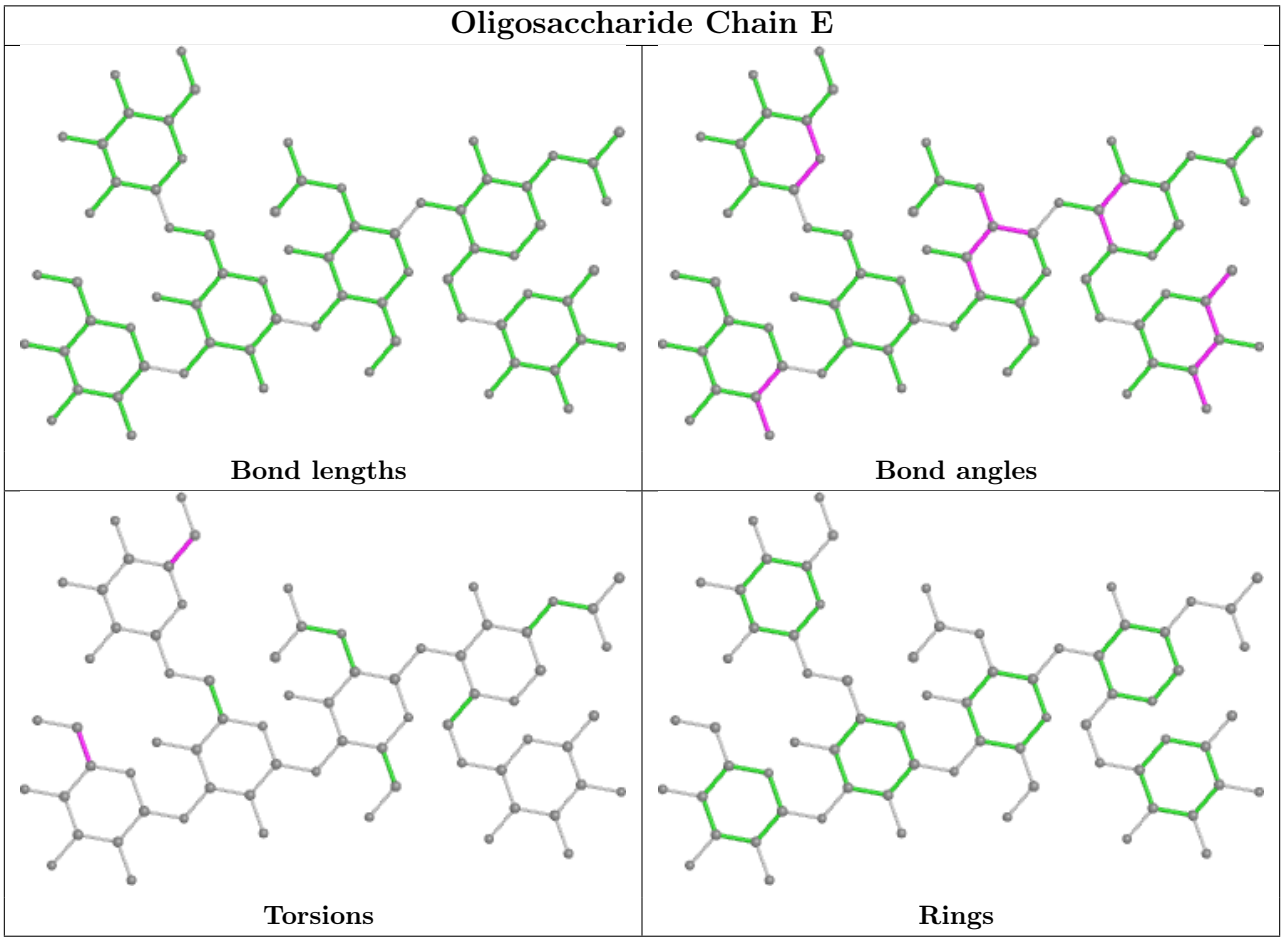
There are no ring outliers.

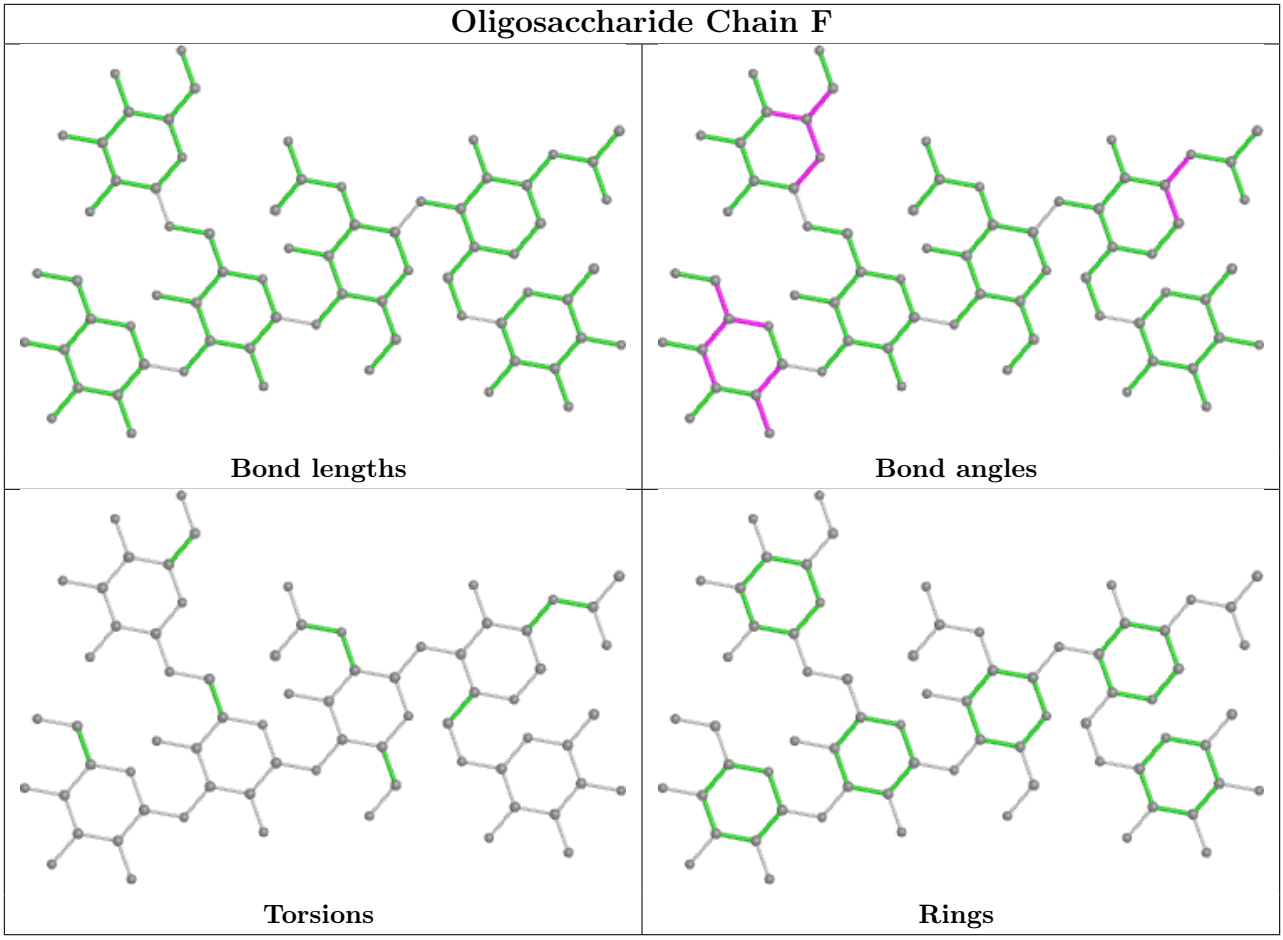
1 monomer is involved in 1 short contact:

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.

Oligosaccharide Chain E





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	$\#\|Z\| > 2$
4	NAG	B	620	2	14,14,15	0.94	0	17,19,21	1.43	2 (11%)
4	NAG	B	630	2	14,14,15	1.05	1 (7%)	17,19,21	1.39	3 (17%)
7	HEM	B	605	8,1,2	41,50,50	1.35	6 (14%)	45,82,82	0.98	2 (4%)
4	NAG	A	620	2	14,14,15	0.80	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	A	630	2	14,14,15	1.17	2 (14%)	17,19,21	2.00	5 (29%)
7	HEM	A	605	8,1,2	41,50,50	1.25	6 (14%)	45,82,82	1.09	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	620	2	-	1/6/23/26	0/1/1/1
4	NAG	B	630	2	-	0/6/23/26	0/1/1/1
7	HEM	B	605	8,1,2	-	4/12/54/54	-
4	NAG	A	620	2	-	2/6/23/26	0/1/1/1
4	NAG	A	630	2	-	0/6/23/26	0/1/1/1
7	HEM	A	605	8,1,2	-	6/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	630	NAG	C1-C2	-3.31	1.47	1.52
7	B	605	HEM	CBB-CAB	3.07	1.45	1.30
7	A	605	HEM	CBB-CAB	2.93	1.44	1.30
7	B	605	HEM	C3C-CAC	-2.85	1.42	1.47
4	B	630	NAG	C1-C2	-2.76	1.48	1.52
7	A	605	HEM	C3C-CAC	-2.75	1.42	1.47
7	A	605	HEM	CAB-C3B	-2.66	1.40	1.47
7	A	605	HEM	CBC-CAC	2.64	1.46	1.29
7	B	605	HEM	O2A-CGA	-2.51	1.22	1.30
7	B	605	HEM	CBC-CAC	2.48	1.45	1.29
7	B	605	HEM	CAB-C3B	-2.44	1.40	1.47
7	A	605	HEM	O2A-CGA	-2.41	1.22	1.30
7	A	605	HEM	O2D-CGD	-2.19	1.23	1.30
4	A	630	NAG	O5-C1	-2.12	1.40	1.43
7	B	605	HEM	O2D-CGD	-2.11	1.23	1.30
4	A	620	NAG	C1-C2	2.07	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	620	NAG	C1-O5-C5	4.44	118.20	112.19
4	A	630	NAG	C6-C5-C4	3.67	121.60	113.00
4	A	630	NAG	C3-C4-C5	-3.51	103.98	110.24
7	A	605	HEM	C4C-CHD-C1D	3.49	127.16	122.56
4	A	630	NAG	C1-C2-N2	-3.48	104.55	110.49
4	A	630	NAG	O4-C4-C3	-2.95	103.52	110.35
4	A	630	NAG	O4-C4-C5	2.88	116.45	109.30
4	B	630	NAG	C2-N2-C7	-2.60	119.20	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	620	NAG	C1-O5-C5	2.32	115.33	112.19
4	B	630	NAG	C3-C4-C5	-2.26	106.22	110.24
4	B	630	NAG	C6-C5-C4	2.24	118.26	113.00
7	A	605	HEM	C2C-C3C-C4C	-2.16	105.39	106.90
7	B	605	HEM	C4B-CHC-C1C	2.15	125.40	122.56
4	B	620	NAG	C2-N2-C7	-2.14	119.85	122.90
7	B	605	HEM	CMC-C2C-C3C	2.03	128.47	124.68
7	A	605	HEM	CMC-C2C-C3C	2.01	128.44	124.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

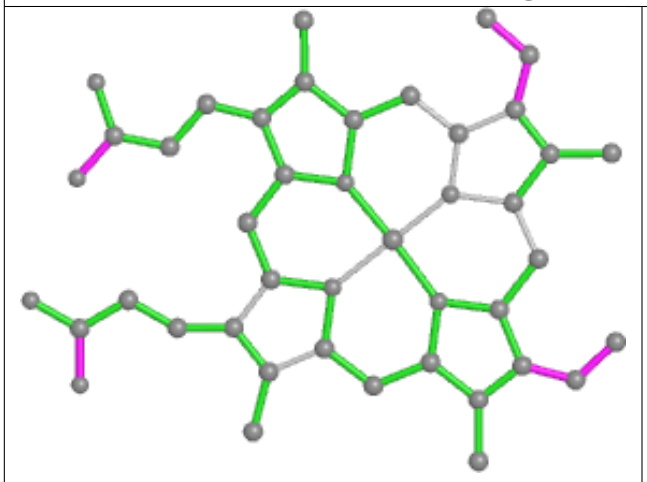
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	605	HEM	1	0
7	A	605	HEM	2	0

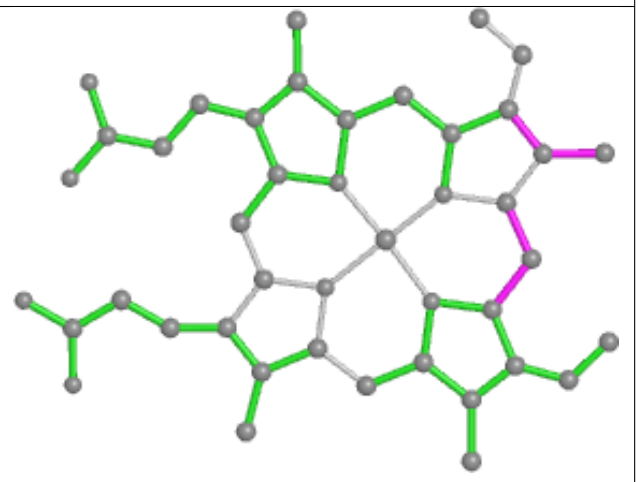
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

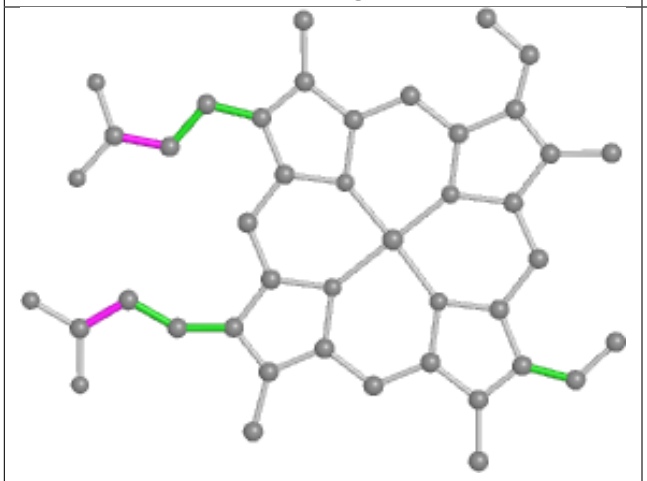
Ligand HEM B 605



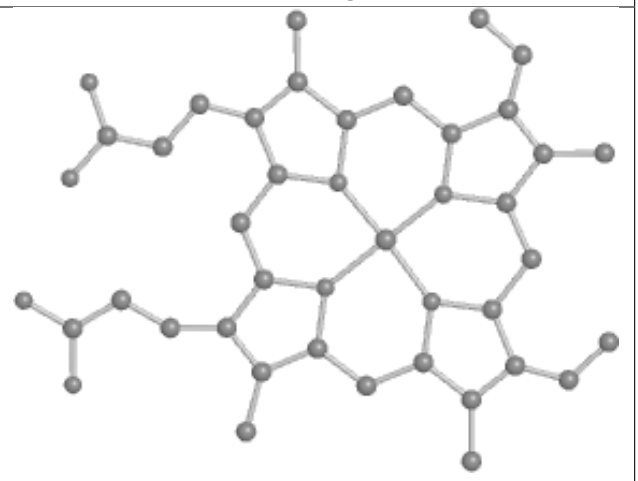
Bond lengths



Bond angles

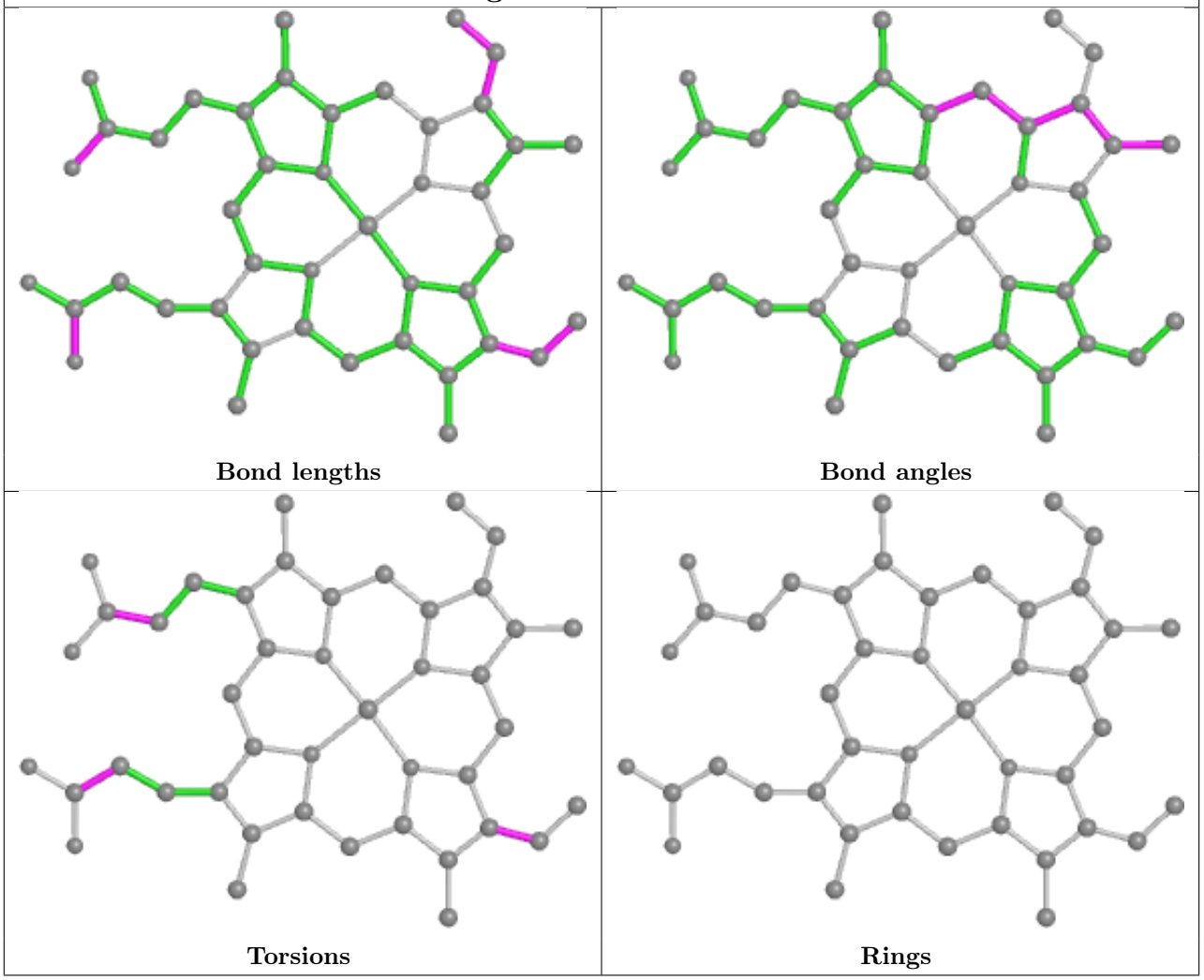


Torsions



Rings

Ligand HEM A 605



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.