



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:33 AM UTC

PDB ID : 2HLO / pdb_00002hlo
Title : Crystal Structure of Fragment D-dimer from Human Fibrin Complexed with Gly-hydroxyPro-Arg-Pro-amide
Authors : Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.
Deposited on : 2006-07-08
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

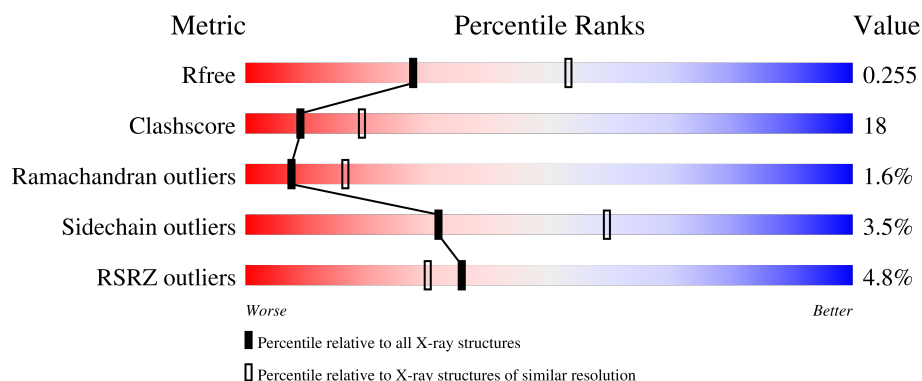
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	87	9% 41% 31% 5% 23%
1	D	87	3% 38% 20% 5% 38%
2	B	328	6% 60% 28% • 8%
2	E	328	4% 59% 29% •• 10%
3	C	324	3% 63% 25% • 10%

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Mol	Chain	Length	Quality of chain
3	F	324	2% 64% 21% • 12%
4	G	5	40% 40% 20%
4	H	5	80% 20%
5	I	2	50% 50%
6	J	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10750 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			547	337	103	104	3			
1	D	54	Total	C	N	O	S	0	0	0
			441	269	84	85	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2428	1515	429	462	22			
2	E	296	Total	C	N	O	S	0	0	0
			2377	1484	420	451	22			

- Molecule 3 is a protein called Isoform Gamma-A of Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	0	0
			2343	1485	396	451	11			
3	F	285	Total	C	N	O	S	0	0	0
			2287	1453	384	439	11			

- Molecule 4 is a protein called GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	H	5	Total	C	N	O	0	0	1
			31	18	8	5			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	C	2	Total	Ca	0	0
			2	2		
7	E	2	Total	Ca	0	0
			2	2		
7	F	1	Total	Ca	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	55	Total	O	0	0
			55	55		
8	C	44	Total	O	0	0
			44	44		
8	D	13	Total	O	0	0
			13	13		

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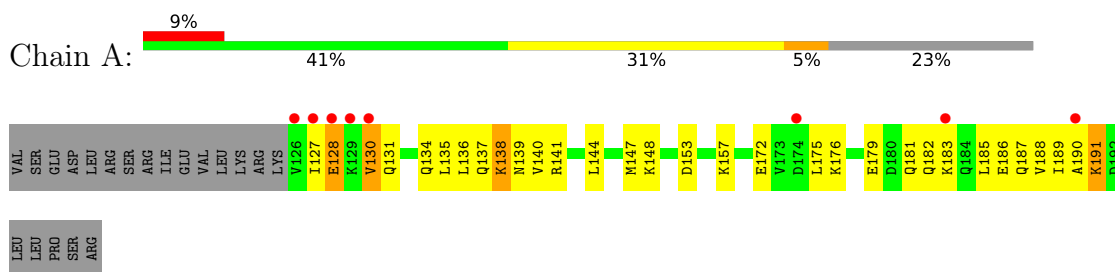
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	46	Total 46	O 46	0	0
8	F	33	Total 33	O 33	0	0
8	G	1	Total 1	O 1	0	0
8	H	2	Total 2	O 2	0	0

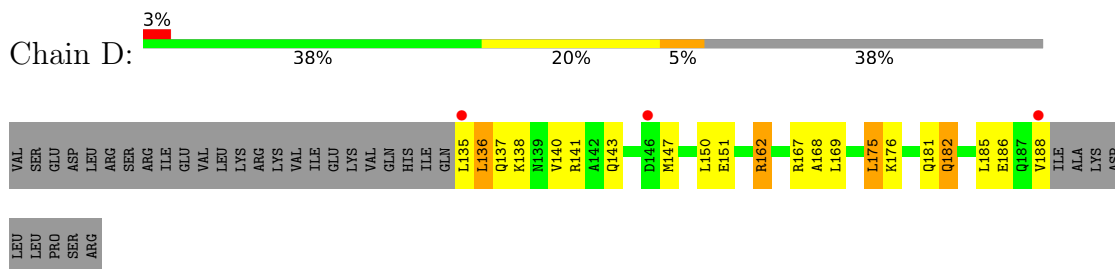
3 Residue-property plots [i](#)

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

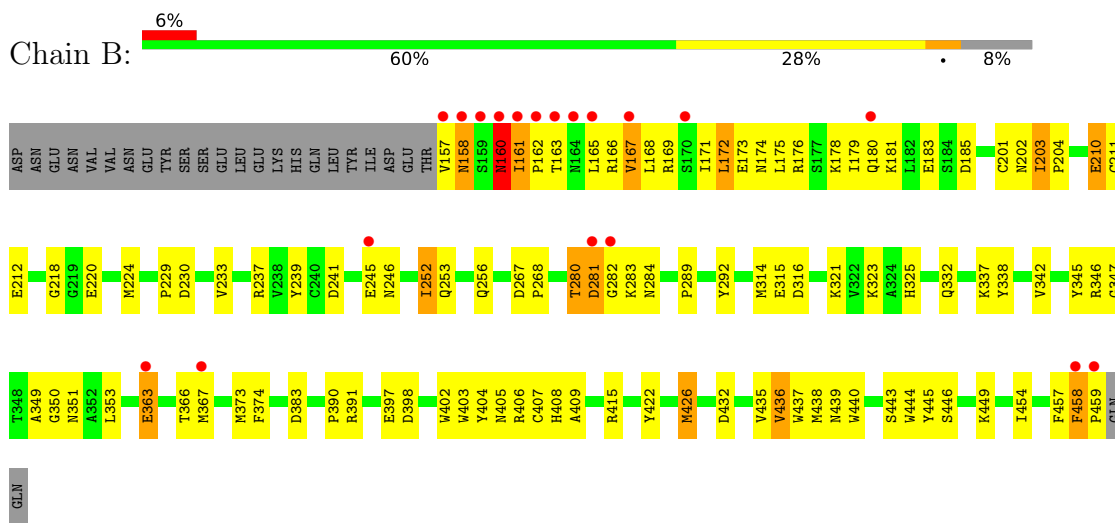
- Molecule 1: Fibrinogen alpha chain



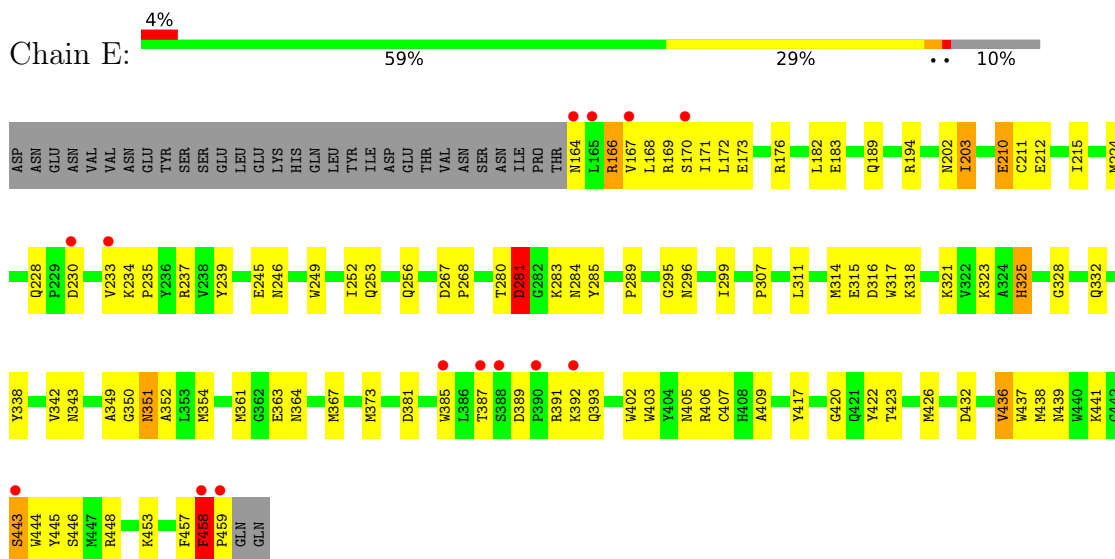
- Molecule 1: Fibrinogen alpha chain



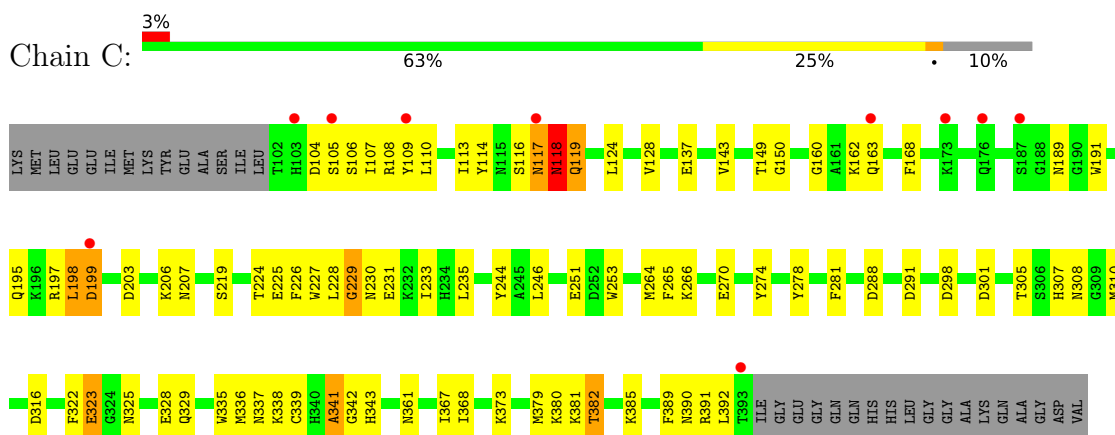
- Molecule 2: Fibrinogen beta chain



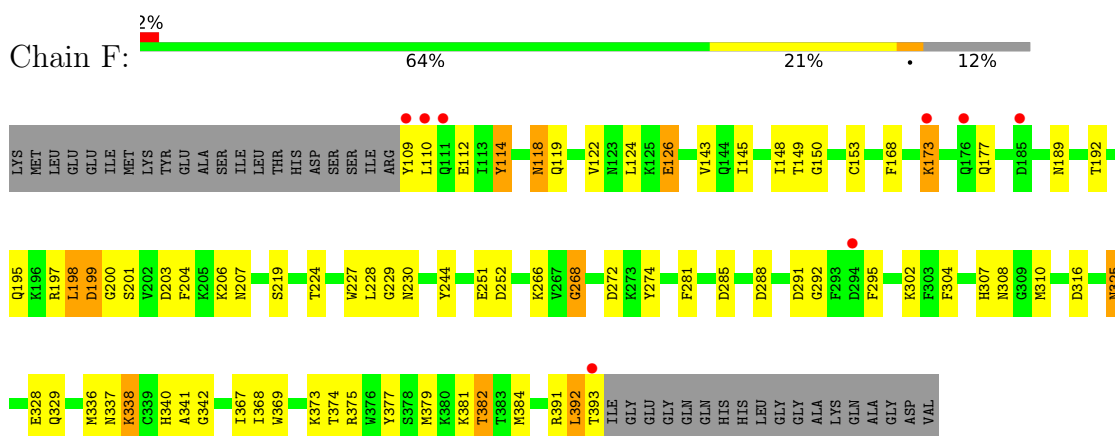
- Molecule 2: Fibrinogen beta chain



• Molecule 3: Isoform Gamma-A of Fibrinogen gamma chain



• Molecule 3: Isoform Gamma-A of Fibrinogen gamma chain

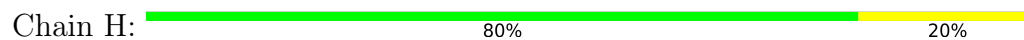


• Molecule 4: GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND





- Molecule 4: GLY-HYP-ARG-PRO-AMIDE PEPTIDE LIGAND



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.69Å 149.48Å 232.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.60) 93.8 (30.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	34.39 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.268 0.200 , 0.255	Depositor DCC
R_{free} test set	2825 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10750	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, NH2, NDG, NAG, CA

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	0.36	0/548	0.81	2/731 (0.3%)
1	D	0.39	0/441	0.83	2/587 (0.3%)
2	B	0.43	0/2490	0.96	11/3364 (0.3%)
2	E	0.42	0/2438	0.96	12/3291 (0.4%)
3	C	0.41	0/2408	0.93	7/3257 (0.2%)
3	F	0.41	0/2351	0.90	7/3180 (0.2%)
4	G	0.62	0/21	0.86	0/25
4	H	0.61	0/21	0.72	0/25
All	All	0.41	0/10718	0.93	41/14460 (0.3%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	ILE	N-CA-C	10.83	117.94	108.63
2	E	349	ALA	N-CA-C	-9.29	98.54	110.53
3	C	228	LEU	N-CA-C	-9.11	97.66	110.50
2	E	203	ILE	N-CA-C	9.02	116.39	108.63
2	B	349	ALA	N-CA-C	-8.32	98.53	110.59
2	E	436	VAL	N-CA-C	7.84	121.13	108.97
2	B	409	ALA	N-CA-C	-7.73	104.08	113.97
2	E	443	SER	N-CA-C	7.58	120.64	111.40
3	F	228	LEU	N-CA-C	-7.51	99.17	110.28
3	C	118	ASN	N-CA-C	-7.26	104.67	113.97
2	B	436	VAL	N-CA-C	7.12	119.71	108.89
3	F	340	HIS	N-CA-C	6.76	119.14	108.79
2	E	409	ALA	N-CA-C	-6.71	105.66	114.31
3	C	341	ALA	N-CA-C	-6.66	106.36	114.75
2	B	166	ARG	N-CA-C	-6.56	104.50	113.30
3	C	229	GLY	N-CA-C	6.29	120.59	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	368	ILE	N-CA-C	6.27	118.92	109.20
2	B	211	CYS	N-CA-C	6.15	119.89	112.38
3	F	229	GLY	N-CA-C	6.15	119.09	112.33
3	F	368	ILE	N-CA-C	6.07	117.84	109.46
3	F	268	GLY	CA-C-N	5.91	125.89	120.21
3	F	268	GLY	C-N-CA	5.91	125.89	120.21
2	B	167	VAL	N-CA-C	-5.82	103.89	112.04
1	A	130	VAL	N-CA-C	5.80	115.99	110.42
2	B	347	GLY	N-CA-C	5.69	117.66	110.38
2	B	426	MET	N-CA-C	-5.67	106.91	113.88
1	D	176	LYS	N-CA-C	-5.35	106.58	113.01
1	D	141	ARG	N-CA-C	-5.31	106.64	113.23
2	E	318	LYS	N-CA-C	-5.22	106.94	113.72
2	E	228	GLN	CA-C-N	5.18	125.22	119.32
2	E	228	GLN	C-N-CA	5.18	125.22	119.32
3	C	119	GLN	N-CA-C	-5.17	106.12	112.90
2	E	211	CYS	N-CA-C	5.16	117.64	111.71
2	E	170	SER	N-CA-C	-5.16	107.06	113.55
3	C	336	MET	N-CA-C	5.14	117.32	110.53
3	F	338	LYS	N-CA-C	5.10	121.67	110.80
2	B	408	HIS	N-CA-C	5.10	116.59	108.79
1	A	138	LYS	N-CA-C	-5.05	105.47	111.69
2	E	194	ARG	N-CA-C	-5.02	107.11	113.18
2	E	296	ASN	N-CA-C	5.01	116.74	111.28
2	B	292	TYR	N-CA-C	5.00	116.13	108.42

There are no chirality outliers.

There are no planarity outliers.

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	547	0	573	35	0
1	D	441	0	458	22	0
2	B	2428	0	2295	90	0
2	E	2377	0	2244	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2343	0	2188	84	0
3	F	2287	0	2136	62	0
4	G	31	0	32	4	0
4	H	31	0	32	2	0
5	I	28	0	25	2	0
6	J	28	0	24	3	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
8	A	8	0	0	2	0
8	B	55	0	0	2	0
8	C	44	0	0	2	0
8	D	13	0	0	1	0
8	E	46	0	0	4	0
8	F	33	0	0	6	0
8	G	1	0	0	0	0
8	H	2	0	0	0	0
All	All	10750	0	10007	378	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 18.

All (378) 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:141:ARG:HH21	1:A:189:ILE:HD13	1.25	1.02
3:C:338:LYS:N	3:C:339:CYS:HA	1.85	0.89
1:A:136:LEU:HD22	2:B:168:LEU:HD21	1.56	0.85
2:B:160:ASN:HB2	2:B:161:ILE:HD13	1.59	0.84
1:D:175:LEU:HD23	1:D:175:LEU:H	1.46	0.81
2:E:166:ARG:HE	2:E:166:ARG:HA	1.47	0.79
2:B:161:ILE:HD13	2:B:161:ILE:H	1.48	0.78
3:F:325:ASN:HD22	3:F:325:ASN:C	1.90	0.78
2:E:230:ASP:O	2:E:233:VAL:HG22	1.84	0.78
2:E:167:VAL:HG23	2:E:168:LEU:HD12	1.65	0.77
2:B:179:ILE:HD12	3:C:117:ASN:HB2	1.66	0.76
2:E:385:TRP:CB	2:E:406:ARG:HD3	2.15	0.76
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.66	0.76
2:E:224:MET:HE2	2:E:237:ARG:HD3	1.68	0.76
3:C:149:THR:HG22	3:C:150:GLY:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.68	0.74
2:E:458:PHE:H	2:E:459:PRO:CD	1.99	0.74
2:E:457:PHE:O	2:E:458:PHE:HB3	1.88	0.73
3:F:310:MET:HG3	3:F:337:ASN:HB2	1.71	0.72
2:E:183:GLU:HG2	3:F:124:LEU:HD13	1.72	0.72
3:C:244:TYR:H	3:C:266:LYS:HZ3	1.38	0.72
3:C:329:GLN:HE22	4:G:3:ARG:HE	1.35	0.71
3:C:244:TYR:H	3:C:266:LYS:NZ	1.88	0.71
1:A:137:GLN:HA	1:A:140:VAL:HG22	1.71	0.71
1:A:128:GLU:C	1:A:131:GLN:HE22	1.97	0.71
2:B:158:ASN:H	2:B:158:ASN:HD22	1.40	0.70
1:D:150:LEU:HD21	3:F:124:LEU:HD23	1.74	0.70
2:B:282:GLY:C	2:B:283:LYS:HD2	2.17	0.69
3:C:149:THR:HG22	3:C:150:GLY:N	2.05	0.69
2:E:373:MET:HE2	2:E:405:ASN:HA	1.74	0.69
2:E:385:TRP:HB2	2:E:406:ARG:HD3	1.72	0.69
2:E:389:ASP:OD2	2:E:392:LYS:HG3	1.93	0.69
3:F:304:PHE:O	3:F:337:ASN:O	2.11	0.69
3:C:329:GLN:NE2	4:G:3:ARG:HH11	1.91	0.69
2:E:441:LYS:HD3	2:E:445:TYR:CE1	2.28	0.69
3:F:307:HIS:HE1	3:F:341:ALA:H	1.41	0.68
1:A:144:LEU:HD23	2:B:175:LEU:HD21	1.73	0.68
2:B:438:MET:HE3	2:B:443:SER:HB3	1.75	0.68
3:C:329:GLN:HE21	4:G:3:ARG:HH11	1.40	0.68
3:C:338:LYS:H	3:C:339:CYS:HA	1.57	0.68
2:B:183:GLU:HG2	3:C:124:LEU:HD13	1.76	0.67
1:D:140:VAL:HG23	1:D:185:LEU:HD21	1.76	0.67
2:E:210:GLU:OE2	2:E:212:GLU:HB3	1.96	0.66
2:E:423:THR:H	2:E:426:MET:HE3	1.61	0.66
6:J:1:NAG:C7	6:J:2:NDG:H8C1	2.26	0.66
2:E:173:GLU:HA	2:E:176:ARG:HH12	1.61	0.65
2:E:315:GLU:HG3	2:E:321:LYS:HG2	1.77	0.65
3:F:195:GLN:OE1	3:F:382:THR:HG22	1.96	0.65
3:F:244:TYR:H	3:F:266:LYS:NZ	1.94	0.65
3:F:336:MET:HA	8:F:429:HOH:O	1.97	0.65
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.43	0.64
3:C:163:GLN:CD	3:C:163:GLN:H	2.05	0.64
3:C:265:PHE:C	3:C:266:LYS:HD2	2.22	0.64
2:B:172:LEU:HB3	3:C:113:ILE:HG21	1.80	0.63
5:I:1:NAG:H61	5:I:2:NAG:O5	1.98	0.63
2:E:423:THR:N	2:E:426:MET:HE3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LEU:H	1:D:175:LEU:CD2	2.11	0.63
2:B:373:MET:HE2	2:B:405:ASN:HA	1.81	0.63
2:B:161:ILE:N	2:B:162:PRO:CD	2.62	0.62
3:F:268:GLY:O	3:F:274:TYR:HA	1.99	0.62
2:B:158:ASN:HD22	2:B:158:ASN:N	1.96	0.62
2:E:203:ILE:CD1	3:F:145:ILE:HD11	2.31	0.61
3:F:307:HIS:CE1	3:F:341:ALA:H	2.17	0.61
3:C:117:ASN:C	3:C:117:ASN:HD22	2.07	0.61
3:C:195:GLN:OE1	3:C:382:THR:HG22	2.00	0.61
2:E:438:MET:HE3	2:E:443:SER:OG	2.00	0.61
2:E:458:PHE:N	2:E:459:PRO:CD	2.61	0.61
3:F:392:LEU:HD13	3:F:392:LEU:O	2.01	0.61
3:C:310:MET:SD	3:C:337:ASN:HB2	2.41	0.60
3:C:337:ASN:O	3:C:337:ASN:CG	2.44	0.60
2:E:387:THR:C	2:E:389:ASP:H	2.08	0.60
3:F:199:ASP:O	3:F:201:SER:N	2.31	0.60
3:C:149:THR:HG23	3:C:168:PHE:O	2.01	0.60
3:C:329:GLN:O	3:C:361:ASN:ND2	2.33	0.60
2:B:157:VAL:HG22	2:B:158:ASN:H	1.66	0.60
2:B:210:GLU:OE2	2:B:212:GLU:HB3	2.02	0.60
1:D:137:GLN:HA	2:E:168:LEU:HD21	1.84	0.60
3:F:329:GLN:HE22	4:H:3:ARG:HE	1.50	0.60
2:B:201:CYS:HB3	2:B:224:MET:HE3	1.85	0.59
2:E:252:ILE:HB	8:E:493:HOH:O	2.02	0.59
1:A:153:ASP:O	1:A:157:LYS:HG2	2.02	0.59
2:E:457:PHE:O	2:E:458:PHE:CB	2.51	0.59
1:A:175:LEU:O	1:A:179:GLU:HG2	2.03	0.59
1:D:169:LEU:H	2:E:189:GLN:HE22	1.50	0.59
2:B:158:ASN:H	2:B:158:ASN:ND2	2.00	0.59
2:B:161:ILE:N	2:B:162:PRO:HD3	2.16	0.59
2:B:282:GLY:O	2:B:283:LYS:HD2	2.02	0.59
2:E:385:TRP:CD1	2:E:406:ARG:NH1	2.70	0.59
1:A:140:VAL:HG23	1:A:185:LEU:HD21	1.85	0.59
6:J:1:NAG:HN2	6:J:2:NDG:H8C1	1.68	0.59
6:J:1:NAG:N2	6:J:2:NDG:H8C1	2.17	0.59
1:A:182:GLN:O	1:A:186:GLU:HG3	2.02	0.58
2:B:230:ASP:O	2:B:233:VAL:HG22	2.03	0.58
3:C:392:LEU:HB2	8:C:450:HOH:O	2.04	0.58
2:E:351:ASN:C	2:E:351:ASN:HD22	2.11	0.58
1:A:136:LEU:HD23	1:A:136:LEU:C	2.29	0.58
2:B:161:ILE:HD13	2:B:161:ILE:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:363:GLU:O	2:E:367:MET:HG2	2.04	0.58
3:F:219:SER:OG	3:F:224:THR:HG22	2.04	0.58
3:F:198:LEU:HD12	3:F:199:ASP:OD1	2.04	0.57
3:C:105:SER:HA	3:C:108:ARG:HD2	1.85	0.57
1:A:139:ASN:HB3	3:C:114:TYR:CE2	2.40	0.57
2:E:173:GLU:HA	2:E:176:ARG:NH1	2.18	0.57
2:B:406:ARG:N	2:B:407:CYS:HA	2.20	0.57
2:E:224:MET:CE	2:E:237:ARG:HD3	2.34	0.57
3:F:325:ASN:C	3:F:325:ASN:ND2	2.62	0.57
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.40	0.57
2:E:391:ARG:HG3	2:E:391:ARG:HH11	1.70	0.57
2:B:161:ILE:H	2:B:162:PRO:HD3	1.70	0.56
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.87	0.56
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.40	0.56
3:C:323:GLU:N	3:C:323:GLU:OE1	2.38	0.56
1:D:181:GLN:HB3	2:E:171:ILE:HD12	1.87	0.56
2:B:157:VAL:HG22	2:B:158:ASN:N	2.19	0.56
2:E:230:ASP:HB3	2:E:233:VAL:HG13	1.86	0.56
2:B:157:VAL:HG22	2:B:158:ASN:HD22	1.71	0.56
3:C:219:SER:OG	3:C:224:THR:HG22	2.06	0.56
2:B:332:GLN:O	2:B:338:TYR:HA	2.04	0.56
1:A:138:LYS:O	1:A:138:LYS:HD3	2.06	0.56
3:F:203:ASP:O	3:F:206:LYS:HE2	2.06	0.56
2:B:353:LEU:HD22	8:B:495:HOH:O	2.05	0.55
3:C:203:ASP:O	3:C:206:LYS:HE2	2.06	0.55
2:B:252:ILE:HD13	2:B:454:ILE:HG12	1.89	0.55
3:F:149:THR:HG23	3:F:168:PHE:O	2.05	0.55
2:B:202:ASN:ND2	2:B:284:ASN:O	2.38	0.55
3:F:244:TYR:H	3:F:266:LYS:HZ2	1.53	0.55
2:B:458:PHE:HB3	2:B:459:PRO:HD3	1.88	0.55
2:E:307:PRO:HD2	2:E:459:PRO:HG3	1.89	0.55
3:C:389:PHE:C	3:C:391:ARG:H	2.14	0.55
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.05	0.55
2:B:280:THR:O	2:B:281:ASP:C	2.51	0.54
3:C:198:LEU:HD12	3:C:199:ASP:OD1	2.06	0.54
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.05	0.54
2:E:307:PRO:CG	2:E:459:PRO:HG3	2.37	0.54
2:B:172:LEU:HD12	3:C:113:ILE:HG22	1.89	0.54
2:E:237:ARG:HG3	2:E:237:ARG:HH11	1.70	0.54
2:E:422:TYR:O	2:E:444:TRP:HB3	2.07	0.54
3:F:325:ASN:ND2	3:F:328:GLU:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:310:MET:CG	3:F:337:ASN:HB2	2.38	0.54
2:B:457:PHE:O	2:B:458:PHE:CB	2.54	0.54
1:A:179:GLU:O	1:A:183:LYS:HG3	2.07	0.54
3:F:189:ASN:OD1	3:F:391:ARG:HG3	2.08	0.54
3:F:272:ASP:HB3	8:F:433:HOH:O	2.08	0.53
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.43	0.53
2:B:457:PHE:O	2:B:458:PHE:HB2	2.07	0.53
1:A:141:ARG:NH2	1:A:189:ILE:HD13	2.09	0.53
2:B:174:ASN:HD21	2:B:178:LYS:HZ3	1.55	0.53
2:B:443:SER:HG	2:B:444:TRP:CD1	2.26	0.53
1:D:136:LEU:HD13	1:D:136:LEU:C	2.33	0.53
3:C:116:SER:C	3:C:118:ASN:H	2.16	0.53
2:E:458:PHE:H	2:E:459:PRO:HD3	1.72	0.53
3:F:198:LEU:O	3:F:199:ASP:HB3	2.09	0.53
1:A:136:LEU:HD22	2:B:168:LEU:CD2	2.35	0.52
3:F:149:THR:HG22	3:F:150:GLY:N	2.24	0.52
1:A:137:GLN:CA	1:A:140:VAL:HG22	2.40	0.52
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.44	0.52
3:C:124:LEU:O	3:C:128:VAL:HG23	2.09	0.52
2:E:166:ARG:HG3	2:E:169:ARG:HB2	1.90	0.52
2:E:406:ARG:N	2:E:407:CYS:HA	2.24	0.52
2:B:373:MET:HE2	2:B:404:TYR:O	2.10	0.52
3:C:149:THR:CG2	3:C:150:GLY:H	2.22	0.52
2:E:212:GLU:O	2:E:215:ILE:HG22	2.09	0.52
2:E:458:PHE:H	2:E:459:PRO:HD2	1.74	0.52
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.09	0.52
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.10	0.51
2:E:252:ILE:HG23	2:E:299:ILE:HG12	1.92	0.51
2:B:229:PRO:HD2	2:B:233:VAL:HG21	1.92	0.51
3:C:149:THR:CG2	3:C:150:GLY:N	2.74	0.51
2:E:436:VAL:HG12	2:E:437:TRP:N	2.26	0.51
3:F:195:GLN:HB3	3:F:384:MET:HB2	1.92	0.51
3:C:231:GLU:HG2	8:C:421:HOH:O	2.10	0.51
3:C:310:MET:HG3	3:C:337:ASN:HB2	1.93	0.51
1:A:136:LEU:HD23	1:A:136:LEU:O	2.10	0.51
3:C:264:MET:HE3	3:F:308:ASN:ND2	2.26	0.51
2:E:361:MET:O	2:E:364:ASN:HB2	2.11	0.51
1:A:137:GLN:HA	1:A:140:VAL:CG2	2.41	0.51
2:E:436:VAL:CG1	2:E:437:TRP:N	2.74	0.51
2:B:363:GLU:O	2:B:367:MET:HG2	2.12	0.50
2:E:423:THR:OG1	2:E:426:MET:HE3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:LYS:O	3:C:338:LYS:HG2	2.12	0.50
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.60	0.50
3:C:373:LYS:HG3	3:C:379:MET:HE1	1.94	0.50
4:G:3:ARG:O	4:G:4:PRO:C	2.55	0.50
3:F:310:MET:SD	3:F:337:ASN:HB2	2.51	0.50
1:D:136:LEU:C	1:D:138:LYS:H	2.18	0.49
1:A:130:VAL:O	1:A:134:GLN:HG2	2.12	0.49
2:E:252:ILE:CG2	2:E:299:ILE:HG12	2.42	0.49
2:B:224:MET:HE2	2:B:237:ARG:HD3	1.94	0.49
2:B:422:TYR:OH	2:B:432:ASP:HB2	2.12	0.49
2:B:350:GLY:HA3	2:B:439:ASN:HB3	1.95	0.49
3:C:163:GLN:CD	3:C:163:GLN:N	2.71	0.49
1:A:189:ILE:HG22	1:A:189:ILE:O	2.13	0.49
2:E:245:GLU:O	2:E:246:ASN:HB2	2.13	0.49
3:C:191:TRP:CE3	3:C:385:LYS:HG3	2.48	0.48
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.48	0.48
2:E:351:ASN:C	2:E:351:ASN:ND2	2.71	0.48
2:B:345:TYR:CG	2:B:346:ARG:N	2.81	0.48
3:C:281:PHE:CD2	3:C:288:ASP:HB2	2.49	0.48
3:F:119:GLN:HG2	8:F:440:HOH:O	2.12	0.48
1:D:188:VAL:HG12	1:D:188:VAL:O	2.14	0.48
2:B:165:LEU:N	2:B:165:LEU:HD12	2.28	0.48
2:E:381:ASP:OD2	2:E:393:GLN:HG2	2.12	0.48
2:E:458:PHE:CG	2:E:458:PHE:O	2.66	0.48
3:C:337:ASN:O	3:C:338:LYS:HB3	2.13	0.48
2:E:280:THR:O	2:E:281:ASP:C	2.57	0.48
2:E:385:TRP:CG	2:E:406:ARG:HD3	2.48	0.48
3:C:338:LYS:N	3:C:339:CYS:CA	2.69	0.48
2:B:168:LEU:O	2:B:172:LEU:HD23	2.13	0.48
3:C:163:GLN:H	3:C:163:GLN:NE2	2.12	0.48
1:A:144:LEU:CD2	2:B:175:LEU:HD21	2.44	0.48
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.78	0.48
2:E:392:LYS:C	2:E:393:GLN:HG3	2.38	0.47
2:E:385:TRP:CH2	2:E:392:LYS:HB3	2.48	0.47
3:C:137:GLU:HA	3:C:137:GLU:OE1	2.14	0.47
2:E:245:GLU:OE2	2:E:323:LYS:NZ	2.47	0.47
2:E:351:ASN:ND2	2:E:354:MET:H	2.13	0.47
2:B:167:VAL:O	2:B:171:ILE:HG12	2.14	0.47
2:E:441:LYS:HD3	2:E:445:TYR:CD1	2.50	0.47
2:E:385:TRP:CA	2:E:406:ARG:HD3	2.44	0.47
1:A:137:GLN:C	1:A:140:VAL:HG22	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:HG3	8:A:199:HOH:O	2.15	0.47
3:C:197:ARG:HB2	3:C:382:THR:HB	1.97	0.47
3:C:265:PHE:O	3:C:266:LYS:HD2	2.14	0.47
1:D:182:GLN:O	1:D:186:GLU:HG3	2.15	0.47
2:E:169:ARG:HH11	2:E:169:ARG:HG2	1.79	0.47
2:E:311:LEU:HD13	2:E:325:HIS:CD2	2.50	0.47
2:E:332:GLN:O	2:E:338:TYR:HA	2.15	0.47
3:F:126:GLU:OE2	3:F:126:GLU:N	2.48	0.47
3:F:292:GLY:C	3:F:302:LYS:HD2	2.39	0.47
2:B:174:ASN:HD21	2:B:178:LYS:NZ	2.13	0.47
3:C:305:THR:HB	3:C:341:ALA:HB2	1.96	0.47
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.29	0.47
2:B:169:ARG:O	2:B:173:GLU:HG2	2.15	0.47
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.80	0.47
3:C:307:HIS:HE1	3:C:341:ALA:H	1.63	0.46
2:E:387:THR:O	2:E:387:THR:HG23	2.14	0.46
2:E:458:PHE:N	2:E:459:PRO:HD3	2.29	0.46
3:F:119:GLN:HA	3:F:119:GLN:NE2	2.30	0.46
1:A:187:GLN:O	1:A:190:ALA:HB3	2.15	0.46
1:A:191:LYS:NZ	2:B:161:ILE:HG13	2.30	0.46
8:A:199:HOH:O	2:B:165:LEU:HD11	2.15	0.46
3:C:343:HIS:O	3:C:367:ILE:HA	2.15	0.46
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.50	0.46
3:C:143:VAL:HG23	3:C:143:VAL:O	2.14	0.46
1:A:148:LYS:NZ	1:A:182:GLN:HE22	2.13	0.46
3:C:114:TYR:O	3:C:118:ASN:HB2	2.15	0.46
3:C:307:HIS:CE1	3:C:341:ALA:H	2.33	0.46
2:B:201:CYS:O	3:C:143:VAL:HG21	2.14	0.46
2:B:363:GLU:HA	2:B:366:THR:OG1	2.16	0.46
3:C:307:HIS:HE1	3:C:342:GLY:H	1.62	0.46
2:E:295:GLY:O	2:E:299:ILE:HG13	2.16	0.46
2:E:385:TRP:CZ2	2:E:392:LYS:HB3	2.51	0.46
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.16	0.46
1:D:169:LEU:H	2:E:189:GLN:NE2	2.11	0.46
3:C:229:GLY:O	3:C:233:ILE:HG13	2.16	0.46
2:E:391:ARG:HG3	2:E:391:ARG:NH1	2.31	0.45
3:F:114:TYR:CD1	3:F:114:TYR:C	2.94	0.45
2:B:201:CYS:CB	2:B:224:MET:HE3	2.45	0.45
3:C:246:LEU:HD22	3:C:265:PHE:CE1	2.51	0.45
2:B:168:LEU:HD23	3:C:110:LEU:HD23	1.99	0.45
3:C:189:ASN:OD1	3:C:391:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ILE:HA	2:B:204:PRO:HD3	1.86	0.45
2:E:439:ASN:HD22	2:E:439:ASN:H	1.62	0.45
2:B:241:ASP:C	2:B:241:ASP:OD2	2.59	0.45
3:C:253:TRP:CH2	3:C:380:LYS:HG3	2.52	0.45
1:A:175:LEU:HD13	2:B:426:MET:HE2	1.99	0.45
1:A:176:LYS:O	1:A:176:LYS:HD3	2.16	0.45
2:E:402:TRP:CG	2:E:403:TRP:N	2.85	0.45
3:F:367:ILE:O	3:F:379:MET:HG2	2.17	0.45
2:E:249:TRP:HB3	2:E:453:LYS:HB3	1.99	0.45
2:B:422:TYR:O	2:B:444:TRP:HB3	2.17	0.45
3:C:105:SER:HB3	3:C:109:TYR:CE2	2.52	0.45
2:E:283:LYS:HG2	2:E:285:TYR:CE1	2.52	0.44
2:E:350:GLY:HA3	2:E:439:ASN:HB3	1.99	0.44
3:F:118:ASN:O	3:F:122:VAL:HG23	2.18	0.44
2:B:245:GLU:OE2	2:B:323:LYS:NZ	2.50	0.44
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.53	0.44
3:F:307:HIS:CE1	3:F:342:GLY:H	2.36	0.44
2:B:351:ASN:C	2:B:351:ASN:HD22	2.26	0.44
2:E:252:ILE:CB	8:E:493:HOH:O	2.61	0.44
2:E:387:THR:C	2:E:389:ASP:N	2.71	0.44
1:D:167:ARG:CZ	8:D:201:HOH:O	2.66	0.44
2:E:307:PRO:CD	2:E:459:PRO:HG3	2.46	0.44
2:E:343:ASN:OD1	2:E:343:ASN:C	2.61	0.44
3:F:110:LEU:N	3:F:112:GLU:OE2	2.51	0.44
3:F:112:GLU:HB3	8:F:442:HOH:O	2.17	0.44
3:F:168:PHE:HB3	3:F:177:GLN:HE21	1.82	0.44
2:B:391:ARG:HA	2:B:391:ARG:NE	2.33	0.43
2:B:398:ASP:HB3	8:B:514:HOH:O	2.18	0.43
2:B:383:ASP:OD1	2:B:383:ASP:C	2.61	0.43
3:C:298:ASP:HB3	3:C:301:ASP:OD1	2.18	0.43
3:C:307:HIS:CE1	3:C:342:GLY:H	2.36	0.43
1:D:143:GLN:O	1:D:147:MET:HB2	2.19	0.43
5:I:1:NAG:H4	5:I:2:NAG:H2	1.80	0.43
1:D:162:ARG:HH11	1:D:162:ARG:HB2	1.82	0.43
3:F:392:LEU:O	3:F:393:THR:HB	2.18	0.43
3:C:278:TYR:CE2	3:C:308:ASN:HB2	2.53	0.43
3:C:143:VAL:O	3:C:143:VAL:CG2	2.67	0.43
2:E:432:ASP:O	2:E:432:ASP:OD2	2.36	0.43
2:B:218:GLY:O	2:B:220:GLU:HG3	2.18	0.43
2:B:245:GLU:O	2:B:246:ASN:HB2	2.19	0.43
2:E:169:ARG:HG2	2:E:169:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:GLU:C	2:E:210:GLU:OE1	2.61	0.43
1:D:136:LEU:C	1:D:138:LYS:N	2.76	0.43
2:E:385:TRP:CD1	2:E:406:ARG:CZ	3.02	0.43
3:C:160:GLY:O	3:C:162:LYS:HG3	2.19	0.42
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.19	0.42
2:B:402:TRP:CG	2:B:403:TRP:H	2.36	0.42
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.99	0.42
2:B:325:HIS:O	2:B:345:TYR:HA	2.19	0.42
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.17	0.42
3:F:369:TRP:HB3	8:F:416:HOH:O	2.19	0.42
3:F:173:LYS:NZ	3:F:173:LYS:HB3	2.35	0.42
3:F:295:PHE:HD2	3:F:375:ARG:NH1	2.17	0.42
1:D:140:VAL:HG12	2:E:172:LEU:HD21	2.01	0.42
2:E:457:PHE:O	2:E:458:PHE:CD1	2.73	0.42
2:E:307:PRO:HG2	2:E:459:PRO:HG3	2.01	0.42
2:B:390:PRO:C	2:B:391:ARG:HE	2.28	0.42
3:C:207:ASN:HB2	3:C:316:ASP:OD2	2.19	0.42
2:E:417:TYR:HB2	2:E:446:SER:HB3	2.02	0.42
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.20	0.42
2:B:398:ASP:OD2	2:B:415:ARG:HD3	2.20	0.42
2:B:435:VAL:O	2:B:446:SER:HA	2.19	0.42
3:C:117:ASN:C	3:C:117:ASN:ND2	2.76	0.42
3:F:148:ILE:HG23	8:F:430:HOH:O	2.20	0.42
2:B:436:VAL:CG1	2:B:437:TRP:N	2.82	0.42
1:D:147:MET:HE2	2:E:182:LEU:CD1	2.50	0.42
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.55	0.42
3:C:322:PHE:CD2	3:C:323:GLU:N	2.87	0.42
2:E:167:VAL:HG23	2:E:168:LEU:CD1	2.43	0.42
2:E:392:LYS:HG2	8:E:483:HOH:O	2.19	0.42
2:B:402:TRP:CG	2:B:403:TRP:N	2.88	0.41
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.34	0.41
2:B:337:LYS:HE3	2:B:374:PHE:CE1	2.55	0.41
3:C:199:ASP:O	3:C:225:GLU:CD	2.62	0.41
1:A:188:VAL:C	1:A:190:ALA:H	2.27	0.41
2:B:181:LYS:HE2	2:B:185:ASP:OD2	2.19	0.41
3:C:310:MET:CG	3:C:337:ASN:HB2	2.51	0.41
3:F:295:PHE:CD2	3:F:375:ARG:NH1	2.88	0.41
2:B:438:MET:C	2:B:440:TRP:H	2.28	0.41
3:C:226:PHE:CD1	3:C:226:PHE:C	2.99	0.41
2:E:202:ASN:HD22	2:E:284:ASN:HB2	1.86	0.41
2:E:405:ASN:HB3	2:E:406:ARG:H	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:317:TRP:CE3	2:E:448:ARG:HD3	2.56	0.41
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.36	0.41
2:E:389:ASP:CG	2:E:392:LYS:HE2	2.45	0.41
2:B:161:ILE:C	2:B:163:THR:N	2.79	0.41
3:C:107:ILE:HG22	3:C:107:ILE:O	2.21	0.41
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.20	0.41
1:A:147:MET:HG3	2:B:175:LEU:HD22	2.02	0.41
1:A:188:VAL:C	1:A:190:ALA:N	2.79	0.41
3:C:231:GLU:O	3:C:235:LEU:HG	2.21	0.41
2:E:164:ASN:C	2:E:166:ARG:H	2.25	0.41
2:E:166:ARG:HE	2:E:166:ARG:CA	2.21	0.41
2:E:166:ARG:HA	2:E:166:ARG:NE	2.27	0.41
2:E:392:LYS:HA	8:E:483:HOH:O	2.19	0.41
1:D:147:MET:HE1	1:D:150:LEU:HD23	2.02	0.41
1:D:186:GLU:C	1:D:188:VAL:H	2.28	0.41
2:E:234:LYS:HA	2:E:235:PRO:HD3	1.94	0.41
2:E:328:GLY:O	2:E:342:VAL:HA	2.21	0.41
3:F:109:TYR:CD1	3:F:109:TYR:N	2.89	0.41
3:F:373:LYS:HG3	3:F:379:MET:HE1	2.03	0.41
3:F:391:ARG:C	3:F:393:THR:H	2.27	0.41
3:F:122:VAL:O	3:F:126:GLU:OE2	2.39	0.41
3:F:199:ASP:O	3:F:199:ASP:CG	2.64	0.41
3:F:329:GLN:NE2	4:H:3:ARG:HE	2.15	0.41
1:A:140:VAL:HG12	2:B:172:LEU:HD21	2.03	0.40
1:A:181:GLN:HB3	2:B:171:ILE:HD12	2.02	0.40
2:E:406:ARG:HA	2:E:406:ARG:HD2	1.88	0.40
3:F:197:ARG:HD3	3:F:204:PHE:CZ	2.56	0.40
1:A:140:VAL:CG1	2:B:172:LEU:HD21	2.51	0.40
2:B:176:ARG:O	2:B:180:GLN:HG2	2.22	0.40
3:C:325:ASN:OD1	3:C:328:GLU:HB2	2.21	0.40
2:B:314:MET:HA	2:B:449:LYS:O	2.22	0.40
2:B:315:GLU:HG3	2:B:321:LYS:HB3	2.03	0.40
3:F:153:CYS:SG	3:F:192:THR:HA	2.61	0.40
3:C:307:HIS:HD2	3:C:335:TRP:O	2.05	0.40
2:E:420:GLY:HA2	2:E:446:SER:O	2.21	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	65/87 (75%)	60 (92%)	2 (3%)	3 (5%)	2	2
1	D	52/87 (60%)	50 (96%)	2 (4%)	0	100	100
2	B	301/328 (92%)	274 (91%)	23 (8%)	4 (1%)	9	21
2	E	294/328 (90%)	272 (92%)	19 (6%)	3 (1%)	12	28
3	C	290/324 (90%)	266 (92%)	19 (7%)	5 (2%)	7	15
3	F	283/324 (87%)	262 (93%)	17 (6%)	4 (1%)	9	19
4	G	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	H	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1289/1488 (87%)	1187 (92%)	82 (6%)	20 (2%)	7	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	191	LYS
2	B	281	ASP
2	B	458	PHE
3	C	104	ASP
2	E	281	ASP
2	E	458	PHE
3	F	338	LYS
1	A	128	GLU
2	B	160	ASN
3	C	106	SER
3	F	199	ASP
3	F	200	GLY
2	B	256	GLN
3	C	390	ASN
2	E	256	GLN
3	C	199	ASP

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Mol	Chain	Res	Type
3	F	198	LEU
3	C	198	LEU
4	G	4	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/82 (76%)	60 (97%)	2 (3%)	34	62
1	D	50/82 (61%)	45 (90%)	5 (10%)	7	16
2	B	261/286 (91%)	250 (96%)	11 (4%)	26	52
2	E	254/286 (89%)	247 (97%)	7 (3%)	38	66
3	C	246/270 (91%)	242 (98%)	4 (2%)	55	79
3	F	239/270 (88%)	229 (96%)	10 (4%)	26	52
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	1116/1280 (87%)	1077 (96%)	39 (4%)	32	59

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	172	GLU
2	B	158	ASN
2	B	160	ASN
2	B	161	ILE
2	B	172	LEU
2	B	210	GLU
2	B	252	ILE
2	B	253	GLN
2	B	280	THR
2	B	342	VAL
2	B	363	GLU

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Mol	Chain	Res	Type
2	B	397	GLU
3	C	117	ASN
3	C	118	ASN
3	C	323	GLU
3	C	382	THR
1	D	135	LEU
1	D	136	LEU
1	D	162	ARG
1	D	175	LEU
1	D	182	GLN
2	E	166	ARG
2	E	210	GLU
2	E	253	GLN
2	E	281	ASP
2	E	325	HIS
2	E	351	ASN
2	E	458	PHE
3	F	114	TYR
3	F	118	ASN
3	F	126	GLU
3	F	143	VAL
3	F	173	LYS
3	F	285	ASP
3	F	325	ASN
3	F	374	THR
3	F	382	THR
3	F	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	137	GLN
1	A	182	GLN
1	A	184	GLN
2	B	158	ASN
2	B	164	ASN
2	B	174	ASN
2	B	189	GLN
2	B	228	GLN
2	B	253	GLN
2	B	256	GLN

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Mol	Chain	Res	Type
2	B	296	ASN
2	B	301	GLN
2	B	325	HIS
2	B	339	GLN
2	B	351	ASN
2	B	439	ASN
3	C	103	HIS
3	C	117	ASN
3	C	118	ASN
3	C	119	GLN
3	C	123	ASN
3	C	136	GLN
3	C	144	GLN
3	C	146	HIS
3	C	163	GLN
3	C	177	GLN
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	329	GLN
1	D	143	GLN
1	D	182	GLN
1	D	187	GLN
2	E	174	ASN
2	E	180	GLN
2	E	189	GLN
2	E	202	ASN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	296	ASN
2	E	301	GLN
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	439	ASN
3	F	115	ASN
3	F	118	ASN
3	F	119	GLN

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Mol	Chain	Res	Type
3	F	123	ASN
3	F	130	GLN
3	F	163	GLN
3	F	177	GLN
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN
3	F	307	HIS
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	HYP	H	2	4	7,8,9	0.76	0	5,10,12	1.15	0
4	HYP	G	2	4	7,8,9	0.99	0	5,10,12	1.32	1 (20%)

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	HYP	H	2	4	-	0/0/11/13	0/1/1/1
4	HYP	G	2	4	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	HYP	CG-CB-CA	-2.42	100.96	103.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

4 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
5	NAG	I	1	2,5	14,14,15	0.74	0	17,19,21	1.09	2 (11%)
5	NAG	I	2	5	14,14,15	0.63	0	17,19,21	0.65	0
6	NAG	J	1	2,6	14,14,15	0.56	0	17,19,21	0.63	1 (5%)
6	NDG	J	2	6	14,14,15	0.70	0	17,19,21	0.78	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	I	1	2,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	2,6	-	2/6/23/26	0/1/1/1
6	NDG	J	2	6	-	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(°)
6	J	2	NDG	C2-N2-C7	-2.20	119.95	122.90
5	I	1	NAG	C3-C4-C5	2.15	114.14	110.23
6	J	1	NAG	C2-N2-C7	-2.07	120.12	122.90
5	I	1	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

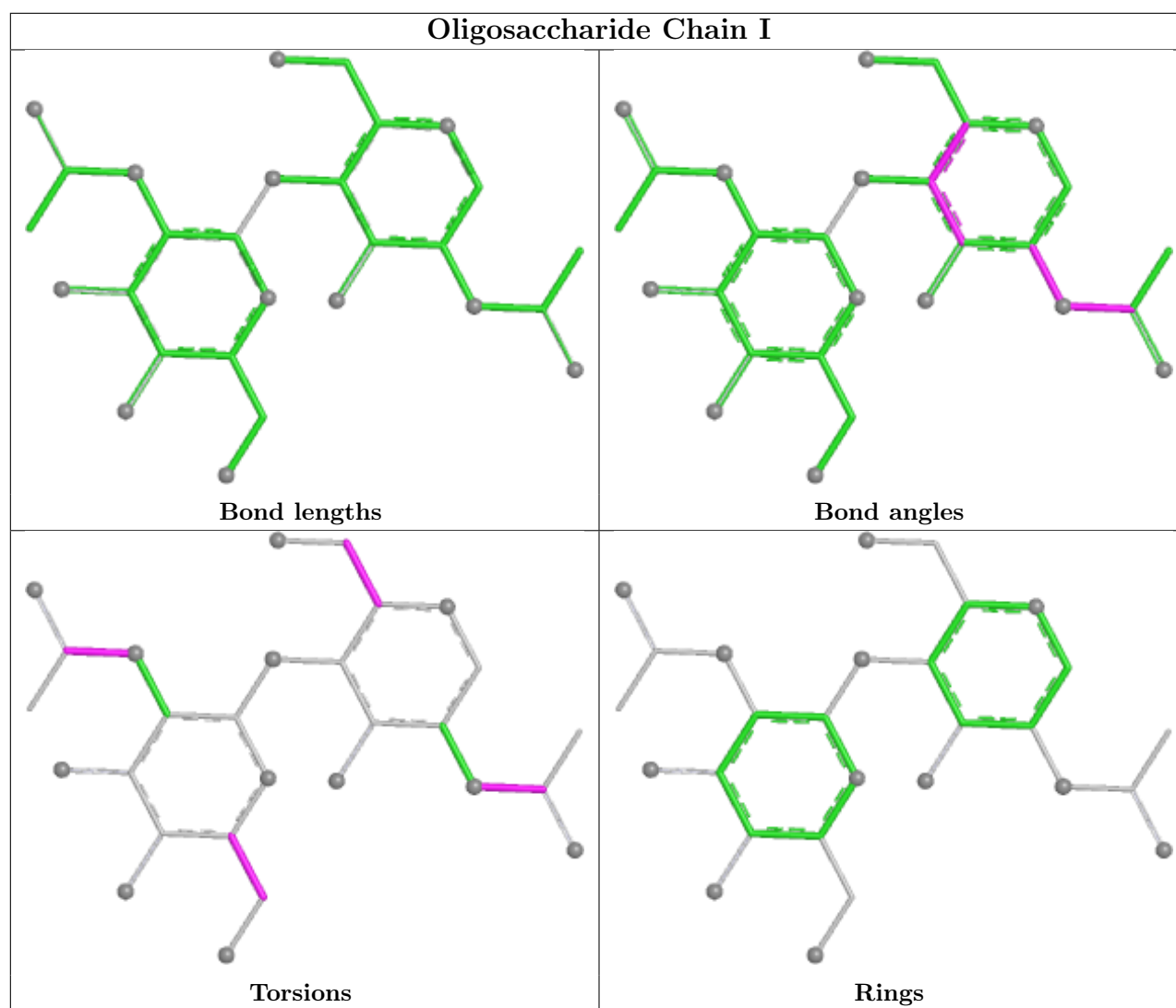
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	1	NAG	C8-C7-N2-C2
6	J	1	NAG	O7-C7-N2-C2
6	J	2	NDG	C8-C7-N2-C2
6	J	2	NDG	O7-C7-N2-C2
5	I	2	NAG	C4-C5-C6-O6
6	J	2	NDG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	J	2	NDG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6

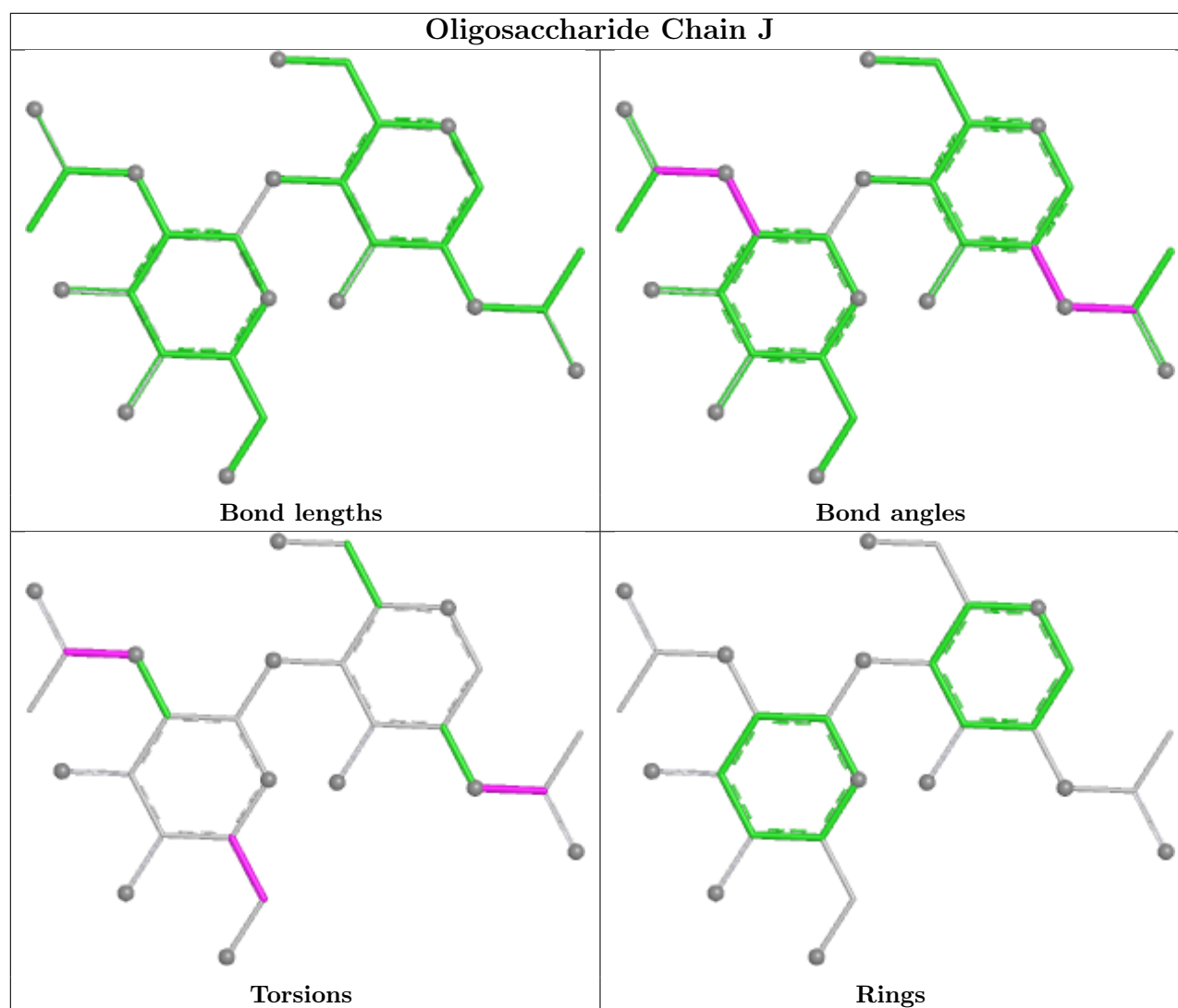
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	2	0
6	J	1	NAG	3	0
5	I	2	NAG	2	0
6	J	2	NDG	3	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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	67/87 (77%)	0.70	8 (11%) 9 7	33, 68, 124, 158	0
1	D	54/87 (62%)	0.50	3 (5%) 30 24	29, 65, 111, 139	0
2	B	303/328 (92%)	0.02	19 (6%) 26 20	23, 41, 103, 166	0
2	E	296/328 (90%)	-0.05	14 (4%) 36 30	24, 40, 99, 142	0
3	C	292/324 (90%)	-0.08	10 (3%) 48 42	24, 44, 79, 129	0
3	F	285/324 (87%)	-0.05	8 (2%) 55 49	26, 45, 78, 123	0
4	G	3/5 (60%)	-0.04	0 100 100	48, 48, 51, 69	0
4	H	3/5 (60%)	-0.21	0 100 100	42, 42, 46, 61	0
All	All	1303/1488 (87%)	0.02	62 (4%) 35 30	23, 44, 99, 166	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	110	LEU	6.7
1	D	188	VAL	4.9
2	E	385	TRP	4.9
1	A	127	ILE	4.6
3	C	393	THR	4.5
2	E	165	LEU	4.4
3	C	109	TYR	4.1
2	E	459	PRO	4.1
2	E	170	SER	4.0
2	B	458	PHE	4.0
1	A	126	VAL	4.0
2	E	233	VAL	3.8
1	D	135	LEU	3.8
2	B	157	VAL	3.6
2	B	161	ILE	3.5
2	B	459	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	390	PRO	3.4
3	F	176	GLN	3.4
2	B	159	SER	3.3
2	E	167	VAL	3.2
3	F	393	THR	3.1
2	B	167	VAL	3.0
2	B	363	GLU	2.9
2	B	165	LEU	2.9
3	C	187	SER	2.8
3	F	109	TYR	2.8
3	C	173	LYS	2.8
3	C	117	ASN	2.8
2	B	245	GLU	2.8
2	E	388	SER	2.7
2	B	158	ASN	2.7
2	E	458	PHE	2.7
1	A	130	VAL	2.6
3	F	111	GLN	2.6
1	A	183	LYS	2.6
3	C	103	HIS	2.5
1	A	190	ALA	2.5
2	B	367	MET	2.5
2	B	180	GLN	2.5
2	B	163	THR	2.4
2	B	164	ASN	2.4
3	F	294	ASP	2.4
3	C	199	ASP	2.4
3	C	105	SER	2.4
1	A	129	LYS	2.3
1	A	174	ASP	2.3
1	D	146	ASP	2.3
2	E	387	THR	2.3
2	E	392	LYS	2.2
2	B	282	GLY	2.2
3	F	173	LYS	2.2
2	E	443	SER	2.2
3	F	185	ASP	2.2
2	B	160	ASN	2.2
2	B	281	ASP	2.2
2	B	162	PRO	2.1
2	B	170	SER	2.1
3	C	176	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	163	GLN	2.1
1	A	128	GLU	2.0
2	E	230	ASP	2.0
2	E	164	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HYP	G	2	8/9	0.93	0.07	37,47,50,52	0
4	HYP	H	2	8/9	0.95	0.08	40,46,50,53	0

6.3 Carbohydrates [i](#)

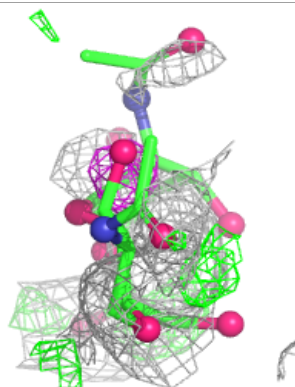
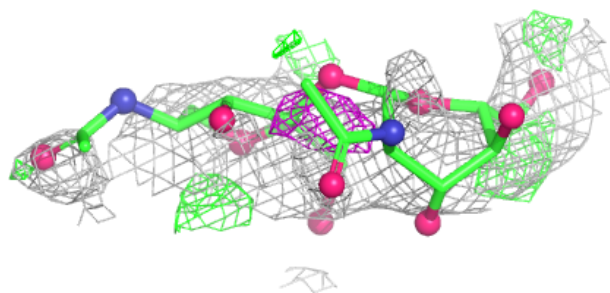
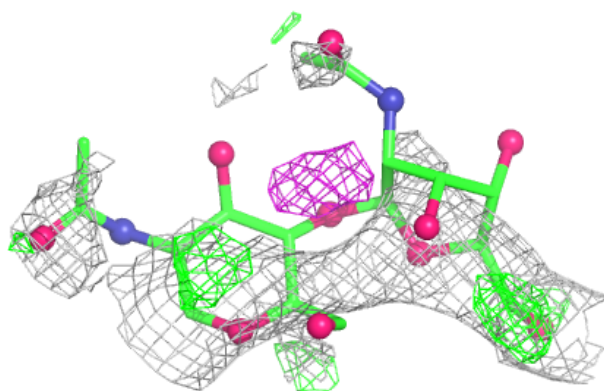
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

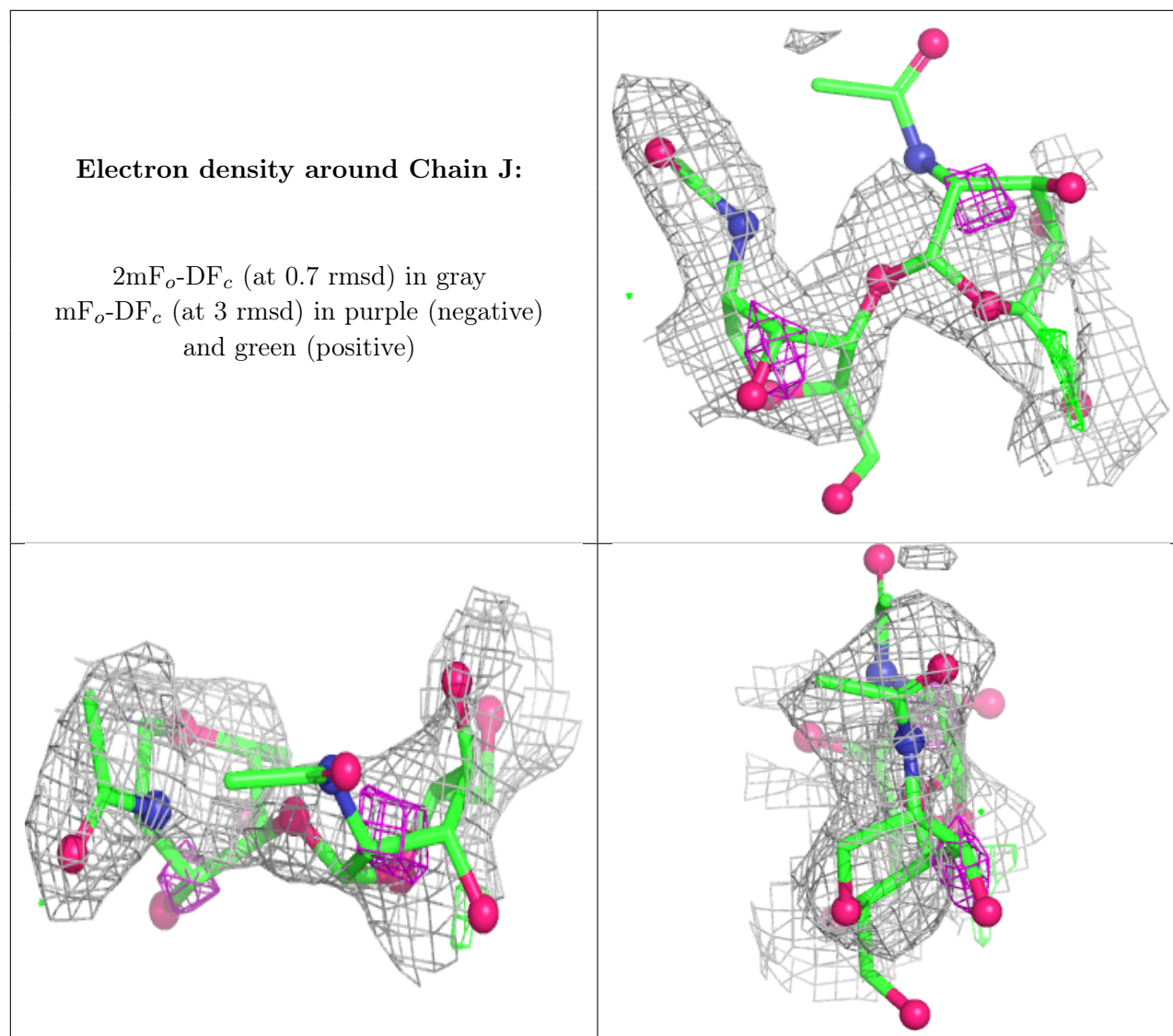
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	I	2	14/15	0.48	0.20	120,154,156,157	0
5	NAG	I	1	14/15	0.56	0.20	121,132,143,154	0
6	NDG	J	2	14/15	0.71	0.18	105,118,126,127	0
6	NAG	J	1	14/15	0.80	0.15	65,85,107,114	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	C	1	1/1	0.90	0.14	61,61,61,61	0
7	CA	B	2	1/1	0.95	0.13	56,56,56,56	0
7	CA	E	2	1/1	0.95	0.07	58,58,58,58	0
7	CA	C	4	1/1	0.97	0.13	55,55,55,55	0
7	CA	B	3	1/1	0.97	0.09	53,53,53,53	0
7	CA	E	3	1/1	0.97	0.12	47,47,47,47	0
7	CA	F	1	1/1	0.97	0.12	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.