



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:37 PM UTC

PDB ID : 6MX4 / pdb_00006mx4
EMDB ID : EMD-9280
Title : CryoEM structure of chimeric Eastern Equine Encephalitis Virus
Authors : Hasan, S.S.; Sun, C.; Kim, A.S.; Watanabe, Y.; Chen, C.L.; Klose, T.; Buda, G.; Crispin, M.; Diamond, M.S.; Klimstra, W.B.; Rossmann, M.G.
Deposited on : 2018-10-30
Resolution : 4.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

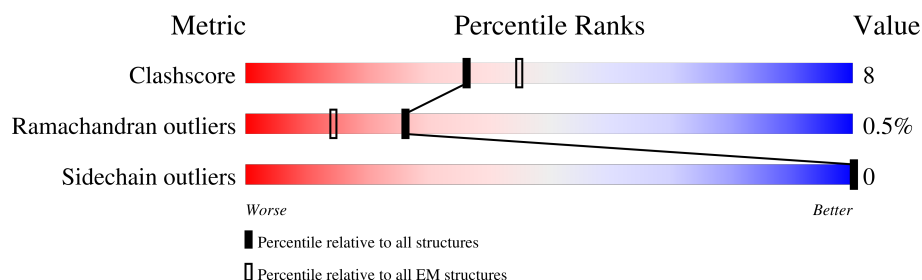
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	441	 77% 20% .
1	D	441	 75% 22% .
1	G	441	 76% 20% .
1	J	441	 78% 20% .
2	B	420	 79% 20%
2	E	420	 77% 23%
2	H	420	 80% 20%
2	K	420	 80% 20%
3	C	260	 52% 10% 38%

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Mol	Chain	Length	Quality of chain
3	F	260	
3	I	260	
3	L	260	
4	M	3	
4	N	3	
4	O	3	
4	P	3	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31491 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	430	Total	C	N	O	S	0	0
			3286	2096	544	626	20		
1	D	430	Total	C	N	O	S	0	0
			3286	2096	544	626	20		
1	G	430	Total	C	N	O	S	0	0
			3286	2096	544	626	20		
1	J	430	Total	C	N	O	S	0	0
			3286	2096	544	626	20		

- Molecule 2 is a protein called E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3294	2084	595	591	24		
2	E	420	Total	C	N	O	S	0	0
			3294	2084	595	591	24		
2	H	420	Total	C	N	O	S	0	0
			3294	2084	595	591	24		
2	K	420	Total	C	N	O	S	0	0
			3294	2084	595	591	24		

- Molecule 3 is a protein called Capsid.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
3	F	159	Total	C	N	O	S	0	0
			1230	773	219	231	7		
3	I	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		
3	L	160	Total	C	N	O	S	0	0
			1239	778	221	233	7		

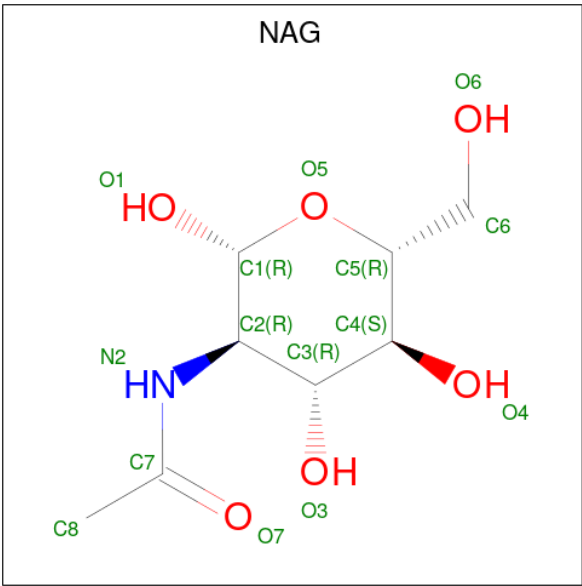
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	3	Total	C	N	O	0	0
			42	24	3	15		
4	N	3	Total	C	N	O	0	0
			42	24	3	15		
4	O	3	Total	C	N	O	0	0
			42	24	3	15		
4	P	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



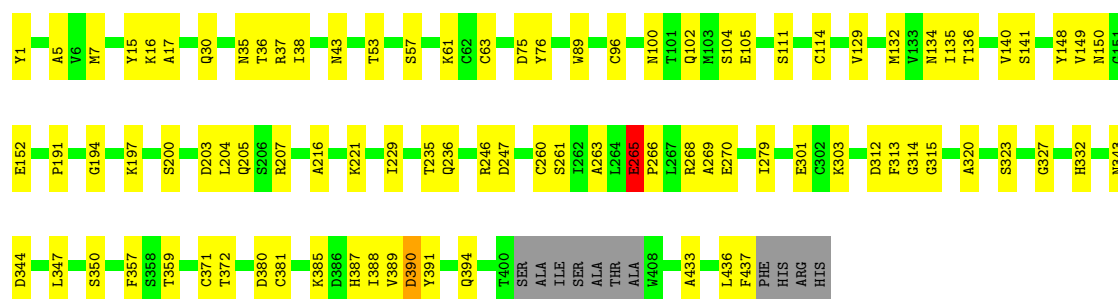
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	K	1	Total	C	N	O	0
			14	8	1	5	

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.

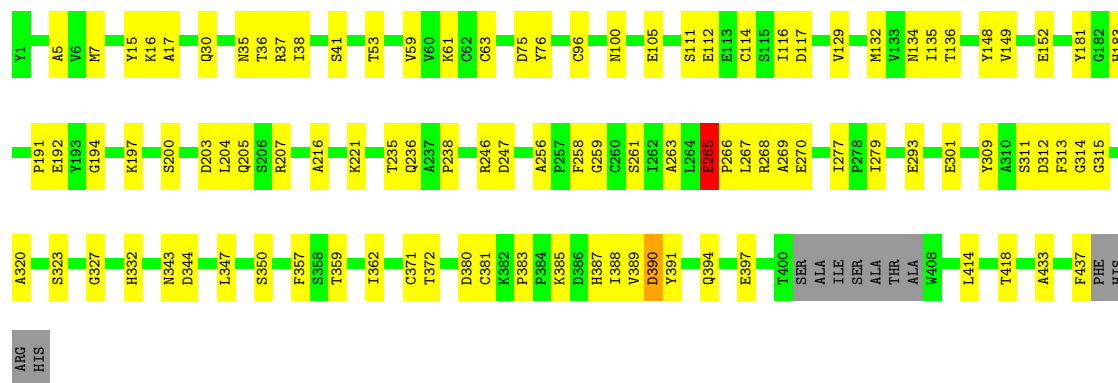
• Molecule 1: E1

Chain A: 



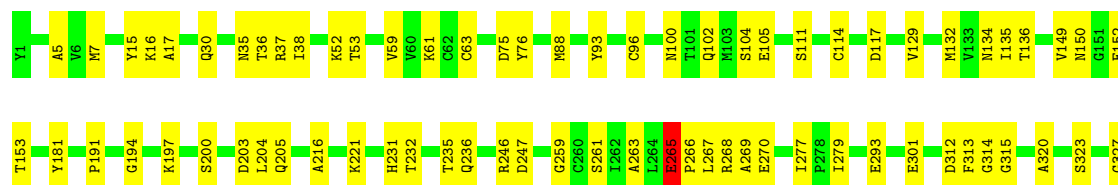
• Molecule 1: E1

Chain D: 



• Molecule 1: E1

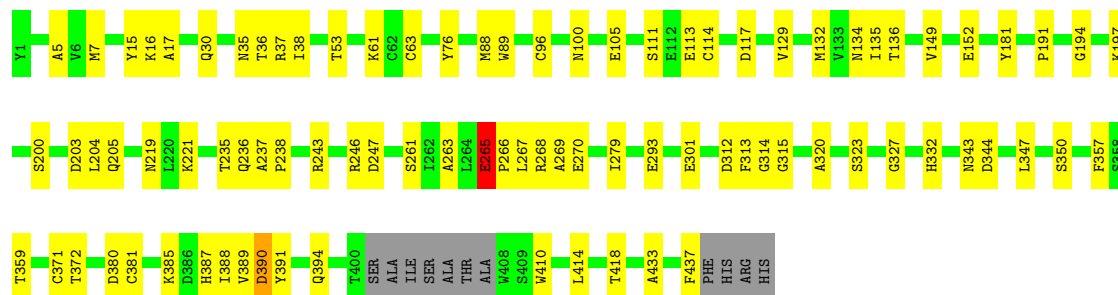
Chain G: 





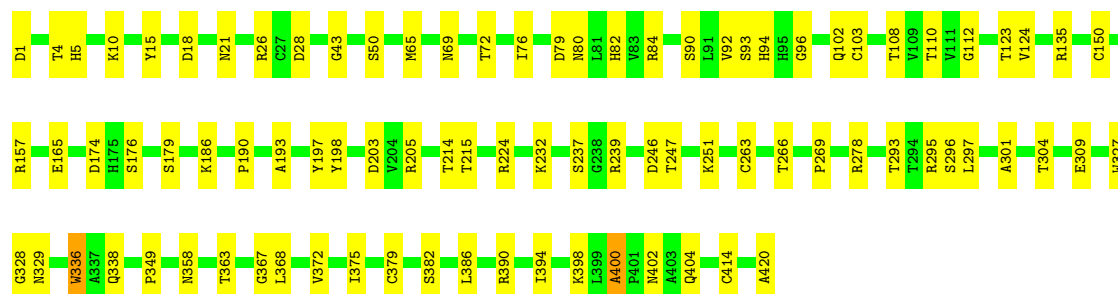
• Molecule 1: E1

Chain J: 78% 20%



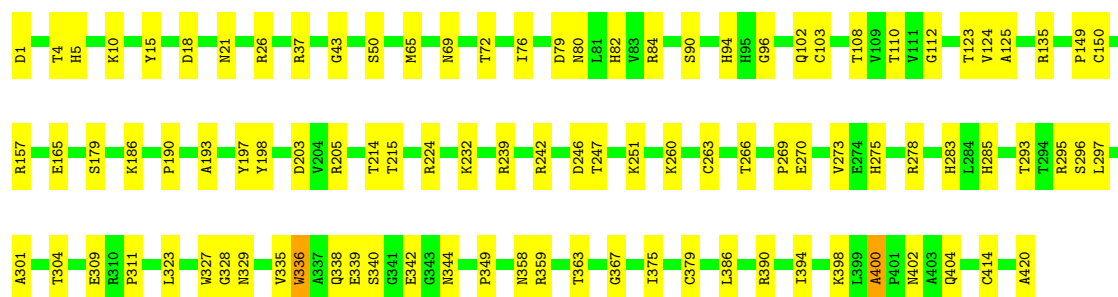
• Molecule 2: E2

Chain B: 79% 20%



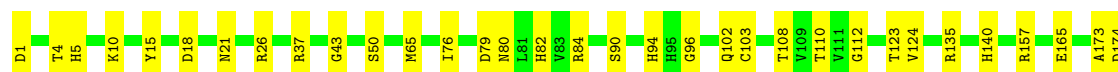
• Molecule 2: E2

Chain E: 77% 23%

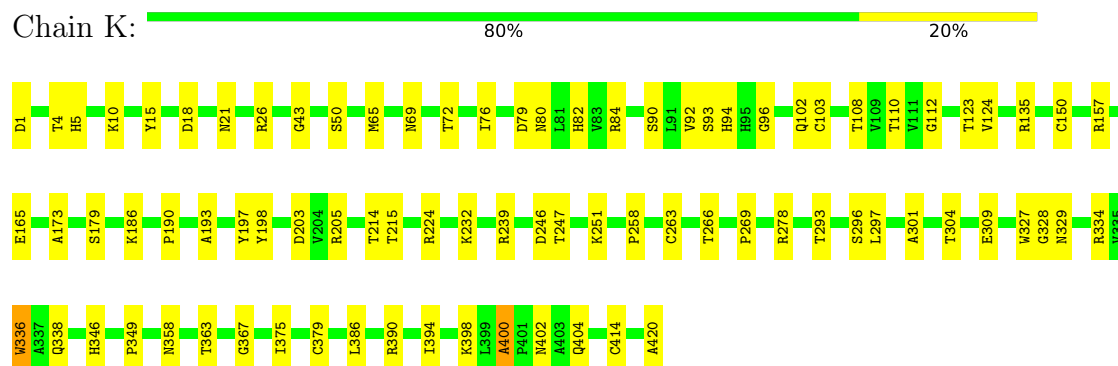


• Molecule 2: E2

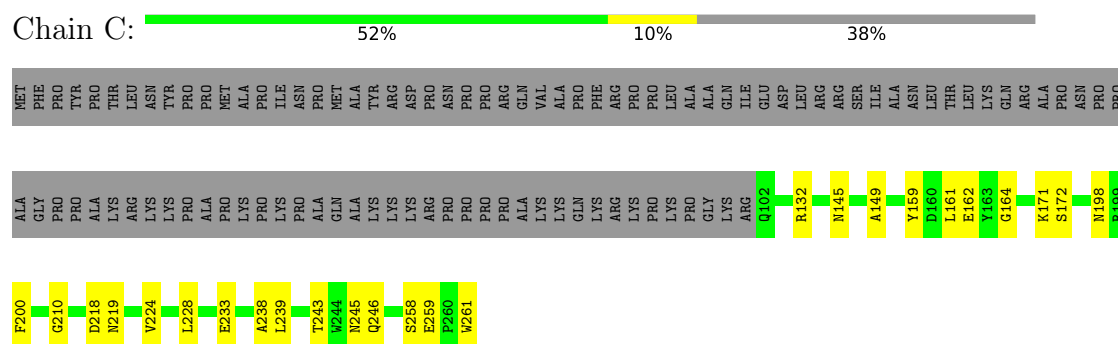
Chain H: 80% 20%



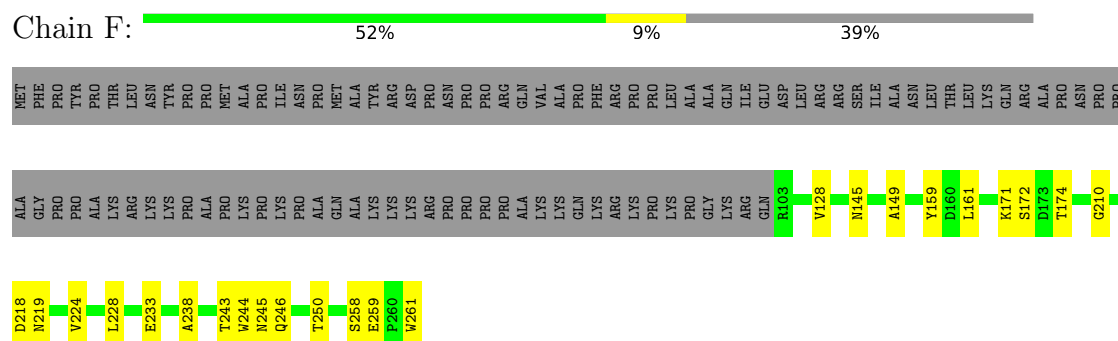
- Molecule 2: E2



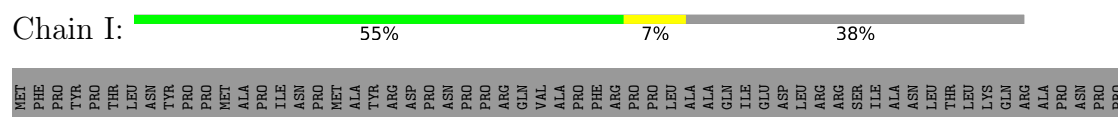
- Molecule 3: Capsid

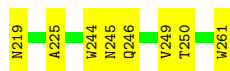


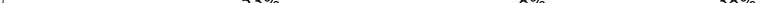
- Molecule 3: Capsid

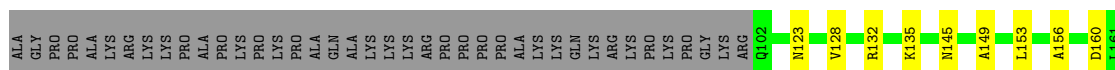


- Molecule 3: Capsid



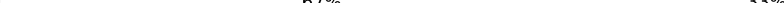


Chain L:  53% 8% 38%

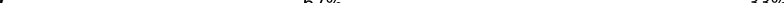


Chain M: 67% 33%

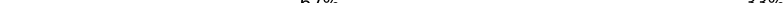


Chain N:  67% 33%



Chain O:  67% 33%



Chain P:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/3375	0.62	1/4607 (0.0%)
1	D	0.43	0/3375	0.62	1/4607 (0.0%)
1	G	0.43	0/3375	0.62	1/4607 (0.0%)
1	J	0.43	0/3375	0.62	1/4607 (0.0%)
2	B	0.41	0/3389	0.64	2/4624 (0.0%)
2	E	0.41	0/3389	0.64	2/4624 (0.0%)
2	H	0.41	0/3389	0.64	2/4624 (0.0%)
2	K	0.41	0/3389	0.64	2/4624 (0.0%)
3	C	0.30	0/1266	0.58	0/1711
3	F	0.31	0/1257	0.56	0/1699
3	I	0.31	0/1266	0.57	0/1711
3	L	0.38	0/1266	0.57	0/1711
All	All	0.41	0/32111	0.62	12/43756 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	G	0	1
1	J	0	1
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
3	C	0	1
3	L	0	1
All	All	0	14

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	265	GLU	N-CA-C	-6.85	94.68	109.81
1	J	265	GLU	N-CA-C	-6.84	94.69	109.81
1	A	265	GLU	N-CA-C	-6.83	94.72	109.81
1	G	265	GLU	N-CA-C	-6.83	94.72	109.81
2	E	198	TYR	CA-CB-CG	5.82	124.37	113.90
2	B	198	TYR	CA-CB-CG	5.79	124.32	113.90
2	H	198	TYR	CA-CB-CG	5.78	124.31	113.90
2	K	198	TYR	CA-CB-CG	5.78	124.31	113.90
2	B	336	TRP	CA-CB-CG	5.07	123.23	113.60
2	H	336	TRP	CA-CB-CG	5.07	123.23	113.60
2	K	336	TRP	CA-CB-CG	5.07	123.22	113.60
2	E	336	TRP	CA-CB-CG	5.06	123.22	113.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	LYS	Peptide
2	B	400	ALA	Peptide
2	B	414	CYS	Peptide
3	C	162	GLU	Peptide
1	D	385	LYS	Peptide
2	E	400	ALA	Peptide
2	E	414	CYS	Peptide
1	G	385	LYS	Peptide
2	H	400	ALA	Peptide
2	H	414	CYS	Peptide
1	J	385	LYS	Peptide
2	K	400	ALA	Peptide
2	K	414	CYS	Peptide
3	L	164	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3286	0	3193	65	0
1	D	3286	0	3193	91	0
1	G	3286	0	3193	59	0
1	J	3286	0	3193	58	0
2	B	3294	0	3251	57	0
2	E	3294	0	3251	86	0
2	H	3294	0	3251	57	0
2	K	3294	0	3251	52	0
3	C	1239	0	1225	15	0
3	F	1230	0	1217	12	0
3	I	1239	0	1225	10	0
3	L	1239	0	1225	11	0
4	M	42	0	37	0	0
4	N	42	0	37	0	0
4	O	42	0	37	0	0
4	P	42	0	37	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
5	H	14	0	13	0	0
5	K	14	0	13	0	0
All	All	31491	0	30868	479	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 8.

All (479) 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:437:PHE:O	2:H:419:ARG:NH1	1.95	0.98
1:D:390:ASP:O	2:E:336:TRP:N	2.09	0.85
1:A:207:ARG:NH2	1:D:148:TYR:OH	2.11	0.83
1:G:93:TYR:HB3	2:H:173:ALA:HB2	1.62	0.82
1:D:259:GLY:HA2	2:E:297:LEU:HD22	1.61	0.81
1:D:311:SER:H	2:E:338:GLN:HE22	1.31	0.78
1:D:387:HIS:ND1	2:E:340:SER:OG	2.15	0.78
1:A:389:VAL:O	2:B:336:TRP:N	2.13	0.78
1:D:311:SER:N	2:E:338:GLN:HE22	1.82	0.78
3:C:132:ARG:NE	3:C:164:GLY:O	2.16	0.77
2:K:269:PRO:O	2:K:327:TRP:NE1	2.18	0.77
2:B:197:TYR:OH	2:B:214:THR:OG1	2.03	0.76
2:H:205:ARG:O	2:H:224:ARG:NH2	2.19	0.76
2:H:108:THR:OG1	2:H:124:VAL:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:PRO:O	2:H:327:TRP:NE1	2.18	0.76
2:E:205:ARG:O	2:E:224:ARG:NH2	2.19	0.76
2:K:205:ARG:O	2:K:224:ARG:NH2	2.19	0.76
2:E:108:THR:OG1	2:E:124:VAL:O	2.04	0.76
2:B:205:ARG:O	2:B:224:ARG:NH2	2.19	0.76
2:E:269:PRO:O	2:E:327:TRP:NE1	2.18	0.75
2:K:108:THR:OG1	2:K:124:VAL:O	2.03	0.75
2:B:269:PRO:O	2:B:327:TRP:NE1	2.18	0.75
3:L:128:VAL:O	3:L:174:THR:OG1	2.04	0.75
2:B:108:THR:OG1	2:B:124:VAL:O	2.04	0.75
2:B:266:THR:OG1	2:B:329:ASN:ND2	2.20	0.75
2:K:266:THR:OG1	2:K:329:ASN:ND2	2.20	0.75
2:H:266:THR:OG1	2:H:329:ASN:ND2	2.20	0.75
2:H:197:TYR:OH	2:H:214:THR:OG1	2.03	0.75
2:K:197:TYR:OH	2:K:214:THR:OG1	2.03	0.74
2:E:266:THR:OG1	2:E:329:ASN:ND2	2.20	0.74
2:E:197:TYR:OH	2:E:214:THR:OG1	2.03	0.74
1:J:30:GLN:OE1	1:J:136:THR:OG1	2.06	0.74
1:D:30:GLN:OE1	1:D:136:THR:OG1	2.06	0.74
1:J:410:TRP:HE1	2:K:346:HIS:CE1	2.06	0.74
1:G:30:GLN:OE1	1:G:136:THR:OG1	2.06	0.73
2:B:10:LYS:O	2:B:232:LYS:NZ	2.22	0.72
2:E:10:LYS:O	2:E:232:LYS:NZ	2.22	0.72
2:B:135:ARG:NH2	2:B:328:GLY:O	2.23	0.72
2:K:10:LYS:O	2:K:232:LYS:NZ	2.22	0.72
2:H:10:LYS:O	2:H:232:LYS:NZ	2.22	0.72
2:H:135:ARG:NH2	2:H:328:GLY:O	2.23	0.72
1:A:30:GLN:OE1	1:A:136:THR:OG1	2.06	0.72
2:E:135:ARG:NH2	2:E:328:GLY:O	2.23	0.71
1:G:76:TYR:OH	1:G:105:GLU:OE1	2.08	0.71
2:K:135:ARG:NH2	2:K:328:GLY:O	2.23	0.71
1:D:76:TYR:OH	1:D:105:GLU:OE1	2.08	0.71
2:K:296:SER:OG	2:K:301:ALA:O	2.06	0.71
1:J:76:TYR:OH	1:J:105:GLU:OE1	2.08	0.70
1:A:76:TYR:OH	1:A:105:GLU:OE1	2.08	0.70
2:E:278:ARG:NH2	2:E:358:ASN:O	2.25	0.70
2:B:278:ARG:NH2	2:B:358:ASN:O	2.25	0.70
2:H:278:ARG:NH2	2:H:358:ASN:O	2.25	0.69
1:J:111:SER:N	1:J:114:CYS:SG	2.66	0.69
3:L:123:ASN:OD1	3:L:209:LYS:NZ	2.25	0.69
2:K:278:ARG:NH2	2:K:358:ASN:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:SER:N	1:G:114:CYS:SG	2.66	0.69
1:A:111:SER:N	1:A:114:CYS:SG	2.66	0.69
1:D:111:SER:N	1:D:114:CYS:SG	2.66	0.69
1:A:207:ARG:NH2	1:D:148:TYR:HH	1.91	0.69
1:J:359:THR:O	1:J:394:GLN:NE2	2.26	0.69
2:B:65:MET:N	2:B:76:ILE:O	2.26	0.69
2:E:65:MET:N	2:E:76:ILE:O	2.26	0.69
1:G:359:THR:O	1:G:394:GLN:NE2	2.26	0.69
2:H:404:GLN:HG2	2:H:420:ALA:HB1	1.75	0.68
1:D:359:THR:O	1:D:394:GLN:NE2	2.26	0.68
1:D:383:PRO:HG2	2:E:342:GLU:HA	1.75	0.68
2:K:404:GLN:HG2	2:K:420:ALA:HB1	1.75	0.68
1:A:359:THR:O	1:A:394:GLN:NE2	2.26	0.68
1:A:391:TYR:OH	2:B:297:LEU:HD11	1.94	0.68
2:B:296:SER:OG	2:B:301:ALA:O	2.06	0.68
1:A:436:LEU:O	2:H:419:ARG:NH1	2.27	0.68
2:B:394:ILE:O	2:B:398:LYS:N	2.27	0.68
1:D:391:TYR:OH	2:E:323:LEU:O	2.09	0.68
2:E:296:SER:OG	2:E:301:ALA:O	2.06	0.67
2:E:394:ILE:O	2:E:398:LYS:N	2.27	0.67
2:B:404:GLN:HG2	2:B:420:ALA:HB1	1.75	0.67
2:K:65:MET:N	2:K:76:ILE:O	2.26	0.67
2:H:65:MET:N	2:H:76:ILE:O	2.26	0.67
2:E:404:GLN:HG2	2:E:420:ALA:HB1	1.75	0.66
2:K:394:ILE:O	2:K:398:LYS:N	2.27	0.66
1:A:43:ASN:OD1	1:D:41:SER:OG	2.05	0.66
2:H:394:ILE:O	2:H:398:LYS:N	2.27	0.66
2:H:296:SER:OG	2:H:301:ALA:O	2.06	0.65
1:D:388:ILE:HD13	2:E:273:VAL:HG11	1.79	0.65
1:D:383:PRO:CG	2:E:342:GLU:HA	2.27	0.64
1:D:387:HIS:H	2:E:275:HIS:CD2	2.16	0.63
1:D:388:ILE:HD13	2:E:273:VAL:CG1	2.28	0.63
1:D:387:HIS:HB2	2:E:275:HIS:NE2	2.14	0.63
2:B:21:ASN:OD1	2:B:123:THR:OG1	2.11	0.63
1:J:88:MET:O	2:K:173:ALA:HB3	1.97	0.62
2:K:18:ASP:O	2:K:239:ARG:NH1	2.32	0.62
2:H:18:ASP:O	2:H:239:ARG:NH1	2.32	0.62
1:D:53:THR:OG1	1:D:236:GLN:OE1	2.18	0.62
1:A:53:THR:OG1	1:A:236:GLN:OE1	2.18	0.62
2:E:18:ASP:O	2:E:239:ARG:NH1	2.32	0.62
1:G:53:THR:OG1	1:G:236:GLN:OE1	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:LEU:O	2:B:390:ARG:N	2.33	0.61
3:C:228:LEU:O	3:C:261:TRP:NE1	2.32	0.61
1:J:53:THR:OG1	1:J:236:GLN:OE1	2.18	0.61
2:B:18:ASP:O	2:B:239:ARG:NH1	2.32	0.61
1:D:259:GLY:CA	2:E:297:LEU:HD22	2.29	0.61
2:K:386:LEU:O	2:K:390:ARG:N	2.33	0.61
2:H:386:LEU:O	2:H:390:ARG:N	2.33	0.61
2:H:94:HIS:NE2	2:H:96:GLY:O	2.34	0.61
2:K:94:HIS:NE2	2:K:96:GLY:O	2.34	0.60
1:D:259:GLY:HA2	2:E:297:LEU:CD2	2.30	0.60
2:E:94:HIS:NE2	2:E:96:GLY:O	2.34	0.60
2:E:386:LEU:O	2:E:390:ARG:N	2.33	0.60
3:I:132:ARG:NE	3:I:164:GLY:O	2.33	0.60
1:D:383:PRO:CB	2:E:342:GLU:HA	2.33	0.59
3:F:210:GLY:N	3:F:261:TRP:O	2.35	0.59
2:B:94:HIS:NE2	2:B:96:GLY:O	2.34	0.59
3:F:228:LEU:O	3:F:261:TRP:NE1	2.36	0.59
1:D:38:ILE:HD12	1:D:269:ALA:HB3	1.85	0.58
1:A:57:SER:OG	2:B:237:SER:O	2.16	0.58
2:E:82:HIS:N	2:E:112:GLY:O	2.37	0.58
2:H:21:ASN:OD1	2:H:123:THR:OG1	2.11	0.58
1:J:38:ILE:HD12	1:J:269:ALA:HB3	1.86	0.58
1:A:38:ILE:HD12	1:A:269:ALA:HB3	1.85	0.58
2:E:311:PRO:HG2	1:J:243:ARG:HD2	1.85	0.57
2:E:21:ASN:OD1	2:E:123:THR:OG1	2.11	0.57
2:K:43:GLY:O	2:K:103:CYS:N	2.38	0.57
1:G:38:ILE:HD12	1:G:269:ALA:HB3	1.86	0.57
2:B:90:SER:O	2:B:102:GLN:N	2.37	0.57
2:H:43:GLY:O	2:H:103:CYS:N	2.38	0.57
2:K:90:SER:O	2:K:102:GLN:N	2.37	0.57
2:H:90:SER:O	2:H:102:GLN:N	2.37	0.57
2:E:90:SER:O	2:E:102:GLN:N	2.37	0.57
2:E:125:ALA:HB2	2:H:140:HIS:HD2	1.69	0.57
1:A:387:HIS:CD2	2:B:338:GLN:HE21	2.22	0.57
2:H:82:HIS:N	2:H:112:GLY:O	2.37	0.56
1:A:391:TYR:CZ	2:B:297:LEU:HD11	2.40	0.56
2:E:285:HIS:NE2	1:J:238:PRO:O	2.38	0.56
1:J:221:LYS:O	1:J:235:THR:OG1	2.20	0.56
1:A:150:ASN:ND2	1:D:192:GLU:HG2	2.19	0.56
3:C:198:ASN:ND2	2:H:418:THR:O	2.38	0.56
1:D:194:GLY:N	1:D:205:GLN:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:82:HIS:N	2:K:112:GLY:O	2.37	0.56
1:J:194:GLY:N	1:J:205:GLN:OE1	2.39	0.56
2:E:4:THR:OG1	2:E:157:ARG:NH1	2.39	0.56
2:E:270:GLU:HB2	1:J:219:ASN:ND2	2.21	0.56
3:I:244:TRP:CD1	3:I:250:THR:HG1	2.23	0.56
1:D:238:PRO:O	2:H:285:HIS:NE2	2.39	0.56
1:A:194:GLY:N	1:A:205:GLN:OE1	2.39	0.55
1:G:194:GLY:N	1:G:205:GLN:OE1	2.39	0.55
2:K:4:THR:OG1	2:K:157:ARG:NH1	2.39	0.55
2:E:43:GLY:O	2:E:103:CYS:N	2.38	0.55
2:B:43:GLY:O	2:B:103:CYS:N	2.38	0.55
2:B:82:HIS:N	2:B:112:GLY:O	2.37	0.55
3:C:233:GLU:OE2	3:C:238:ALA:HB2	2.06	0.55
2:H:4:THR:OG1	2:H:157:ARG:NH1	2.39	0.55
2:B:400:ALA:O	2:B:402:ASN:N	2.39	0.55
1:D:389:VAL:O	2:E:336:TRP:N	2.33	0.55
2:K:400:ALA:O	2:K:402:ASN:N	2.39	0.55
2:H:15:TYR:N	2:H:50:SER:O	2.40	0.55
2:B:15:TYR:N	2:B:50:SER:O	2.40	0.55
2:E:15:TYR:N	2:E:50:SER:O	2.40	0.55
2:B:4:THR:OG1	2:B:157:ARG:NH1	2.39	0.54
1:D:238:PRO:HD2	2:H:285:HIS:CD2	2.42	0.54
2:E:400:ALA:O	2:E:402:ASN:N	2.40	0.54
1:J:89:TRP:HD1	2:K:173:ALA:O	1.89	0.54
1:G:221:LYS:O	1:G:235:THR:OG1	2.20	0.54
2:K:15:TYR:N	2:K:50:SER:O	2.40	0.54
2:H:400:ALA:O	2:H:402:ASN:N	2.39	0.54
1:J:117:ASP:OD1	1:J:181:TYR:OH	2.20	0.54
3:L:156:ALA:O	3:L:160:ASP:N	2.38	0.54
1:G:52:LYS:HZ1	2:H:37:ARG:HD2	1.73	0.54
2:B:203:ASP:OD2	2:B:215:THR:N	2.41	0.54
3:F:244:TRP:CD1	3:F:250:THR:HG1	2.26	0.53
2:H:190:PRO:HD2	2:H:193:ALA:HB3	1.90	0.53
2:K:203:ASP:OD2	2:K:215:THR:N	2.41	0.53
2:B:190:PRO:HD2	2:B:193:ALA:HB3	1.90	0.53
3:F:128:VAL:O	3:F:174:THR:OG1	2.25	0.53
2:K:190:PRO:HD2	2:K:193:ALA:HB3	1.90	0.53
2:E:165:GLU:OE2	2:E:251:LYS:NZ	2.41	0.53
1:D:61:LYS:NZ	1:D:63:CYS:O	2.41	0.53
2:B:165:GLU:OE2	2:B:251:LYS:NZ	2.41	0.53
2:E:190:PRO:HD2	2:E:193:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:ASN:OD1	1:G:36:THR:N	2.42	0.53
1:J:61:LYS:NZ	1:J:63:CYS:O	2.41	0.53
2:K:165:GLU:OE2	2:K:251:LYS:NZ	2.41	0.53
3:C:224:VAL:O	3:C:243:THR:OG1	2.19	0.53
2:H:165:GLU:OE2	2:H:251:LYS:NZ	2.41	0.53
1:D:315:GLY:O	1:D:357:PHE:N	2.42	0.53
1:G:197:LYS:O	1:G:200:SER:OG	2.18	0.53
2:H:203:ASP:OD2	2:H:215:THR:N	2.41	0.53
1:A:61:LYS:NZ	1:A:63:CYS:O	2.41	0.52
2:B:398:LYS:O	3:C:132:ARG:NH1	2.42	0.52
1:D:35:ASN:OD1	1:D:36:THR:N	2.42	0.52
2:E:203:ASP:OD2	2:E:215:THR:N	2.41	0.52
2:E:285:HIS:CE1	1:J:243:ARG:HD2	2.44	0.52
1:J:5:ALA:N	1:J:279:ILE:O	2.43	0.52
1:J:35:ASN:OD1	1:J:36:THR:N	2.42	0.52
1:A:343:ASN:OD1	1:A:344:ASP:N	2.42	0.52
1:D:371:CYS:O	1:D:372:THR:OG1	2.25	0.52
1:G:61:LYS:NZ	1:G:63:CYS:O	2.41	0.52
1:D:343:ASN:OD1	1:D:344:ASP:N	2.42	0.52
1:G:343:ASN:OD1	1:G:344:ASP:N	2.42	0.52
1:A:35:ASN:OD1	1:A:36:THR:N	2.42	0.52
3:I:245:ASN:OD1	3:I:246:GLN:N	2.43	0.52
1:J:315:GLY:O	1:J:357:PHE:N	2.42	0.52
1:J:343:ASN:OD1	1:J:344:ASP:N	2.42	0.52
3:L:218:ASP:OD1	3:L:219:ASN:N	2.43	0.52
3:F:218:ASP:OD1	3:F:219:ASN:N	2.43	0.52
3:I:114:PHE:O	3:I:126:ALA:N	2.43	0.52
2:K:398:LYS:O	3:L:132:ARG:NH1	2.43	0.52
1:J:391:TYR:CE2	2:K:334:ARG:HD3	2.44	0.52
1:A:315:GLY:O	1:A:357:PHE:N	2.42	0.51
1:J:203:ASP:OD1	1:J:204:LEU:N	2.43	0.51
2:B:5:HIS:NE2	2:B:157:ARG:O	2.44	0.51
3:C:218:ASP:OD1	3:C:219:ASN:N	2.43	0.51
3:I:218:ASP:OD1	3:I:219:ASN:N	2.44	0.51
2:H:5:HIS:NE2	2:H:157:ARG:O	2.44	0.51
1:G:389:VAL:HG12	1:G:390:ASP:H	1.76	0.51
1:A:221:LYS:O	1:A:235:THR:OG1	2.19	0.51
3:I:210:GLY:N	3:I:261:TRP:O	2.41	0.51
1:A:5:ALA:N	1:A:279:ILE:O	2.42	0.51
1:A:260:CYS:H	2:B:295:ARG:HH22	1.58	0.51
3:C:245:ASN:OD1	3:C:246:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:246:ASP:OD1	2:E:247:THR:N	2.44	0.51
1:J:389:VAL:HG12	1:J:390:ASP:H	1.76	0.51
2:K:5:HIS:NE2	2:K:157:ARG:O	2.44	0.51
2:B:246:ASP:OD1	2:B:247:THR:N	2.44	0.51
2:E:5:HIS:NE2	2:E:157:ARG:O	2.44	0.51
2:B:375:ILE:O	2:B:379:CYS:N	2.44	0.51
2:K:246:ASP:OD1	2:K:247:THR:N	2.44	0.51
1:A:203:ASP:OD1	1:A:204:LEU:N	2.43	0.51
1:A:301:GLU:O	1:A:320:ALA:N	2.43	0.51
1:A:389:VAL:HG12	1:A:390:ASP:H	1.76	0.51
1:D:389:VAL:HG12	1:D:390:ASP:H	1.76	0.51
1:G:15:TYR:O	1:G:17:ALA:N	2.44	0.51
3:L:245:ASN:OD1	3:L:246:GLN:N	2.44	0.50
1:D:389:VAL:O	2:E:335:VAL:HA	2.11	0.50
2:E:82:HIS:O	2:E:112:GLY:N	2.44	0.50
2:H:246:ASP:OD1	2:H:247:THR:N	2.44	0.50
1:D:5:ALA:N	1:D:279:ILE:O	2.42	0.50
1:D:15:TYR:O	1:D:17:ALA:N	2.44	0.50
1:D:116:ILE:HD11	2:E:260:LYS:N	2.25	0.50
1:J:15:TYR:O	1:J:17:ALA:N	2.44	0.50
1:J:433:ALA:O	1:J:437:PHE:N	2.44	0.50
1:A:15:TYR:O	1:A:17:ALA:N	2.44	0.50
3:C:200:PHE:O	3:C:239:LEU:N	2.45	0.50
1:G:5:ALA:N	1:G:279:ILE:O	2.42	0.50
1:J:388:ILE:HD12	1:J:388:ILE:O	2.12	0.50
2:B:82:HIS:O	2:B:112:GLY:N	2.44	0.50
1:G:59:VAL:HG22	2:H:242:ARG:HG2	1.94	0.50
1:J:371:CYS:O	1:J:372:THR:OG1	2.25	0.50
3:F:224:VAL:O	3:F:243:THR:OG1	2.25	0.50
2:K:375:ILE:O	2:K:379:CYS:N	2.44	0.50
1:D:7:MET:SD	1:D:279:ILE:HD12	2.52	0.50
2:K:21:ASN:OD1	2:K:123:THR:OG1	2.11	0.50
1:D:433:ALA:O	1:D:437:PHE:N	2.44	0.50
2:E:375:ILE:O	2:E:379:CYS:N	2.44	0.50
1:G:433:ALA:O	1:G:437:PHE:N	2.44	0.50
2:H:375:ILE:O	2:H:379:CYS:N	2.44	0.50
2:K:82:HIS:O	2:K:112:GLY:N	2.44	0.50
1:D:388:ILE:HD12	1:D:388:ILE:O	2.12	0.49
1:G:7:MET:SD	1:G:279:ILE:HD12	2.52	0.49
1:G:105:GLU:OE2	2:H:242:ARG:NH2	2.45	0.49
1:A:433:ALA:O	1:A:437:PHE:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:GLU:N	2:B:309:GLU:OE1	2.46	0.49
2:H:82:HIS:O	2:H:112:GLY:N	2.44	0.49
1:J:7:MET:SD	1:J:279:ILE:HD12	2.52	0.49
1:D:203:ASP:OD1	1:D:204:LEU:N	2.43	0.49
1:G:203:ASP:OD1	1:G:204:LEU:N	2.43	0.49
1:G:315:GLY:O	1:G:357:PHE:N	2.42	0.49
3:F:245:ASN:OD1	3:F:246:GLN:N	2.45	0.49
1:A:7:MET:SD	1:A:279:ILE:HD12	2.52	0.49
2:E:363:THR:O	2:E:367:GLY:N	2.42	0.49
1:J:197:LYS:O	1:J:200:SER:OG	2.18	0.49
2:K:309:GLU:OE1	2:K:309:GLU:N	2.46	0.49
1:A:265:GLU:OE1	1:A:268:ARG:NH2	2.46	0.49
2:E:293:THR:OG1	2:E:304:THR:O	2.30	0.49
2:K:363:THR:O	2:K:367:GLY:N	2.42	0.49
2:B:174:ASP:OD1	2:B:176:SER:OG	2.28	0.49
1:J:265:GLU:OE1	1:J:268:ARG:NH2	2.46	0.49
1:A:89:TRP:N	2:B:28:ASP:OD2	2.46	0.49
1:D:383:PRO:HG2	2:E:342:GLU:CA	2.40	0.49
1:G:259:GLY:HA2	2:H:297:LEU:HD22	1.94	0.49
2:H:293:THR:OG1	2:H:304:THR:O	2.30	0.49
1:D:197:LYS:O	1:D:200:SER:OG	2.18	0.49
1:D:265:GLU:OE1	1:D:268:ARG:NH2	2.46	0.48
1:G:388:ILE:HD12	1:G:388:ILE:O	2.12	0.48
1:A:268:ARG:NE	1:A:270:GLU:OE2	2.47	0.48
1:A:388:ILE:O	1:A:388:ILE:HD12	2.12	0.48
2:B:363:THR:O	2:B:367:GLY:N	2.42	0.48
1:D:37:ARG:HH12	1:D:132:MET:HG3	1.79	0.48
1:G:37:ARG:HH12	1:G:132:MET:HG3	1.79	0.48
2:E:1:ASP:O	2:E:157:ARG:NH1	2.47	0.48
1:J:37:ARG:HH12	1:J:132:MET:HG3	1.78	0.48
1:A:371:CYS:O	1:A:372:THR:OG1	2.25	0.48
2:B:1:ASP:O	2:B:157:ARG:NH1	2.47	0.48
1:D:311:SER:N	2:E:338:GLN:NE2	2.58	0.48
2:E:270:GLU:HB2	1:J:219:ASN:HD21	1.77	0.48
1:G:265:GLU:OE1	1:G:268:ARG:NH2	2.46	0.48
1:A:148:TYR:OH	1:D:207:ARG:NH2	2.46	0.48
1:D:387:HIS:N	2:E:275:HIS:CD2	2.80	0.48
1:G:301:GLU:O	1:G:320:ALA:N	2.43	0.48
1:J:96:CYS:O	1:J:100:ASN:ND2	2.46	0.48
1:J:129:VAL:HG22	1:J:149:VAL:HG11	1.96	0.48
2:H:1:ASP:O	2:H:157:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:309:GLU:N	2:H:309:GLU:OE1	2.46	0.48
1:G:268:ARG:NE	1:G:270:GLU:OE2	2.47	0.48
1:J:268:ARG:NE	1:J:270:GLU:OE2	2.47	0.48
1:D:96:CYS:O	1:D:100:ASN:ND2	2.46	0.48
2:E:309:GLU:N	2:E:309:GLU:OE1	2.46	0.48
1:A:37:ARG:HH12	1:A:132:MET:HG3	1.79	0.48
1:D:268:ARG:NE	1:D:270:GLU:OE2	2.47	0.47
1:G:231:HIS:HA	2:H:239:ARG:HG2	1.96	0.47
1:G:371:CYS:O	1:G:372:THR:OG1	2.25	0.47
2:K:1:ASP:O	2:K:157:ARG:NH1	2.47	0.47
1:A:260:CYS:H	2:B:295:ARG:NH2	2.11	0.47
1:A:323:SER:N	1:A:350:SER:OG	2.47	0.47
1:D:309:TYR:HD2	2:E:339:GLU:OE2	1.97	0.47
3:I:245:ASN:N	3:I:249:VAL:O	2.42	0.47
1:J:323:SER:N	1:J:350:SER:OG	2.47	0.47
1:A:390:ASP:O	2:B:336:TRP:HB3	2.14	0.47
1:J:312:ASP:OD1	1:J:313:PHE:N	2.48	0.47
1:G:323:SER:N	1:G:350:SER:OG	2.47	0.47
3:C:159:TYR:HB3	3:C:161:LEU:HD13	1.95	0.47
1:D:323:SER:N	1:D:350:SER:OG	2.47	0.47
1:D:387:HIS:C	2:E:275:HIS:HD2	2.23	0.47
1:G:96:CYS:O	1:G:100:ASN:ND2	2.46	0.47
1:G:129:VAL:HG22	1:G:149:VAL:HG11	1.96	0.47
1:G:312:ASP:OD1	1:G:313:PHE:N	2.48	0.47
1:A:129:VAL:HG22	1:A:149:VAL:HG11	1.96	0.47
1:D:129:VAL:HG22	1:D:149:VAL:HG11	1.96	0.47
1:D:301:GLU:O	1:D:320:ALA:N	2.43	0.47
1:D:246:ARG:NH1	1:D:247:ASP:OD2	2.48	0.47
3:F:145:ASN:O	3:F:149:ALA:N	2.47	0.47
1:J:16:LYS:O	1:J:332:HIS:ND1	2.48	0.47
1:A:391:TYR:CE2	2:B:297:LEU:HD11	2.49	0.47
3:I:171:LYS:O	3:I:172:SER:OG	2.30	0.47
3:F:171:LYS:O	3:F:172:SER:OG	2.28	0.46
2:H:363:THR:O	2:H:367:GLY:N	2.42	0.46
3:C:171:LYS:O	3:C:172:SER:OG	2.28	0.46
2:K:293:THR:OG1	2:K:304:THR:O	2.30	0.46
2:B:293:THR:OG1	2:B:304:THR:O	2.30	0.46
1:G:246:ARG:NH1	1:G:247:ASP:OD2	2.48	0.46
1:J:263:ALA:HB3	1:J:268:ARG:HE	1.81	0.46
1:J:387:HIS:HA	2:K:336:TRP:NE1	2.30	0.46
1:D:312:ASP:OD1	1:D:313:PHE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:216:ILE:HG13	3:I:225:ALA:HB3	1.97	0.46
1:A:16:LYS:O	1:A:332:HIS:ND1	2.48	0.46
1:D:16:LYS:O	1:D:332:HIS:ND1	2.48	0.46
1:A:246:ARG:NH1	1:A:247:ASP:OD2	2.48	0.46
3:C:233:GLU:CD	3:C:238:ALA:HB2	2.40	0.46
1:A:312:ASP:OD1	1:A:313:PHE:N	2.48	0.46
1:D:263:ALA:HB3	1:D:268:ARG:HE	1.81	0.46
1:D:391:TYR:HE1	2:E:335:VAL:O	1.99	0.46
1:J:301:GLU:O	1:J:320:ALA:N	2.43	0.46
1:G:16:LYS:O	1:G:332:HIS:ND1	2.48	0.46
1:J:246:ARG:NH1	1:J:247:ASP:OD2	2.48	0.46
1:D:258:PHE:HA	2:E:297:LEU:O	2.16	0.45
1:G:263:ALA:HB3	1:G:268:ARG:HE	1.81	0.45
1:A:229:ILE:HG21	2:B:26:ARG:HE	1.80	0.45
1:A:391:TYR:CZ	2:B:297:LEU:CD1	2.99	0.45
1:A:140:VAL:O	1:A:141:SER:OG	2.32	0.45
2:B:79:ASP:OD1	2:B:80:ASN:N	2.50	0.45
1:D:387:HIS:CE1	2:E:340:SER:OG	2.68	0.45
3:F:258:SER:OG	3:F:259:GLU:N	2.49	0.45
1:A:263:ALA:HB3	1:A:268:ARG:HE	1.81	0.45
1:D:394:GLN:OE1	2:E:338:GLN:OE1	2.35	0.45
2:H:79:ASP:OD1	2:H:80:ASN:N	2.50	0.45
1:J:380:ASP:OD1	1:J:381:CYS:N	2.50	0.45
1:A:261:SER:O	1:A:270:GLU:N	2.50	0.45
1:D:261:SER:O	1:D:270:GLU:N	2.50	0.45
2:E:79:ASP:OD1	2:E:80:ASN:N	2.50	0.44
1:G:261:SER:O	1:G:270:GLU:N	2.50	0.44
2:B:379:CYS:O	2:B:382:SER:OG	2.18	0.44
2:E:84:ARG:HG3	2:E:110:THR:OG1	2.18	0.44
1:J:387:HIS:CD2	2:K:338:GLN:HE21	2.36	0.44
1:A:327:GLY:O	1:A:347:LEU:N	2.50	0.44
1:D:183:HIS:NE2	2:E:149:PRO:HG3	2.33	0.44
2:K:79:ASP:OD1	2:K:80:ASN:N	2.50	0.44
2:E:285:HIS:HD2	1:J:237:ALA:HB1	1.83	0.44
1:A:312:ASP:O	1:A:314:GLY:N	2.50	0.44
1:D:327:GLY:O	1:D:347:LEU:N	2.50	0.44
2:H:84:ARG:HG3	2:H:110:THR:OG1	2.18	0.44
1:J:261:SER:O	1:J:270:GLU:N	2.50	0.44
2:K:21:ASN:CG	2:K:123:THR:HG1	2.17	0.44
3:C:258:SER:OG	3:C:259:GLU:N	2.51	0.44
2:K:69:ASN:O	2:K:72:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASP:OD1	1:D:181:TYR:OH	2.21	0.43
1:D:221:LYS:O	1:D:235:THR:OG1	2.19	0.43
1:D:414:LEU:O	1:D:418:THR:N	2.45	0.43
2:K:84:ARG:HG3	2:K:110:THR:OG1	2.17	0.43
1:A:152:GLU:OE1	1:A:152:GLU:N	2.52	0.43
1:J:327:GLY:O	1:J:347:LEU:N	2.50	0.43
1:A:380:ASP:OD1	1:A:381:CYS:N	2.50	0.43
1:J:312:ASP:O	1:J:314:GLY:N	2.50	0.43
1:A:1:TYR:N	1:G:385:LYS:HD2	2.34	0.43
1:D:380:ASP:OD1	1:D:381:CYS:N	2.50	0.43
3:F:233:GLU:OE2	3:F:238:ALA:HB2	2.18	0.43
1:J:152:GLU:N	1:J:152:GLU:OE1	2.52	0.43
1:J:414:LEU:O	1:J:418:THR:N	2.45	0.43
2:B:84:ARG:HG3	2:B:110:THR:OG1	2.18	0.43
1:G:152:GLU:N	1:G:152:GLU:OE1	2.52	0.43
2:K:400:ALA:HB2	3:L:244:TRP:CD1	2.53	0.43
1:D:152:GLU:N	1:D:152:GLU:OE1	2.52	0.43
1:G:380:ASP:OD1	1:G:381:CYS:N	2.50	0.43
1:D:112:GLU:HB2	2:E:37:ARG:HH22	1.84	0.43
1:G:117:ASP:OD1	1:G:181:TYR:OH	2.20	0.43
1:G:327:GLY:O	1:G:347:LEU:N	2.50	0.43
1:D:309:TYR:CD2	2:E:339:GLU:OE2	2.72	0.43
1:D:312:ASP:O	1:D:314:GLY:N	2.51	0.43
1:D:311:SER:H	2:E:338:GLN:NE2	2.08	0.42
3:F:159:TYR:HB3	3:F:161:LEU:HD13	2.01	0.42
1:G:390:ASP:O	2:H:336:TRP:HB3	2.19	0.42
1:A:197:LYS:O	1:A:200:SER:OG	2.18	0.42
3:C:210:GLY:N	3:C:261:TRP:O	2.50	0.42
1:G:7:MET:O	1:G:277:ILE:N	2.48	0.42
2:H:174:ASP:OD1	2:H:176:SER:OG	2.28	0.42
2:K:179:SER:N	2:K:186:LYS:O	2.52	0.42
1:A:96:CYS:O	1:A:100:ASN:ND2	2.46	0.42
1:G:312:ASP:O	1:G:314:GLY:N	2.51	0.42
3:L:153:LEU:HD21	3:L:164:GLY:O	2.19	0.42
2:B:92:VAL:O	2:B:93:SER:OG	2.33	0.42
1:D:362:ILE:CD1	2:E:344:ASN:HB3	2.50	0.42
2:H:18:ASP:OD2	2:H:26:ARG:NH2	2.53	0.42
1:J:391:TYR:OH	2:K:297:LEU:HD11	2.19	0.42
2:K:18:ASP:OD2	2:K:26:ARG:NH2	2.53	0.42
1:D:75:ASP:HB2	1:D:216:ALA:HB3	2.02	0.42
2:E:18:ASP:OD2	2:E:26:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB2	1:A:216:ALA:HB3	2.02	0.42
2:B:18:ASP:OD2	2:B:26:ARG:NH2	2.53	0.42
2:B:179:SER:N	2:B:186:LYS:O	2.52	0.42
1:G:389:VAL:O	2:H:336:TRP:N	2.33	0.42
2:B:368:LEU:O	2:B:372:VAL:N	2.43	0.42
1:D:362:ILE:HD13	2:E:344:ASN:HB3	2.02	0.42
2:K:92:VAL:O	2:K:93:SER:OG	2.33	0.42
3:L:145:ASN:O	3:L:149:ALA:N	2.46	0.42
1:D:391:TYR:CE1	2:E:335:VAL:O	2.73	0.42
2:H:179:SER:N	2:H:186:LYS:O	2.52	0.42
1:J:38:ILE:HG23	1:J:129:VAL:HG12	2.02	0.42
1:A:38:ILE:HG23	1:A:129:VAL:HG12	2.02	0.41
1:A:301:GLU:OE1	1:A:303:LYS:NZ	2.40	0.41
1:G:391:TYR:OH	2:H:297:LEU:HD11	2.20	0.41
3:L:258:SER:OG	3:L:259:GLU:N	2.49	0.41
2:B:150:CYS:SG	2:B:263:CYS:N	2.93	0.41
1:D:256:ALA:HB3	2:E:295:ARG:NH2	2.36	0.41
2:E:179:SER:N	2:E:186:LYS:O	2.52	0.41
1:G:102:GLN:NE2	1:G:104:SER:OG	2.47	0.41
1:D:391:TYR:OH	2:E:323:LEU:C	2.62	0.41
1:D:397:GLU:HG3	2:E:359:ARG:HH22	1.86	0.41
2:K:150:CYS:SG	2:K:263:CYS:N	2.93	0.41
1:D:293:GLU:N	1:D:293:GLU:OE1	2.54	0.41
1:G:38:ILE:HG23	1:G:129:VAL:HG12	2.02	0.41
1:G:134:ASN:OD1	1:G:135:ILE:N	2.54	0.41
1:G:293:GLU:OE1	1:G:293:GLU:N	2.54	0.41
1:A:134:ASN:OD1	1:A:135:ILE:N	2.54	0.41
1:A:391:TYR:CE2	2:B:297:LEU:CD1	3.04	0.41
1:D:7:MET:O	1:D:277:ILE:N	2.48	0.41
2:E:69:ASN:O	2:E:72:THR:OG1	2.30	0.41
2:E:150:CYS:SG	2:E:263:CYS:N	2.93	0.41
1:A:102:GLN:NE2	1:A:104:SER:OG	2.47	0.41
1:G:88:MET:O	2:H:173:ALA:HB3	2.21	0.41
2:B:69:ASN:O	2:B:72:THR:OG1	2.30	0.41
3:C:145:ASN:O	3:C:149:ALA:N	2.54	0.41
1:G:75:ASP:HB2	1:G:216:ALA:HB3	2.02	0.41
2:H:399:LEU:HD22	3:I:134:PHE:CE1	2.56	0.41
1:J:293:GLU:OE1	1:J:293:GLU:N	2.54	0.41
1:D:134:ASN:OD1	1:D:135:ILE:N	2.54	0.41
1:D:265:GLU:O	1:D:267:LEU:N	2.54	0.41
2:E:84:ARG:N	2:E:110:THR:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ASN:CG	1:G:153:THR:HG1	2.24	0.41
2:H:368:LEU:O	2:H:372:VAL:N	2.43	0.41
2:K:84:ARG:N	2:K:110:THR:O	2.52	0.41
1:D:38:ILE:HG23	1:D:129:VAL:HG12	2.02	0.40
1:G:414:LEU:O	1:G:418:THR:N	2.45	0.40
1:J:113:GLU:HG2	2:K:258:PRO:HG3	2.03	0.40
1:A:43:ASN:OD1	1:D:41:SER:CB	2.69	0.40
2:E:283:HIS:NE2	1:J:200:SER:HB3	2.36	0.40
1:G:265:GLU:O	1:G:267:LEU:N	2.54	0.40
1:J:134:ASN:OD1	1:J:135:ILE:N	2.54	0.40
1:D:59:VAL:HG22	2:E:242:ARG:HG2	2.03	0.40
1:G:232:THR:HG23	2:H:238:GLY:O	2.21	0.40
1:J:265:GLU:O	1:J:267:LEU:N	2.54	0.40
3:L:135:LYS:HB3	3:L:162:GLU:HB2	2.03	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 PDB entries followed by that with respect to all EM entries.

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	426/441 (97%)	346 (81%)	76 (18%)	4 (1%)	14	49
1	D	426/441 (97%)	346 (81%)	76 (18%)	4 (1%)	14	49
1	G	426/441 (97%)	346 (81%)	76 (18%)	4 (1%)	14	49
1	J	426/441 (97%)	346 (81%)	76 (18%)	4 (1%)	14	49
2	B	418/420 (100%)	323 (77%)	94 (22%)	1 (0%)	43	77
2	E	418/420 (100%)	322 (77%)	95 (23%)	1 (0%)	43	77
2	H	418/420 (100%)	322 (77%)	95 (23%)	1 (0%)	43	77
2	K	418/420 (100%)	322 (77%)	95 (23%)	1 (0%)	43	77
3	C	158/260 (61%)	138 (87%)	20 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	157/260 (60%)	137 (87%)	20 (13%)	0	100	100
3	I	158/260 (61%)	130 (82%)	28 (18%)	0	100	100
3	L	158/260 (61%)	136 (86%)	21 (13%)	1 (1%)	21	58
All	All	4007/4484 (89%)	3214 (80%)	772 (19%)	21 (0%)	26	62

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	ASP
1	D	390	ASP
1	G	390	ASP
1	J	390	ASP
3	L	165	ASP
1	A	265	GLU
1	A	266	PRO
1	D	265	GLU
1	D	266	PRO
1	G	265	GLU
1	G	266	PRO
1	J	265	GLU
1	J	266	PRO
2	B	349	PRO
2	E	349	PRO
2	H	349	PRO
2	K	349	PRO
1	A	191	PRO
1	D	191	PRO
1	G	191	PRO
1	J	191	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	362/370 (98%)	362 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	362/370 (98%)	362 (100%)	0	100	100
1	G	362/370 (98%)	362 (100%)	0	100	100
1	J	362/370 (98%)	362 (100%)	0	100	100
2	B	366/367 (100%)	366 (100%)	0	100	100
2	E	366/367 (100%)	366 (100%)	0	100	100
2	H	366/367 (100%)	366 (100%)	0	100	100
2	K	366/367 (100%)	366 (100%)	0	100	100
3	C	134/219 (61%)	134 (100%)	0	100	100
3	F	133/219 (61%)	133 (100%)	0	100	100
3	I	134/219 (61%)	134 (100%)	0	100	100
3	L	134/219 (61%)	134 (100%)	0	100	100
All	All	3447/3824 (90%)	3447 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	102	GLN
1	A	125	HIS
1	A	183	HIS
1	A	328	ASN
1	A	394	GLN
2	B	41	HIS
2	B	151	ASN
2	B	175	HIS
2	B	338	GLN
2	B	344	ASN
2	B	346	HIS
3	C	190	HIS
1	D	102	GLN
1	D	328	ASN
2	E	275	HIS
2	E	338	GLN
2	E	344	ASN
2	E	346	HIS
1	G	102	GLN

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Mol	Chain	Res	Type
1	G	183	HIS
1	G	328	ASN
1	G	394	GLN
2	H	24	HIS
2	H	41	HIS
2	H	151	ASN
2	H	155	HIS
2	H	344	ASN
2	H	346	HIS
3	I	121	GLN
1	J	102	GLN
1	J	328	ASN
1	J	394	GLN
2	K	41	HIS
2	K	151	ASN
2	K	155	HIS
2	K	162	HIS
2	K	338	GLN
2	K	344	ASN
2	K	346	HIS

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
4	NAG	M	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	M	2	4	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	M	3	4	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	N	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	N	2	4	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	N	3	4	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	O	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	O	2	4	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	O	3	4	14,14,15	0.20	0	17,19,21	0.48	0
4	NAG	P	1	4,1	14,14,15	0.76	1 (7%)	17,19,21	0.84	1 (5%)
4	NAG	P	2	4	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	P	3	4	14,14,15	0.22	0	17,19,21	0.48	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
4	NAG	M	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	3	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	3	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	3	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	3	4	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C1	-2.57	1.39	1.43
4	O	1	NAG	O5-C1	-2.56	1.39	1.43
4	P	1	NAG	O5-C1	-2.55	1.39	1.43
4	N	1	NAG	O5-C1	-2.52	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	1	NAG	C2-N2-C7	2.52	126.28	122.90
4	P	1	NAG	C2-N2-C7	2.52	126.28	122.90
4	M	1	NAG	C2-N2-C7	2.50	126.25	122.90
4	O	1	NAG	C2-N2-C7	2.49	126.24	122.90

There are no chirality outliers.

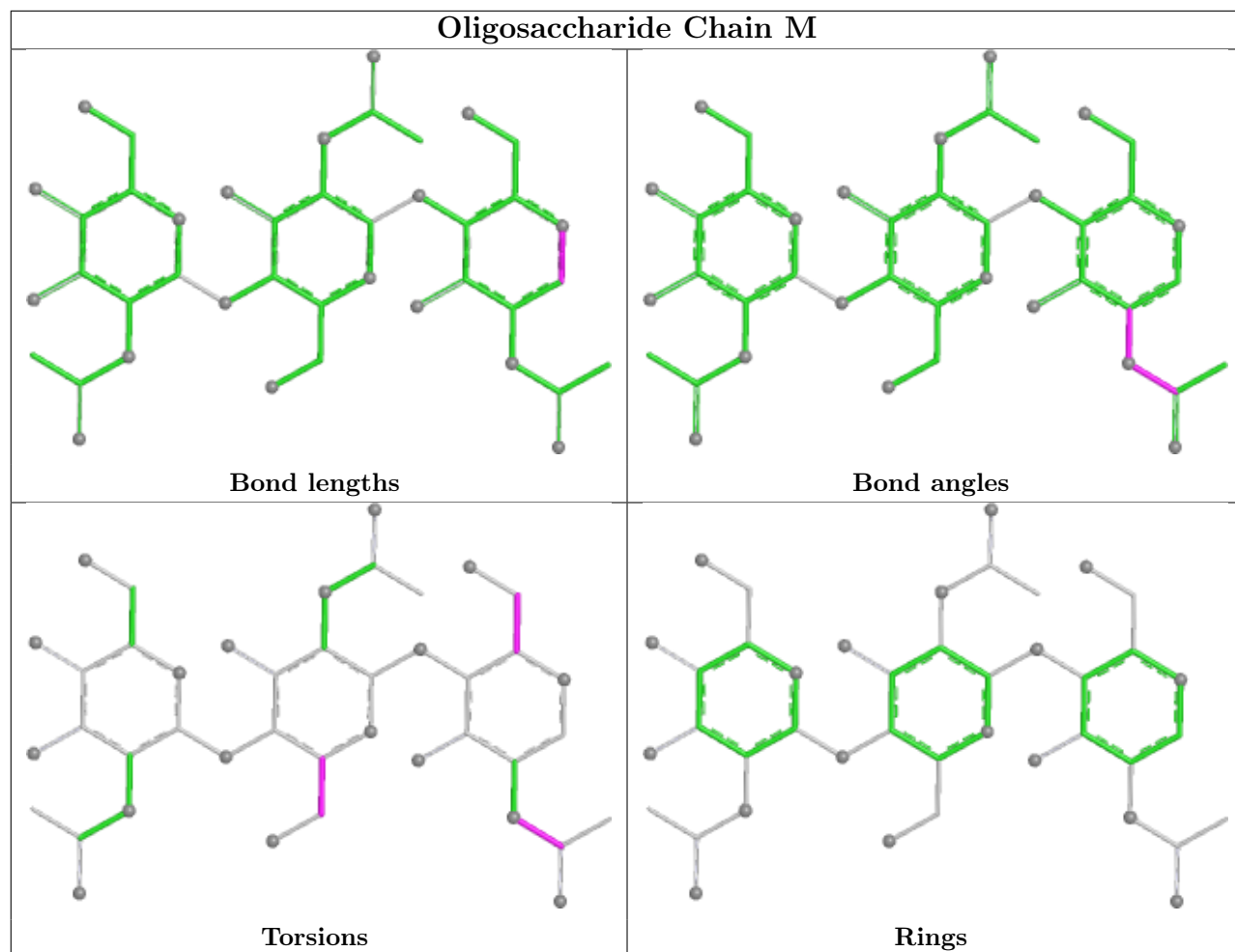
All (20) torsion outliers are listed below:

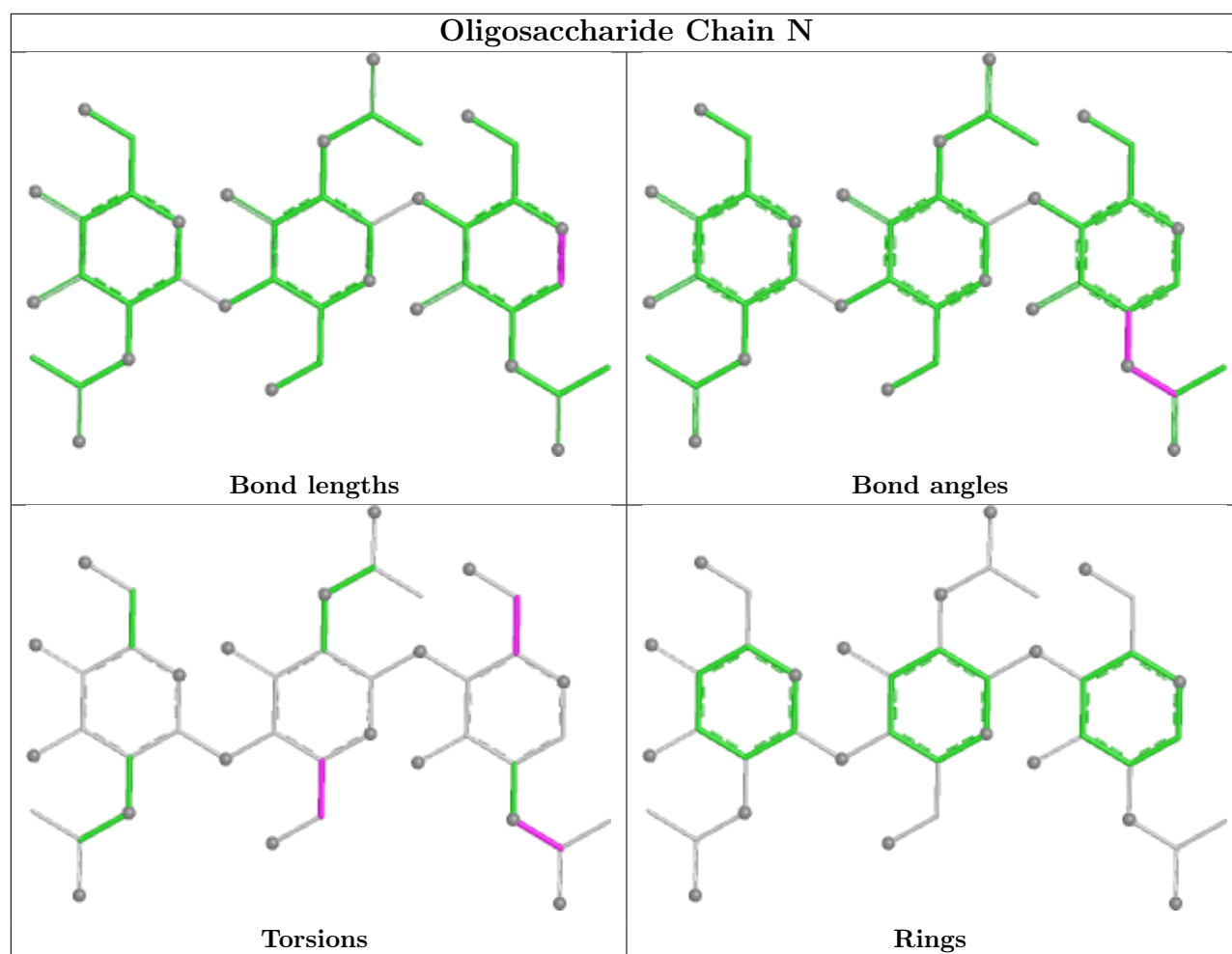
Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	O	1	NAG	C8-C7-N2-C2
4	O	1	NAG	O7-C7-N2-C2
4	P	1	NAG	C8-C7-N2-C2
4	P	1	NAG	O7-C7-N2-C2
4	M	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6

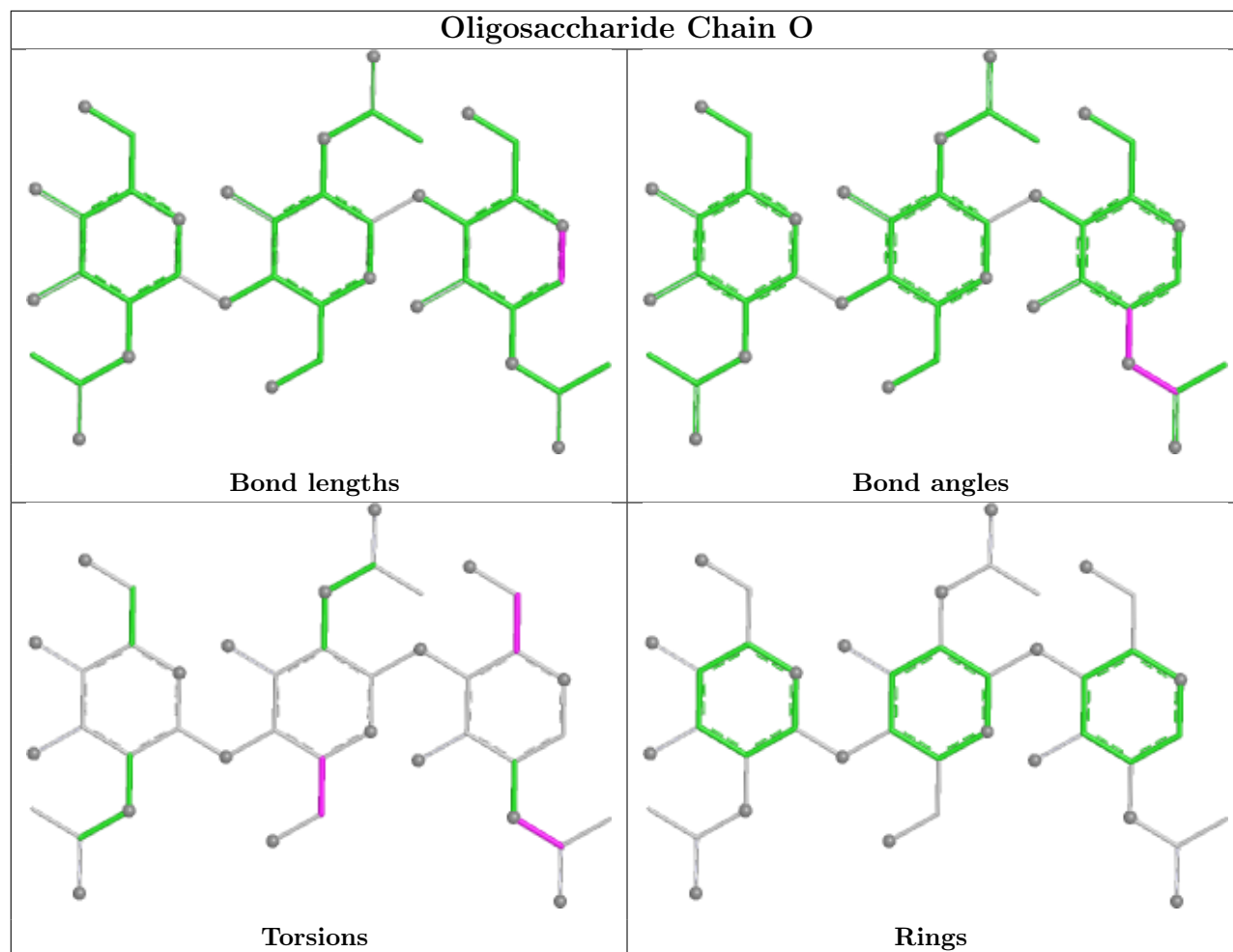
There are no ring outliers.

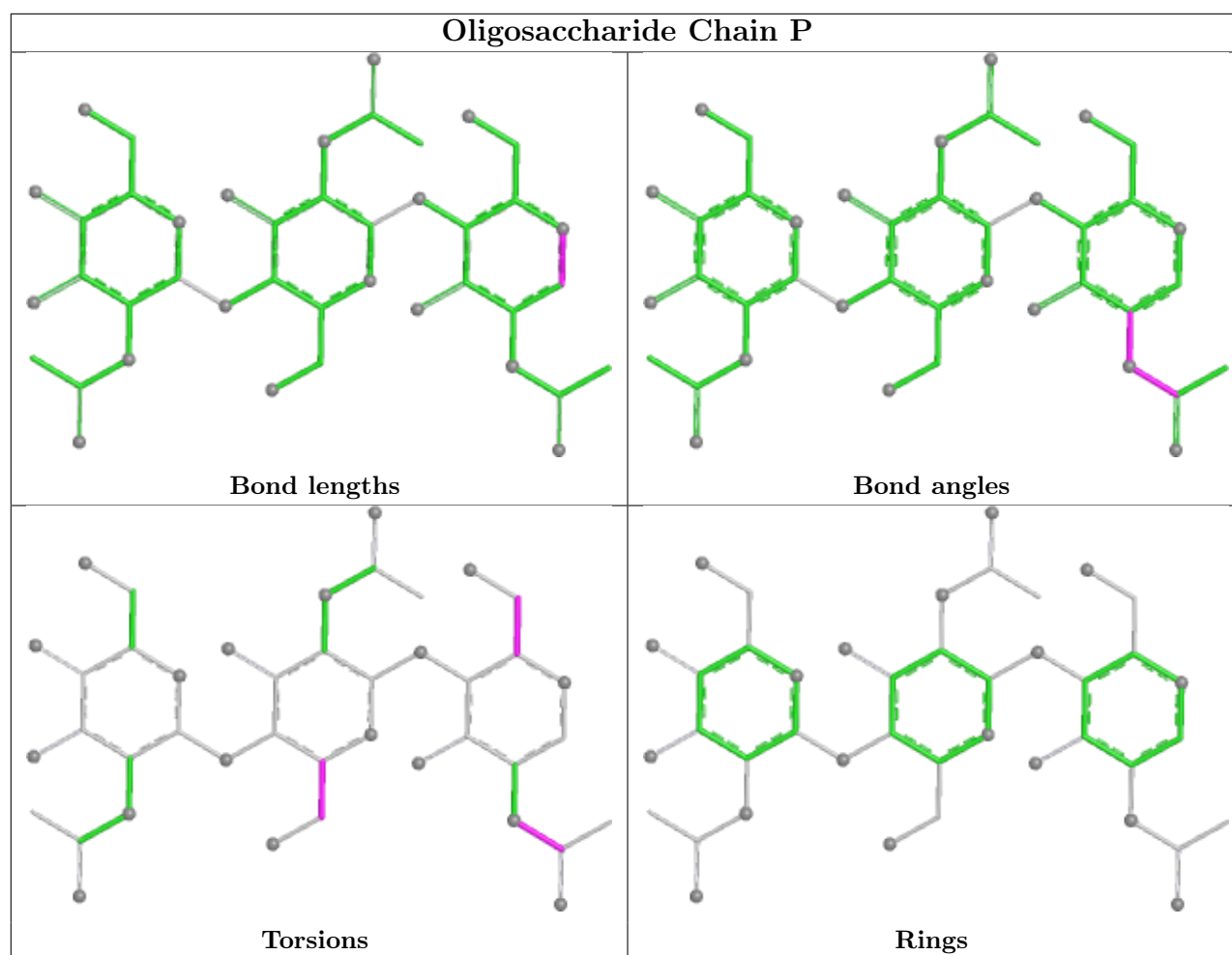
No monomer is involved in short contacts.

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](#)

4 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	$\# Z > 2$
5	NAG	K	501	2	14,14,15	0.27	0	17,19,21	0.78	1 (5%)
5	NAG	E	501	2	14,14,15	0.27	0	17,19,21	0.78	1 (5%)
5	NAG	H	501	2	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
5	NAG	B	501	2	14,14,15	0.27	0	17,19,21	0.77	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
5	NAG	K	501	2	-	4/6/23/26	0/1/1/1
5	NAG	E	501	2	-	4/6/23/26	0/1/1/1
5	NAG	H	501	2	-	4/6/23/26	0/1/1/1
5	NAG	B	501	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	501	NAG	C2-N2-C7	2.62	126.41	122.90
5	H	501	NAG	C2-N2-C7	2.60	126.39	122.90
5	E	501	NAG	C2-N2-C7	2.60	126.38	122.90
5	B	501	NAG	C2-N2-C7	2.60	126.38	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	NAG	C4-C5-C6-O6
5	E	501	NAG	C4-C5-C6-O6
5	H	501	NAG	C4-C5-C6-O6
5	K	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	E	501	NAG	O5-C5-C6-O6
5	H	501	NAG	O5-C5-C6-O6
5	K	501	NAG	O5-C5-C6-O6
5	B	501	NAG	C8-C7-N2-C2
5	B	501	NAG	O7-C7-N2-C2
5	E	501	NAG	C8-C7-N2-C2
5	E	501	NAG	O7-C7-N2-C2
5	H	501	NAG	C8-C7-N2-C2
5	H	501	NAG	O7-C7-N2-C2
5	K	501	NAG	C8-C7-N2-C2
5	K	501	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9280. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.