



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:38 PM UTC

PDB ID : 1MQ8 / pdb_00001mq8
Title : Crystal structure of alphaL I domain in complex with ICAM-1
Authors : Shimaoka, M.; Xiao, T.; Liu, J.-H.; Yang, Y.; Dong, Y.; Jun, C.-D.; McCormack, A.; Zhang, R.; Joachimiak, A.; Takagi, J.; Wang, J.-H.; Springer, T.A.
Deposited on : 2002-09-15
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

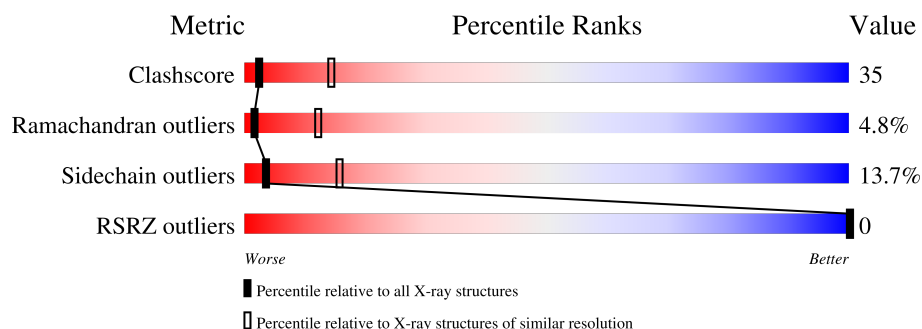
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	291	
1	C	291	
2	B	177	
2	D	177	
3	E	2	
3	F	2	
3	G	2	

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Mol	Chain	Length	Quality of chain
3	H	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	E	1	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5854 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 intercellular adhesion molecule-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1421	889	250	275	7			
1	C	184	Total	C	N	O	S	0	0	0
			1421	889	250	275	7			

- Molecule 2 is a protein called Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1419	914	228	271	6			
2	D	177	Total	C	N	O	S	0	0	0
			1419	914	228	271	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	161	CYS	LEU	engineered mutation	UNP P20701
B	299	CYS	PHE	engineered mutation	UNP P20701
D	161	CYS	LEU	engineered mutation	UNP P20701
D	299	CYS	PHE	engineered mutation	UNP P20701

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



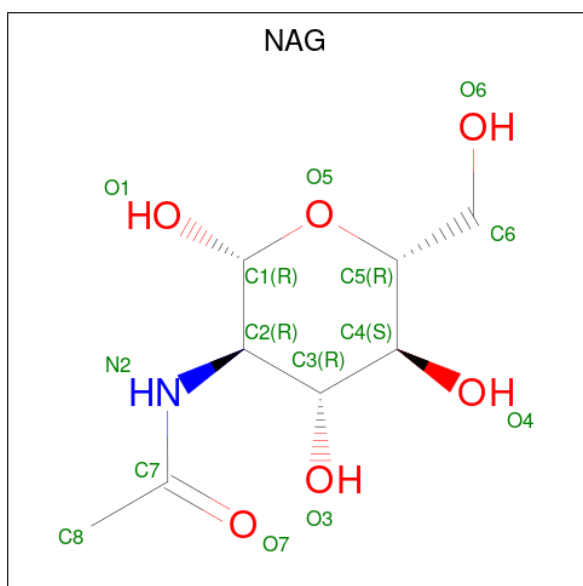
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

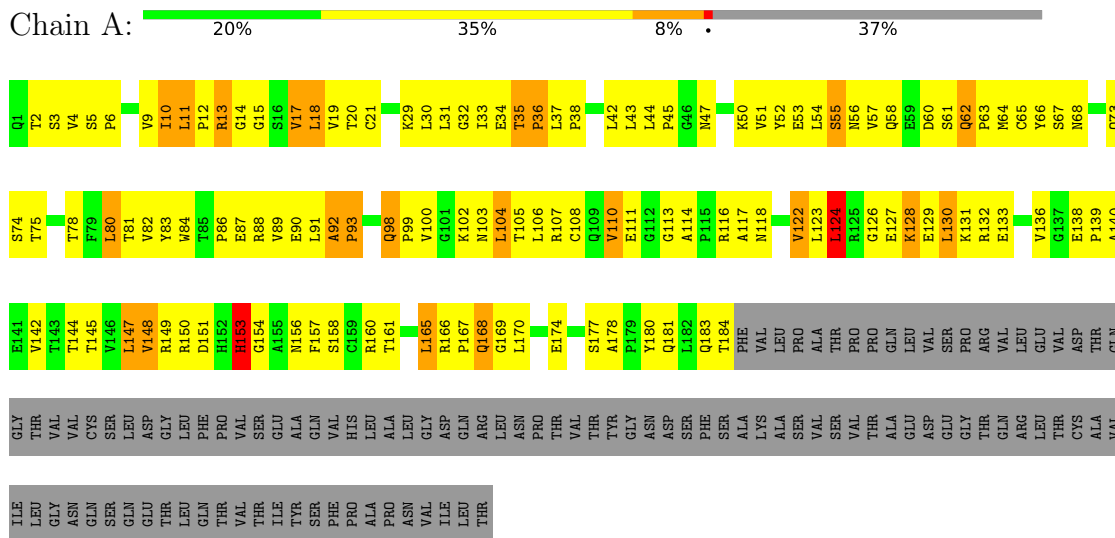
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total 2	O 2	0	0
6	D	2	Total 2	O 2	0	0

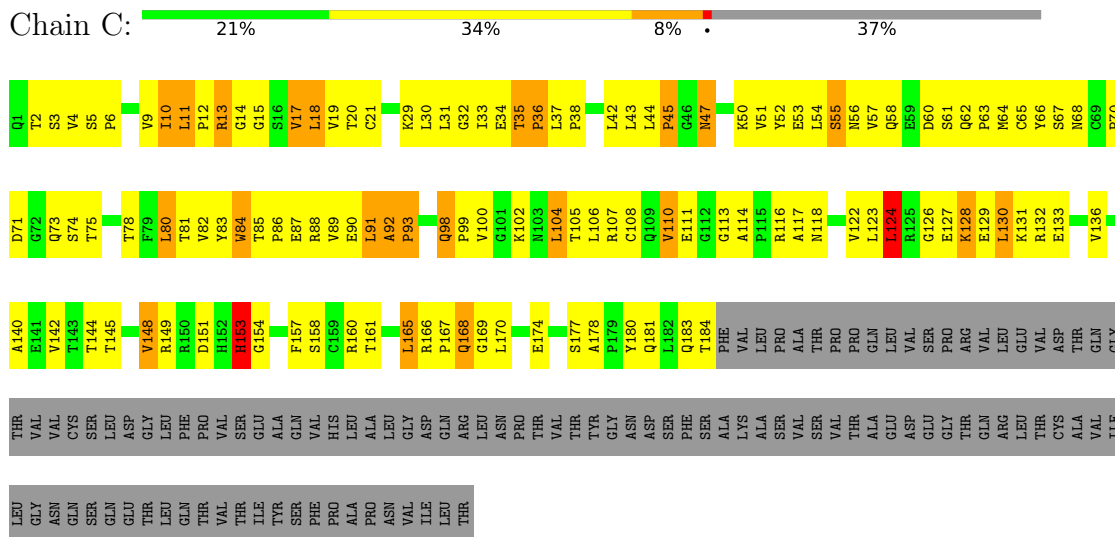
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

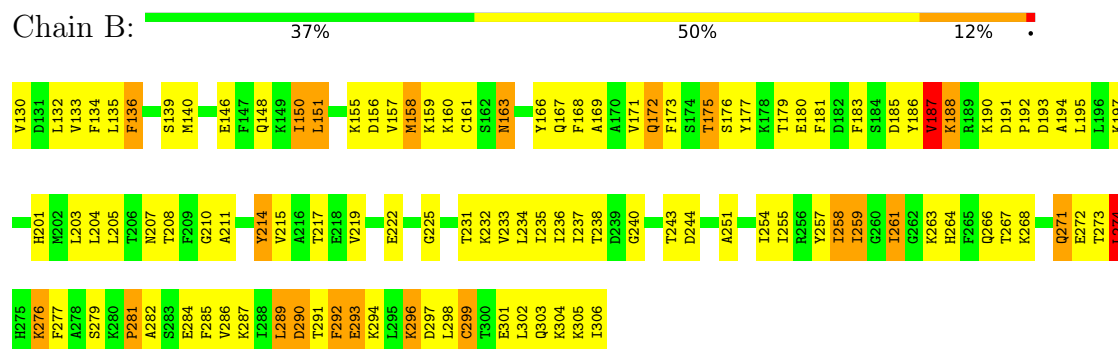
- Molecule 1: intercellular adhesion molecule-1



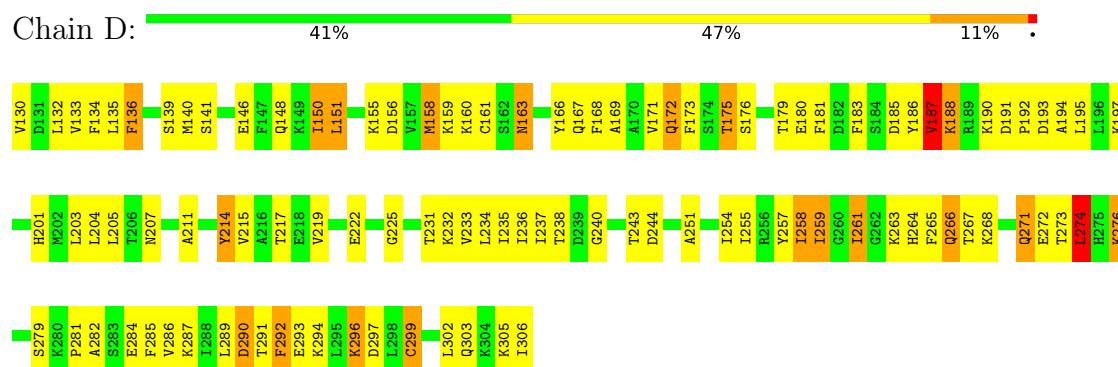
- Molecule 1: intercellular adhesion molecule-1



- Molecule 2: Integrin alpha-L



- Molecule 2: Integrin alpha-L



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.56Å 62.87Å 81.52Å 95.39° 106.67° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.4 (50.00-3.30) 86.2 (50.00-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 3.25Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.264 , 0.313 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 129.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5854	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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: NAG, MG

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	0.66	0/1450	1.22	23/1977 (1.2%)
1	C	0.68	0/1450	1.20	22/1977 (1.1%)
2	B	0.58	1/1445 (0.1%)	1.08	10/1943 (0.5%)
2	D	0.56	0/1445	1.07	9/1943 (0.5%)
All	All	0.62	1/5790 (0.0%)	1.14	64/7840 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	267	THR	N-CA	5.77	1.52	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	LEU	N-CA-C	8.18	115.58	108.22
1	C	11	LEU	N-CA-C	8.01	115.43	108.22
2	D	217	THR	N-CA-C	7.98	119.61	111.07
2	B	217	THR	N-CA-C	7.94	119.57	111.07
2	D	263	LYS	N-CA-C	-7.69	105.85	114.62
2	B	263	LYS	N-CA-C	-7.67	105.87	114.62
2	D	266	GLN	N-CA-C	7.62	122.70	111.34
1	C	92	ALA	N-CA-C	7.47	116.92	108.25
1	A	178	ALA	CA-C-N	7.28	127.71	119.92
1	A	178	ALA	C-N-CA	7.28	127.71	119.92
1	C	92	ALA	C-N-CD	-7.28	104.59	120.60
1	C	178	ALA	CA-C-N	7.11	127.53	119.92
1	C	178	ALA	C-N-CA	7.11	127.53	119.92
1	A	35	THR	CA-C-N	6.54	126.24	119.64
1	A	35	THR	C-N-CA	6.54	126.24	119.64
1	C	35	THR	CA-C-N	6.48	126.18	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	THR	C-N-CA	6.48	126.18	119.64
2	B	290	ASP	N-CA-C	-6.30	105.66	113.15
1	A	149	ARG	N-CA-C	6.21	124.02	110.80
1	A	93	PRO	N-CA-C	6.07	120.78	110.95
1	C	62	GLN	CA-C-N	5.99	126.00	119.89
1	C	62	GLN	C-N-CA	5.99	126.00	119.89
1	C	91	LEU	N-CA-C	-5.94	100.93	110.14
1	A	62	GLN	CA-C-N	5.94	125.95	119.89
1	A	62	GLN	C-N-CA	5.94	125.95	119.89
1	A	92	ALA	CA-C-N	5.93	126.86	119.98
1	A	92	ALA	C-N-CA	5.93	126.86	119.98
2	B	214	TYR	N-CA-C	-5.92	106.09	113.55
1	A	151	ASP	N-CA-C	-5.91	105.83	113.16
1	C	151	ASP	N-CA-C	-5.91	105.83	113.16
2	D	214	TYR	N-CA-C	-5.89	106.12	113.55
2	D	175	THR	N-CA-C	-5.74	106.12	113.23
1	C	36	PRO	N-CA-C	-5.73	106.21	114.18
1	A	36	PRO	N-CA-C	-5.69	106.27	114.18
1	C	149	ARG	N-CA-C	5.69	122.92	110.80
2	B	175	THR	N-CA-C	-5.69	106.18	113.23
2	B	293	GLU	N-CA-C	-5.61	105.70	112.54
2	D	274	LEU	N-CA-C	-5.54	106.48	113.18
2	D	290	ASP	N-CA-C	-5.53	106.57	113.15
2	B	258	ILE	N-CA-C	5.42	116.05	108.89
2	B	274	LEU	N-CA-C	-5.41	106.52	113.01
2	D	258	ILE	N-CA-C	5.37	115.97	108.89
1	A	124	LEU	N-CA-C	5.35	116.54	108.46
1	A	165	LEU	N-CA-C	-5.35	106.06	112.59
1	C	116	ARG	N-CA-C	5.30	119.22	112.87
1	C	124	LEU	N-CA-C	5.27	116.42	108.46
1	A	35	THR	CB-CA-C	-5.25	101.83	109.97
1	A	116	ARG	N-CA-C	5.23	119.15	112.87
1	C	165	LEU	N-CA-C	-5.18	106.27	112.59
1	A	150	ARG	N-CA-C	-5.18	106.90	113.43
1	C	133	GLU	CA-C-N	5.18	124.94	119.76
1	C	133	GLU	C-N-CA	5.18	124.94	119.76
1	A	133	GLU	CA-C-N	5.17	124.93	119.76
1	A	133	GLU	C-N-CA	5.17	124.93	119.76
2	B	266	GLN	N-CA-CB	-5.16	101.78	110.49
2	D	193	ASP	N-CA-C	-5.16	106.10	114.09
1	A	98	GLN	CA-C-N	5.14	126.56	120.23
1	A	98	GLN	C-N-CA	5.14	126.56	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	TRP	N-CA-C	5.14	116.88	108.76
1	C	98	GLN	CA-C-N	5.12	126.53	120.23
1	C	98	GLN	C-N-CA	5.12	126.53	120.23
2	B	193	ASP	N-CA-C	-5.10	106.18	114.09
1	C	35	THR	CB-CA-C	-5.09	102.08	109.97
1	A	122	VAL	N-CA-C	5.02	115.25	107.78

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	1421	0	1426	90	0
1	C	1421	0	1426	91	0
2	B	1419	0	1425	124	0
2	D	1419	0	1425	109	0
3	E	28	0	25	7	0
3	F	28	0	25	2	0
3	G	28	0	25	6	0
3	H	28	0	25	1	0
4	A	28	0	26	1	0
4	C	28	0	26	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
All	All	5854	0	5854	412	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 35.

All (412) 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)
2:B:298:LEU:HB3	2:B:302:LEU:HG	1.42	0.99
3:E:1:NAG:H61	3:E:2:NAG:O5	1.63	0.97
1:C:2:THR:HG22	1:C:3:SER:H	1.33	0.94
1:A:2:THR:HG22	1:A:3:SER:H	1.34	0.92
1:A:42:LEU:HD13	1:C:42:LEU:HD13	1.49	0.91
1:C:92:ALA:HB1	1:C:93:PRO:HB3	1.56	0.88
3:G:1:NAG:H61	3:G:2:NAG:O5	1.74	0.87
2:B:130:VAL:HG22	2:B:231:THR:HB	1.58	0.86
2:D:133:VAL:HG22	2:D:169:ALA:HB3	1.58	0.86
2:B:133:VAL:HG22	2:B:169:ALA:HB3	1.58	0.86
2:D:130:VAL:HG22	2:D:231:THR:HB	1.58	0.86
1:A:110:VAL:HG22	1:A:140:ALA:HB3	1.59	0.85
1:C:110:VAL:HG22	1:C:140:ALA:HB3	1.60	0.84
2:D:150:ILE:HA	2:D:292:PHE:CZ	2.15	0.82
2:B:271:GLN:HA	2:B:271:GLN:HE21	1.44	0.82
2:D:271:GLN:HE21	2:D:271:GLN:HA	1.44	0.82
1:C:11:LEU:O	1:C:82:VAL:HA	1.79	0.81
2:B:163:ASN:H	2:B:163:ASN:ND2	1.78	0.80
2:D:163:ASN:H	2:D:163:ASN:ND2	1.78	0.80
2:B:150:ILE:HA	2:B:292:PHE:CZ	2.18	0.79
1:A:11:LEU:O	1:A:82:VAL:HA	1.82	0.79
1:A:167:PRO:HG2	1:A:168:GLN:OE1	1.83	0.78
1:C:167:PRO:HG2	1:C:168:GLN:OE1	1.83	0.78
2:D:158:MET:HE1	2:D:181:PHE:HZ	1.48	0.78
2:B:158:MET:HE1	2:B:181:PHE:HZ	1.48	0.78
1:C:87:GLU:HB2	1:C:111:GLU:HG3	1.67	0.77
1:A:105:THR:HG22	1:A:145:THR:HG22	1.67	0.77
1:C:105:THR:HG22	1:C:145:THR:HG22	1.67	0.77
2:B:136:PHE:HZ	2:B:180:GLU:HG3	1.51	0.76
2:D:150:ILE:HA	2:D:292:PHE:HZ	1.51	0.76
2:D:136:PHE:HZ	2:D:180:GLU:HG3	1.51	0.76
1:A:68:ASN:HD21	2:B:244:ASP:HA	1.51	0.76
1:C:68:ASN:HD21	2:D:244:ASP:HA	1.51	0.76
1:C:68:ASN:ND2	2:D:244:ASP:HA	2.02	0.74
3:G:1:NAG:O3	3:G:2:NAG:H83	1.87	0.74
2:D:240:GLY:HA3	2:D:274:LEU:HD23	1.67	0.74
2:B:240:GLY:HA3	2:B:274:LEU:HD23	1.69	0.73
1:A:68:ASN:ND2	2:B:244:ASP:HA	2.04	0.73
2:B:150:ILE:HA	2:B:292:PHE:HZ	1.55	0.71
2:B:298:LEU:HB3	2:B:302:LEU:CG	2.17	0.71
3:E:1:NAG:C6	3:E:2:NAG:O5	2.37	0.71
1:A:87:GLU:HB2	1:A:111:GLU:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:SER:O	1:C:73:GLN:HA	1.92	0.70
1:A:67:SER:O	1:A:73:GLN:HA	1.92	0.70
2:B:136:PHE:CZ	2:B:180:GLU:HG3	2.27	0.70
2:D:136:PHE:CZ	2:D:180:GLU:HG3	2.27	0.69
2:D:237:ILE:HG12	2:D:259:ILE:HD11	1.73	0.69
2:B:237:ILE:HG12	2:B:259:ILE:HD11	1.73	0.69
2:B:161:CYS:HA	2:B:163:ASN:HD21	1.58	0.69
2:B:303:GLN:HA	2:B:306:ILE:HG12	1.73	0.69
2:D:161:CYS:HA	2:D:163:ASN:HD21	1.58	0.69
2:B:298:LEU:HD13	2:B:302:LEU:HD21	1.75	0.68
2:D:159:LYS:HD3	2:D:192:PRO:HD2	1.76	0.68
2:B:237:ILE:HG23	2:B:259:ILE:HG13	1.76	0.68
2:B:159:LYS:HD3	2:B:192:PRO:HD2	1.76	0.68
1:C:2:THR:HG22	1:C:3:SER:N	2.08	0.68
1:C:35:THR:HG22	1:C:63:PRO:HA	1.76	0.67
1:A:37:LEU:HD11	1:A:61:SER:OG	1.94	0.67
1:A:2:THR:HG22	1:A:3:SER:N	2.09	0.67
2:D:237:ILE:HG23	2:D:259:ILE:HG13	1.77	0.67
2:B:279:SER:H	2:B:285:PHE:HE1	1.42	0.67
1:C:37:LEU:HD11	1:C:61:SER:OG	1.95	0.67
2:D:136:PHE:HD1	2:D:136:PHE:H	1.41	0.66
2:D:235:ILE:HD13	2:D:257:TYR:HB3	1.75	0.66
2:B:136:PHE:HD1	2:B:136:PHE:H	1.42	0.66
2:B:235:ILE:HD13	2:B:257:TYR:HB3	1.75	0.66
1:A:35:THR:HG22	1:A:63:PRO:HA	1.77	0.66
3:E:1:NAG:O3	3:E:2:NAG:H83	1.96	0.66
3:G:1:NAG:C6	3:G:2:NAG:O5	2.44	0.66
2:B:185:ASP:HA	2:B:188:LYS:HZ2	1.61	0.65
1:A:31:LEU:HG	1:A:50:LYS:HE2	1.78	0.65
2:B:236:ILE:O	2:B:258:ILE:HA	1.97	0.65
2:D:236:ILE:O	2:D:258:ILE:HA	1.97	0.65
2:D:185:ASP:HA	2:D:188:LYS:HZ2	1.61	0.65
1:A:64:MET:HE1	2:B:204:LEU:HA	1.78	0.65
2:B:261:ILE:HD12	2:B:290:ASP:O	1.97	0.64
2:B:268:LYS:O	2:B:272:GLU:HG3	1.98	0.64
1:C:64:MET:HE1	2:D:204:LEU:HA	1.79	0.64
1:C:89:VAL:HG13	1:C:177:SER:HB3	1.80	0.63
1:C:118:ASN:HA	3:G:1:NAG:O7	1.98	0.63
2:B:134:PHE:CE2	2:B:158:MET:HE3	2.33	0.63
2:D:134:PHE:CE2	2:D:158:MET:HE3	2.33	0.63
1:C:157:PHE:HB2	1:C:180:TYR:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:LYS:HD3	2:B:197:LYS:H	1.62	0.63
1:A:157:PHE:HB2	1:A:180:TYR:HB3	1.81	0.63
2:D:197:LYS:H	2:D:197:LYS:HD3	1.62	0.63
2:D:303:GLN:HA	2:D:306:ILE:HG12	1.80	0.62
2:B:271:GLN:HA	2:B:271:GLN:NE2	2.11	0.62
1:C:31:LEU:HG	1:C:50:LYS:HE2	1.81	0.62
1:A:103:ASN:HA	1:A:147:LEU:CD1	2.29	0.62
2:B:299:CYS:O	2:B:303:GLN:HG2	2.00	0.62
2:D:271:GLN:HA	2:D:271:GLN:NE2	2.11	0.61
1:C:122:VAL:HA	1:C:131:LYS:O	2.00	0.61
2:D:261:ILE:HD12	2:D:290:ASP:O	2.00	0.61
2:B:157:VAL:HG11	2:B:302:LEU:HD12	1.83	0.61
2:D:136:PHE:CZ	2:D:172:GLN:HB2	2.36	0.61
2:D:268:LYS:O	2:D:272:GLU:HG3	2.01	0.61
2:B:136:PHE:CZ	2:B:172:GLN:HB2	2.36	0.60
2:B:251:ALA:HB1	2:B:254:ILE:HD12	1.83	0.60
1:A:122:VAL:HA	1:A:131:LYS:O	2.01	0.60
1:C:100:VAL:HA	1:C:148:VAL:HB	1.83	0.60
1:A:91:LEU:HD23	1:A:91:LEU:H	1.67	0.60
1:C:91:LEU:HB2	1:C:107:ARG:O	2.01	0.60
2:D:299:CYS:O	2:D:303:GLN:HG2	2.01	0.60
1:A:20:THR:HG22	1:A:51:VAL:HG22	1.83	0.60
2:D:251:ALA:HB1	2:D:254:ILE:HD12	1.84	0.59
2:D:185:ASP:HA	2:D:188:LYS:NZ	2.18	0.59
1:A:37:LEU:HD22	1:A:54:LEU:HB3	1.85	0.59
1:A:100:VAL:HA	1:A:148:VAL:HB	1.84	0.59
1:C:166:ARG:N	1:C:167:PRO:HD2	2.18	0.59
2:B:185:ASP:HA	2:B:188:LYS:NZ	2.18	0.59
2:B:215:VAL:O	2:B:219:VAL:HB	2.03	0.59
2:B:136:PHE:HB3	2:B:237:ILE:HD12	1.83	0.58
1:C:117:ALA:C	1:C:118:ASN:HD22	2.11	0.58
1:C:92:ALA:HB1	1:C:93:PRO:CB	2.31	0.58
2:D:136:PHE:HB3	2:D:237:ILE:HD12	1.83	0.58
2:D:215:VAL:O	2:D:219:VAL:HB	2.03	0.58
2:B:291:THR:HG22	2:B:293:GLU:HB3	1.84	0.58
1:A:124:LEU:HA	1:A:130:LEU:HB2	1.85	0.58
2:D:279:SER:H	2:D:285:PHE:HE1	1.50	0.58
1:C:124:LEU:HA	1:C:130:LEU:HB2	1.85	0.58
1:A:166:ARG:N	1:A:167:PRO:HD2	2.19	0.58
1:C:37:LEU:HD22	1:C:54:LEU:HB3	1.86	0.57
2:D:271:GLN:HE21	2:D:271:GLN:CA	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:THR:HG22	2:D:293:GLU:HB3	1.87	0.57
1:A:13:ARG:HG3	1:A:58:GLN:HA	1.87	0.57
2:B:132:LEU:HB3	2:B:168:PHE:CD1	2.39	0.57
2:B:279:SER:N	2:B:285:PHE:CE1	2.72	0.57
2:B:303:GLN:HA	2:B:306:ILE:CG1	2.35	0.57
2:D:132:LEU:HB3	2:D:168:PHE:CD1	2.39	0.57
1:C:13:ARG:HG3	1:C:58:GLN:HA	1.87	0.56
1:A:91:LEU:HB2	1:A:107:ARG:O	2.05	0.56
1:C:84:TRP:O	1:C:113:GLY:HA2	2.06	0.56
1:A:84:TRP:O	1:A:113:GLY:HA2	2.06	0.56
1:C:20:THR:HG22	1:C:51:VAL:HG22	1.87	0.56
1:C:183:GLN:O	1:C:184:THR:HB	2.04	0.56
2:B:132:LEU:O	2:B:168:PHE:HA	2.06	0.56
2:B:271:GLN:HE21	2:B:271:GLN:CA	2.12	0.56
1:A:183:GLN:O	1:A:184:THR:HB	2.04	0.56
2:D:132:LEU:O	2:D:168:PHE:HA	2.06	0.56
2:B:279:SER:N	2:B:285:PHE:HE1	2.04	0.56
1:A:2:THR:CG2	1:A:3:SER:H	2.15	0.56
2:D:132:LEU:HB3	2:D:168:PHE:HD1	1.71	0.56
2:B:132:LEU:HB3	2:B:168:PHE:HD1	1.71	0.55
1:C:124:LEU:HB2	1:C:128:LYS:O	2.06	0.55
2:B:156:ASP:O	2:B:160:LYS:HD2	2.05	0.55
2:B:298:LEU:CB	2:B:302:LEU:HG	2.26	0.55
1:A:103:ASN:HA	1:A:147:LEU:HD12	1.88	0.55
1:A:124:LEU:HD23	1:A:158:SER:O	2.07	0.55
2:B:276:LYS:HB3	2:B:276:LYS:NZ	2.22	0.55
2:D:156:ASP:O	2:D:160:LYS:HD2	2.05	0.55
1:A:36:PRO:HG3	2:B:140:MET:O	2.06	0.55
1:C:124:LEU:HD23	1:C:158:SER:O	2.07	0.55
2:D:303:GLN:HA	2:D:306:ILE:CG1	2.37	0.55
1:A:124:LEU:HB2	1:A:128:LYS:O	2.07	0.55
1:C:33:ILE:HG22	1:C:52:TYR:CE1	2.42	0.54
1:C:37:LEU:HD11	1:C:61:SER:CB	2.38	0.54
1:A:117:ALA:C	1:A:118:ASN:HD22	2.16	0.54
2:B:132:LEU:HD23	2:B:133:VAL:N	2.22	0.54
2:D:132:LEU:HD23	2:D:133:VAL:N	2.22	0.54
1:A:33:ILE:HG22	1:A:52:TYR:CE1	2.42	0.54
2:B:264:HIS:O	2:B:271:GLN:HG3	2.08	0.54
1:A:37:LEU:HD11	1:A:61:SER:CB	2.38	0.54
2:D:289:LEU:C	2:D:291:THR:H	2.13	0.54
1:C:91:LEU:HD23	1:C:91:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:LYS:HG3	2:B:254:ILE:HG12	1.88	0.53
1:A:18:LEU:HD23	1:C:18:LEU:HD23	1.89	0.53
2:D:232:LYS:HG3	2:D:254:ILE:HG12	1.89	0.53
2:B:289:LEU:C	2:B:291:THR:H	2.14	0.53
1:C:21:CYS:HB3	1:C:31:LEU:HD11	1.91	0.52
2:D:133:VAL:HG11	2:D:215:VAL:HG13	1.91	0.52
1:C:85:THR:HG21	3:H:1:NAG:H5	1.90	0.52
2:D:235:ILE:HD13	2:D:257:TYR:CB	2.40	0.52
1:A:21:CYS:HB3	1:A:31:LEU:HD11	1.91	0.52
1:A:106:LEU:HD11	1:A:157:PHE:CD1	2.44	0.52
2:D:163:ASN:ND2	2:D:163:ASN:N	2.53	0.52
2:B:235:ILE:HD13	2:B:257:TYR:CB	2.40	0.52
2:B:133:VAL:HG11	2:B:215:VAL:HG13	1.91	0.52
2:B:284:GLU:HA	2:B:287:LYS:HE3	1.92	0.52
1:C:106:LEU:HD11	1:C:157:PHE:CD1	2.45	0.52
1:C:88:ARG:HH21	1:C:90:GLU:HB3	1.75	0.52
2:B:163:ASN:ND2	2:B:163:ASN:N	2.53	0.51
2:D:134:PHE:HD1	2:D:235:ILE:HB	1.76	0.51
2:D:136:PHE:HA	2:D:237:ILE:HB	1.93	0.51
2:B:175:THR:HA	2:B:207:ASN:ND2	2.26	0.51
1:C:63:PRO:HD2	1:C:78:THR:HG23	1.93	0.51
2:D:135:LEU:HD23	2:D:236:ILE:HG12	1.93	0.51
2:B:298:LEU:HB3	2:B:302:LEU:CD1	2.40	0.51
2:B:298:LEU:HD13	2:B:302:LEU:HD11	1.92	0.51
1:A:11:LEU:HB2	1:A:12:PRO:HD2	1.92	0.51
1:A:118:ASN:HA	3:E:1:NAG:O7	2.10	0.51
2:B:134:PHE:HD1	2:B:235:ILE:HB	1.76	0.51
2:B:136:PHE:HA	2:B:237:ILE:HB	1.93	0.51
1:C:38:PRO:HD2	1:C:55:SER:O	2.12	0.50
2:B:135:LEU:HD23	2:B:236:ILE:HG12	1.93	0.50
1:C:43:LEU:HB3	1:C:45:PRO:HD2	1.92	0.50
2:D:179:THR:HG23	2:D:214:TYR:HE1	1.76	0.50
2:B:167:GLN:HA	2:B:186:TYR:HE1	1.75	0.50
2:B:179:THR:HG23	2:B:214:TYR:HE1	1.76	0.50
2:B:291:THR:HB	2:B:294:LYS:HE3	1.94	0.50
1:C:36:PRO:HG3	2:D:140:MET:O	2.11	0.50
1:A:63:PRO:HD2	1:A:78:THR:HG23	1.94	0.50
2:D:175:THR:HA	2:D:207:ASN:ND2	2.27	0.50
2:D:264:HIS:O	2:D:271:GLN:HG3	2.12	0.50
2:B:296:LYS:HG3	2:B:297:ASP:N	2.27	0.50
2:D:167:GLN:HA	2:D:186:TYR:HE1	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:NAG:O3	3:F:2:NAG:O5	2.28	0.49
2:D:134:PHE:HE2	2:D:158:MET:HE3	1.74	0.49
2:D:284:GLU:HA	2:D:287:LYS:HE3	1.95	0.49
1:A:14:GLY:HA2	1:A:56:ASN:HA	1.94	0.49
1:A:38:PRO:HD2	1:A:55:SER:O	2.13	0.49
1:C:108:CYS:HB2	1:C:123:LEU:HD21	1.95	0.49
2:D:291:THR:HB	2:D:294:LYS:HE3	1.95	0.49
1:A:108:CYS:HB2	1:A:123:LEU:HD21	1.95	0.49
2:B:134:PHE:HE2	2:B:158:MET:HE3	1.74	0.49
1:C:11:LEU:HB2	1:C:12:PRO:HD2	1.94	0.48
2:D:195:LEU:HA	2:D:197:LYS:NZ	2.28	0.48
1:A:4:VAL:CG2	1:A:65:CYS:SG	3.01	0.48
1:A:89:VAL:HG13	1:A:177:SER:HB3	1.95	0.48
1:C:63:PRO:HB2	1:C:78:THR:CG2	2.44	0.48
1:A:63:PRO:HB2	1:A:78:THR:CG2	2.44	0.48
2:D:188:LYS:NZ	2:D:188:LYS:HB2	2.27	0.48
1:C:14:GLY:HA2	1:C:56:ASN:HA	1.95	0.48
2:D:130:VAL:HG13	2:D:231:THR:O	2.13	0.48
2:D:167:GLN:HB3	2:D:183:PHE:CE1	2.48	0.48
2:B:167:GLN:HB3	2:B:183:PHE:CE1	2.48	0.48
2:B:195:LEU:HA	2:B:197:LYS:NZ	2.29	0.48
2:D:183:PHE:O	2:D:186:TYR:HB3	2.14	0.48
1:A:43:LEU:HB3	1:A:45:PRO:HD2	1.95	0.48
2:B:183:PHE:O	2:B:186:TYR:HB3	2.14	0.48
1:C:4:VAL:CG2	1:C:65:CYS:SG	3.02	0.48
2:B:130:VAL:HG13	2:B:231:THR:O	2.13	0.48
2:D:205:LEU:HB3	2:D:243:THR:HG21	1.95	0.48
2:D:297:ASP:OD2	2:D:299:CYS:HB2	2.14	0.48
2:B:157:VAL:HG11	2:B:302:LEU:CD1	2.44	0.48
2:B:205:LEU:HB3	2:B:243:THR:HG21	1.96	0.48
2:D:279:SER:N	2:D:285:PHE:CE1	2.78	0.48
2:B:232:LYS:O	2:B:254:ILE:HG23	2.13	0.47
1:A:66:TYR:CD1	1:A:66:TYR:C	2.92	0.47
2:B:188:LYS:NZ	2:B:188:LYS:HB2	2.28	0.47
2:D:234:LEU:HB2	2:D:254:ILE:CG2	2.44	0.47
1:C:66:TYR:CD1	1:C:66:TYR:C	2.92	0.47
1:A:13:ARG:C	1:A:15:GLY:H	2.22	0.47
1:C:44:LEU:N	1:C:45:PRO:CD	2.78	0.47
2:B:234:LEU:HB2	2:B:254:ILE:CG2	2.45	0.47
1:C:9:VAL:HG11	1:C:17:VAL:HG11	1.96	0.47
1:C:13:ARG:C	1:C:15:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:GLY:HA3	2:D:274:LEU:CD2	2.39	0.47
1:A:9:VAL:HG11	1:A:17:VAL:HG11	1.96	0.47
1:A:90:GLU:HG2	1:A:91:LEU:N	2.30	0.47
2:B:261:ILE:HA	2:B:290:ASP:O	2.14	0.47
1:C:10:ILE:HA	1:C:81:THR:HB	1.97	0.47
1:C:42:LEU:HD12	1:C:51:VAL:CG1	2.45	0.47
1:A:44:LEU:N	1:A:45:PRO:CD	2.78	0.47
3:E:1:NAG:H61	3:E:2:NAG:O6	2.14	0.46
1:A:106:LEU:HD11	1:A:157:PHE:HD1	1.81	0.46
2:B:186:TYR:CD1	2:B:187:VAL:HG22	2.50	0.46
1:C:47:ASN:N	1:C:47:ASN:OD1	2.48	0.46
1:C:122:VAL:HB	1:C:132:ARG:HG2	1.96	0.46
2:D:186:TYR:CD1	2:D:187:VAL:HG22	2.50	0.46
2:B:240:GLY:O	2:B:271:GLN:NE2	2.48	0.46
2:B:298:LEU:O	2:B:302:LEU:HB2	2.16	0.46
2:D:133:VAL:HG11	2:D:215:VAL:CG1	2.45	0.46
1:A:83:TYR:HA	1:A:114:ALA:O	2.16	0.46
2:B:305:LYS:C	2:B:306:ILE:HD13	2.40	0.46
1:C:83:TYR:HA	1:C:114:ALA:O	2.16	0.46
1:C:123:LEU:HD13	1:C:144:THR:HG22	1.97	0.46
2:D:148:GLN:HA	2:D:151:LEU:HG	1.98	0.46
2:D:232:LYS:O	2:D:254:ILE:HG23	2.15	0.46
1:A:64:MET:HE1	2:B:204:LEU:CA	2.43	0.46
1:A:122:VAL:HB	1:A:132:ARG:HG2	1.97	0.46
1:A:123:LEU:HD13	1:A:144:THR:HG22	1.97	0.46
2:B:233:VAL:HG22	2:B:255:ILE:HD12	1.98	0.46
1:C:2:THR:CG2	1:C:3:SER:H	2.15	0.46
2:D:233:VAL:HG22	2:D:255:ILE:HD12	1.98	0.46
1:C:110:VAL:HG22	1:C:140:ALA:CB	2.41	0.46
2:D:240:GLY:O	2:D:271:GLN:NE2	2.48	0.46
2:D:276:LYS:NZ	2:D:276:LYS:HB3	2.31	0.46
1:C:166:ARG:N	1:C:167:PRO:CD	2.80	0.45
2:D:302:LEU:O	2:D:302:LEU:HD23	2.15	0.45
2:D:292:PHE:CD1	2:D:292:PHE:N	2.83	0.45
2:B:298:LEU:HD22	2:B:302:LEU:HG	1.98	0.45
1:C:106:LEU:HD11	1:C:157:PHE:HD1	1.81	0.45
2:B:133:VAL:HG11	2:B:215:VAL:CG1	2.46	0.45
2:D:296:LYS:HG3	2:D:297:ASP:N	2.31	0.45
2:B:130:VAL:HG21	2:B:306:ILE:HD12	1.98	0.45
2:B:157:VAL:CG1	2:B:302:LEU:HD12	2.45	0.45
2:D:267:THR:O	2:D:271:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:N	1:A:153:HIS:ND1	2.65	0.45
1:A:17:VAL:O	1:A:53:GLU:HA	2.17	0.45
1:C:34:GLU:HB3	1:C:64:MET:HB3	1.99	0.45
2:D:130:VAL:HG22	2:D:231:THR:CB	2.39	0.45
2:B:130:VAL:HG22	2:B:231:THR:CB	2.39	0.45
2:B:148:GLN:HA	2:B:151:LEU:HG	1.99	0.45
1:A:34:GLU:HB3	1:A:64:MET:HB3	1.99	0.45
2:D:150:ILE:HG12	2:D:292:PHE:CZ	2.52	0.45
2:D:264:HIS:O	2:D:266:GLN:N	2.48	0.45
2:B:155:LYS:HE2	2:B:192:PRO:O	2.16	0.45
2:B:234:LEU:O	2:B:257:TYR:HB2	2.17	0.45
2:B:240:GLY:HA3	2:B:274:LEU:CD2	2.41	0.45
1:C:136:VAL:O	1:C:140:ALA:HA	2.17	0.45
1:C:153:HIS:ND1	1:C:153:HIS:N	2.65	0.45
1:C:10:ILE:HG12	1:C:81:THR:HB	1.99	0.44
2:D:155:LYS:HE2	2:D:192:PRO:O	2.16	0.44
2:D:234:LEU:O	2:D:257:TYR:HB2	2.17	0.44
1:A:62:GLN:O	2:B:140:MET:HE1	2.18	0.44
1:A:10:ILE:HA	1:A:81:THR:HB	1.99	0.44
1:A:10:ILE:HG12	1:A:81:THR:HB	1.99	0.44
1:A:160:ARG:CG	1:A:161:THR:N	2.80	0.44
1:A:166:ARG:N	1:A:167:PRO:CD	2.81	0.44
1:A:136:VAL:O	1:A:140:ALA:HA	2.18	0.44
1:C:32:GLY:HA2	1:C:52:TYR:OH	2.18	0.44
1:A:32:GLY:HA2	1:A:52:TYR:OH	2.18	0.44
1:C:64:MET:HE1	2:D:204:LEU:CA	2.45	0.44
1:C:160:ARG:CG	1:C:161:THR:N	2.80	0.44
2:D:136:PHE:CD1	2:D:136:PHE:N	2.76	0.44
1:C:17:VAL:O	1:C:53:GLU:HA	2.18	0.44
1:C:17:VAL:HG21	1:C:80:LEU:HD13	2.00	0.44
2:D:158:MET:HE2	2:D:168:PHE:HB2	1.99	0.44
1:A:167:PRO:O	1:C:167:PRO:O	2.36	0.44
2:B:136:PHE:CD1	2:B:136:PHE:N	2.77	0.44
2:B:140:MET:HB2	2:B:203:LEU:O	2.18	0.44
2:D:130:VAL:HG21	2:D:306:ILE:HD12	1.99	0.44
1:A:42:LEU:HD12	1:A:51:VAL:CG1	2.48	0.43
2:B:158:MET:HE2	2:B:168:PHE:HB2	1.99	0.43
1:C:118:ASN:HD22	1:C:118:ASN:N	2.16	0.43
1:C:37:LEU:CD2	1:C:57:VAL:HB	2.48	0.43
1:C:165:LEU:HD13	1:C:170:LEU:HD12	1.98	0.43
2:B:167:GLN:HA	2:B:186:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:N	2:D:151:LEU:HD23	2.33	0.43
2:B:292:PHE:CD1	2:B:292:PHE:N	2.85	0.43
2:D:158:MET:HE1	2:D:181:PHE:CZ	2.39	0.43
2:D:167:GLN:HA	2:D:186:TYR:CE1	2.53	0.43
1:A:50:LYS:HD2	1:A:52:TYR:OH	2.19	0.43
2:D:172:GLN:HE21	2:D:172:GLN:HB3	1.53	0.43
2:D:194:ALA:O	2:D:197:LYS:HD2	2.19	0.43
2:B:150:ILE:HG12	2:B:292:PHE:CZ	2.54	0.43
1:A:165:LEU:HD13	1:A:170:LEU:HD12	1.98	0.43
2:B:194:ALA:O	2:B:197:LYS:HD2	2.19	0.43
2:D:140:MET:HB2	2:D:203:LEU:O	2.19	0.43
1:A:42:LEU:HD23	1:C:43:LEU:HD12	2.01	0.43
1:A:104:LEU:O	1:A:104:LEU:HD23	2.19	0.43
1:C:157:PHE:O	1:C:180:TYR:N	2.52	0.43
1:C:50:LYS:HD2	1:C:52:TYR:OH	2.19	0.43
1:C:64:MET:HG2	1:C:75:THR:CG2	2.49	0.43
1:C:104:LEU:O	1:C:104:LEU:HD23	2.19	0.43
1:A:5:SER:HA	1:A:6:PRO:C	2.44	0.42
2:B:158:MET:HE1	2:B:181:PHE:CZ	2.39	0.42
2:B:273:THR:HG22	2:B:273:THR:O	2.19	0.42
2:D:158:MET:HG3	2:D:168:PHE:CD2	2.54	0.42
2:D:183:PHE:HA	2:D:186:TYR:HB3	2.00	0.42
2:D:279:SER:N	2:D:285:PHE:HE1	2.13	0.42
1:A:4:VAL:HG21	1:A:65:CYS:SG	2.59	0.42
1:A:64:MET:HG2	1:A:75:THR:CG2	2.50	0.42
1:A:88:ARG:HH21	1:A:90:GLU:HB3	1.85	0.42
2:B:158:MET:HG3	2:B:168:PHE:CD2	2.54	0.42
2:B:183:PHE:HA	2:B:186:TYR:HB3	2.00	0.42
2:B:208:THR:HG21	2:B:277:PHE:CE1	2.55	0.42
1:A:89:VAL:O	1:A:89:VAL:HG22	2.19	0.42
2:B:301:GLU:O	2:B:304:LYS:HE3	2.20	0.42
1:A:17:VAL:HG21	1:A:80:LEU:HD13	2.01	0.42
2:D:132:LEU:HD21	2:D:235:ILE:HG13	2.01	0.42
2:B:172:GLN:HE21	2:B:172:GLN:HB3	1.53	0.42
1:C:126:GLY:C	1:C:128:LYS:H	2.27	0.42
1:A:98:GLN:HA	1:A:99:PRO:HD3	1.81	0.42
2:B:274:LEU:HD12	2:B:286:VAL:HG22	2.02	0.42
1:A:157:PHE:O	1:A:180:TYR:N	2.53	0.42
2:B:155:LYS:HG2	2:B:192:PRO:HB2	2.00	0.42
2:D:274:LEU:HD12	2:D:286:VAL:HG22	2.02	0.42
2:B:151:LEU:N	2:B:151:LEU:HD23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:LEU:HD23	2:D:236:ILE:HG23	2.01	0.42
2:D:155:LYS:HG2	2:D:192:PRO:HB2	2.00	0.42
3:E:1:NAG:O4	3:E:2:NAG:C8	2.68	0.42
1:A:37:LEU:CD2	1:A:57:VAL:HB	2.50	0.42
1:C:88:ARG:NH2	1:C:90:GLU:HB3	2.33	0.42
1:C:5:SER:HA	1:C:6:PRO:C	2.45	0.42
2:B:132:LEU:HD21	2:B:235:ILE:HG13	2.02	0.41
1:A:126:GLY:C	1:A:128:LYS:H	2.27	0.41
1:C:91:LEU:HA	1:C:108:CYS:HA	2.02	0.41
2:D:273:THR:O	2:D:273:THR:HG22	2.20	0.41
1:A:92:ALA:HA	1:A:93:PRO:HD2	1.82	0.41
3:E:1:NAG:H61	3:E:2:NAG:C6	2.50	0.41
1:C:4:VAL:HG21	1:C:65:CYS:SG	2.60	0.41
2:D:135:LEU:HD11	2:D:211:ALA:HB1	2.02	0.41
2:B:135:LEU:HD11	2:B:211:ALA:HB1	2.02	0.41
1:C:37:LEU:HD23	1:C:57:VAL:HB	2.03	0.41
2:D:235:ILE:O	2:D:235:ILE:HG22	2.20	0.41
2:D:284:GLU:HG2	2:D:287:LYS:HE3	2.03	0.41
3:G:2:NAG:H82	3:G:2:NAG:H2	1.91	0.41
1:A:156:ASN:ND2	4:A:404:NAG:H83	2.36	0.41
2:B:173:PHE:HZ	2:B:238:THR:HB	1.85	0.41
2:D:173:PHE:HZ	2:D:238:THR:HB	1.85	0.41
1:A:138:GLU:HA	1:A:139:PRO:HA	1.95	0.41
2:B:139:SER:CB	2:B:205:LEU:O	2.69	0.41
2:B:235:ILE:O	2:B:235:ILE:HG22	2.21	0.41
1:C:70:PRO:HG2	1:C:71:ASP:H	1.85	0.41
1:C:161:THR:O	1:C:174:GLU:HA	2.21	0.41
2:B:163:ASN:H	2:B:163:ASN:HD22	1.64	0.40
2:B:238:THR:C	2:B:240:GLY:H	2.30	0.40
2:B:251:ALA:HB1	2:B:254:ILE:CD1	2.51	0.40
2:B:130:VAL:HG13	2:B:233:VAL:HG23	2.04	0.40
2:B:289:LEU:C	2:B:291:THR:N	2.79	0.40
2:D:163:ASN:H	2:D:163:ASN:HD22	1.63	0.40
3:G:1:NAG:H61	3:G:2:NAG:O6	2.20	0.40
1:A:44:LEU:HB3	1:A:45:PRO:HD3	2.03	0.40
2:B:177:TYR:OH	2:B:210:GLY:HA3	2.21	0.40
1:A:161:THR:O	1:A:174:GLU:HA	2.21	0.40
1:C:98:GLN:HA	1:C:99:PRO:HD3	1.81	0.40
2:B:135:LEU:HD23	2:B:236:ILE:HG23	2.03	0.40
2:D:130:VAL:HG13	2:D:233:VAL:HG23	2.04	0.40
2:D:139:SER:CB	2:D:205:LEU:O	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:NAG:O3	3:F:2:NAG:C7	2.69	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	182/291 (62%)	157 (86%)	19 (10%)	6 (3%)	3	19
1	C	182/291 (62%)	155 (85%)	20 (11%)	7 (4%)	2	16
2	B	175/177 (99%)	128 (73%)	37 (21%)	10 (6%)	1	9
2	D	175/177 (99%)	127 (73%)	37 (21%)	11 (6%)	1	8
All	All	714/936 (76%)	567 (79%)	113 (16%)	34 (5%)	2	12

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	289	LEU
1	C	93	PRO
1	A	127	GLU
1	A	154	GLY
2	B	261	ILE
2	B	282	ALA
1	C	127	GLU
1	C	154	GLY
2	D	261	ILE
2	D	265	PHE
2	D	282	ALA
1	A	60	ASP
2	B	190	LYS
1	C	60	ASP

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Mol	Chain	Res	Type
2	D	190	LYS
2	B	225	GLY
2	D	141	SER
2	D	225	GLY
2	D	305	LYS
2	B	146	GLU
1	C	86	PRO
2	D	146	GLU
1	A	153	HIS
2	B	158	MET
2	B	281	PRO
1	C	153	HIS
2	D	158	MET
1	A	86	PRO
2	B	187	VAL
2	B	191	ASP
1	C	169	GLY
2	D	187	VAL
2	D	191	ASP
1	A	169	GLY

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	164/257 (64%)	140 (85%)	24 (15%)	3	14
1	C	164/257 (64%)	140 (85%)	24 (15%)	3	14
2	B	158/158 (100%)	138 (87%)	20 (13%)	4	18
2	D	158/158 (100%)	138 (87%)	20 (13%)	4	18
All	All	644/830 (78%)	556 (86%)	88 (14%)	3	16

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	13	ARG
1	A	17	VAL
1	A	18	LEU
1	A	19	VAL
1	A	29	LYS
1	A	30	LEU
1	A	47	ASN
1	A	55	SER
1	A	74	SER
1	A	80	LEU
1	A	102	LYS
1	A	104	LEU
1	A	110	VAL
1	A	124	LEU
1	A	128	LYS
1	A	129	GLU
1	A	130	LEU
1	A	142	VAL
1	A	147	LEU
1	A	148	VAL
1	A	153	HIS
1	A	168	GLN
1	A	181	GLN
2	B	136	PHE
2	B	150	ILE
2	B	151	LEU
2	B	163	ASN
2	B	166	TYR
2	B	171	VAL
2	B	172	GLN
2	B	176	SER
2	B	187	VAL
2	B	188	LYS
2	B	201	HIS
2	B	222	GLU
2	B	259	ILE
2	B	271	GLN
2	B	274	LEU
2	B	276	LYS
2	B	281	PRO
2	B	292	PHE
2	B	296	LYS

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Mol	Chain	Res	Type
2	B	299	CYS
1	C	10	ILE
1	C	13	ARG
1	C	17	VAL
1	C	18	LEU
1	C	19	VAL
1	C	29	LYS
1	C	30	LEU
1	C	45	PRO
1	C	47	ASN
1	C	55	SER
1	C	74	SER
1	C	80	LEU
1	C	102	LYS
1	C	104	LEU
1	C	110	VAL
1	C	124	LEU
1	C	128	LYS
1	C	129	GLU
1	C	130	LEU
1	C	142	VAL
1	C	148	VAL
1	C	153	HIS
1	C	168	GLN
1	C	181	GLN
2	D	136	PHE
2	D	150	ILE
2	D	151	LEU
2	D	163	ASN
2	D	166	TYR
2	D	171	VAL
2	D	172	GLN
2	D	176	SER
2	D	187	VAL
2	D	188	LYS
2	D	201	HIS
2	D	222	GLU
2	D	259	ILE
2	D	271	GLN
2	D	274	LEU
2	D	276	LYS
2	D	281	PRO

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Mol	Chain	Res	Type
2	D	292	PHE
2	D	296	LYS
2	D	299	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
2	B	148	GLN
2	B	163	ASN
2	B	198	HIS
2	B	207	ASN
2	B	271	GLN
1	C	1	GLN
2	D	148	GLN
2	D	163	ASN
2	D	198	HIS
2	D	207	ASN
2	D	271	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.68	0	17,19,21	2.40	4 (23%)
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	0.73	0
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	0.81	0
3	NAG	F	2	3	14,14,15	0.79	1 (7%)	17,19,21	0.78	0
3	NAG	G	1	1,3	14,14,15	0.90	0	17,19,21	1.07	1 (5%)
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	0.69	0
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.09	1 (5%)
3	NAG	H	2	3	14,14,15	1.05	1 (7%)	17,19,21	0.61	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	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NAG	C1-C2	2.88	1.56	1.52
3	F	2	NAG	C1-C2	2.27	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C4-C3-C2	-7.53	99.99	111.02
3	E	1	NAG	C2-N2-C7	-3.53	118.17	122.90
3	E	1	NAG	C1-O5-C5	3.20	116.48	112.19
3	G	1	NAG	C2-N2-C7	-2.95	118.95	122.90
3	E	1	NAG	O4-C4-C5	2.84	116.33	109.32
3	H	1	NAG	C4-C3-C2	2.30	114.39	111.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

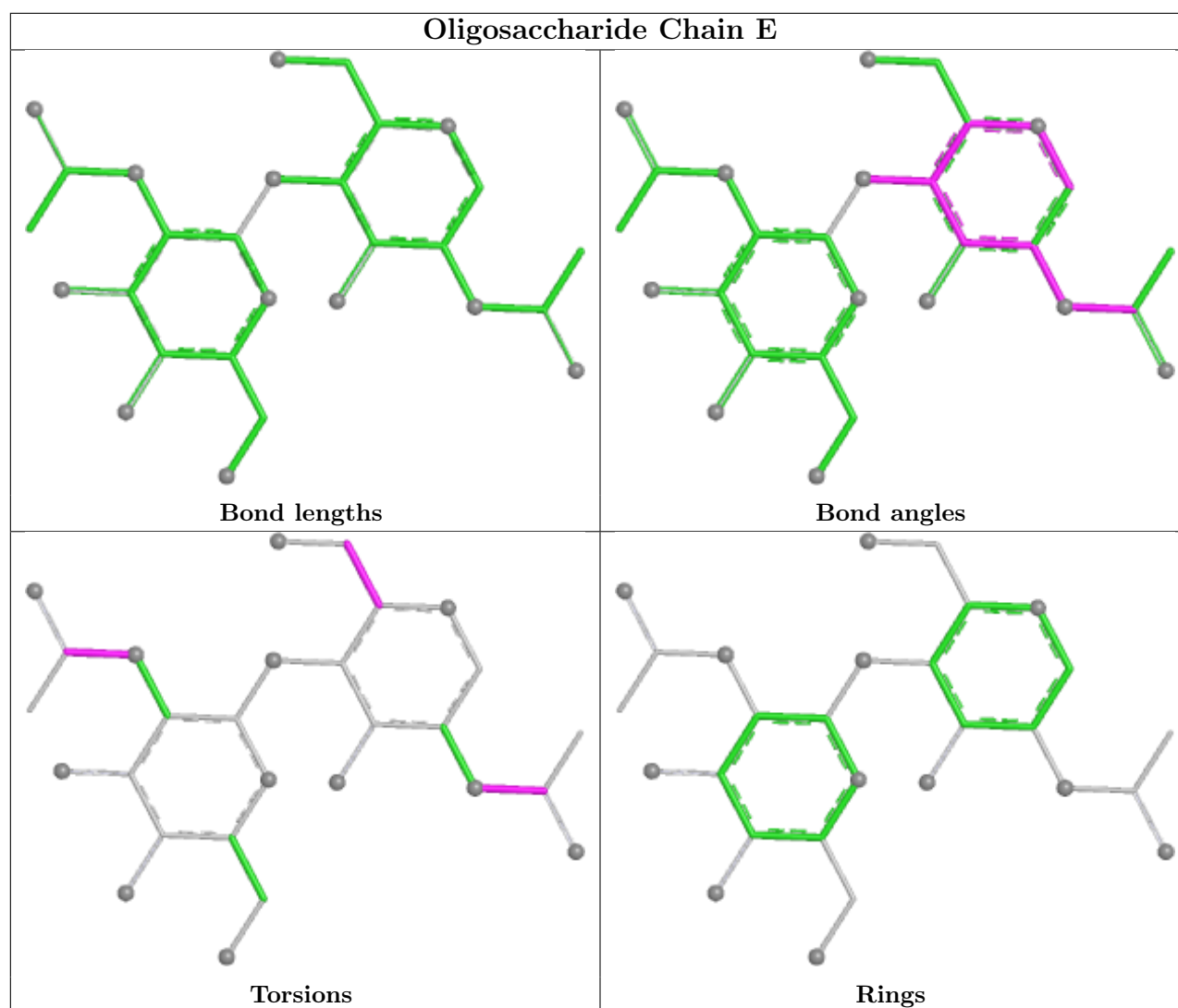
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
3	G	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6

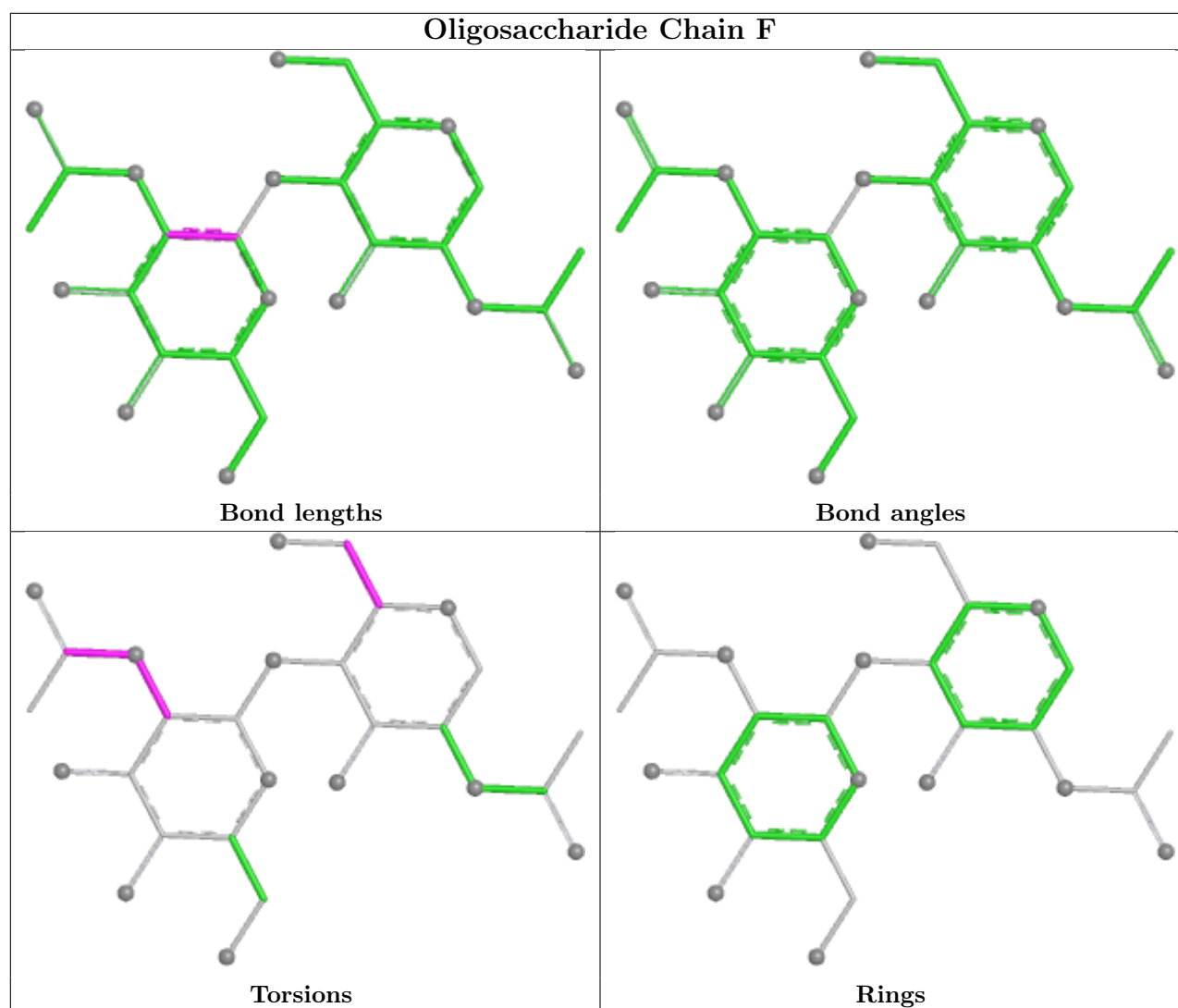
There are no ring outliers.

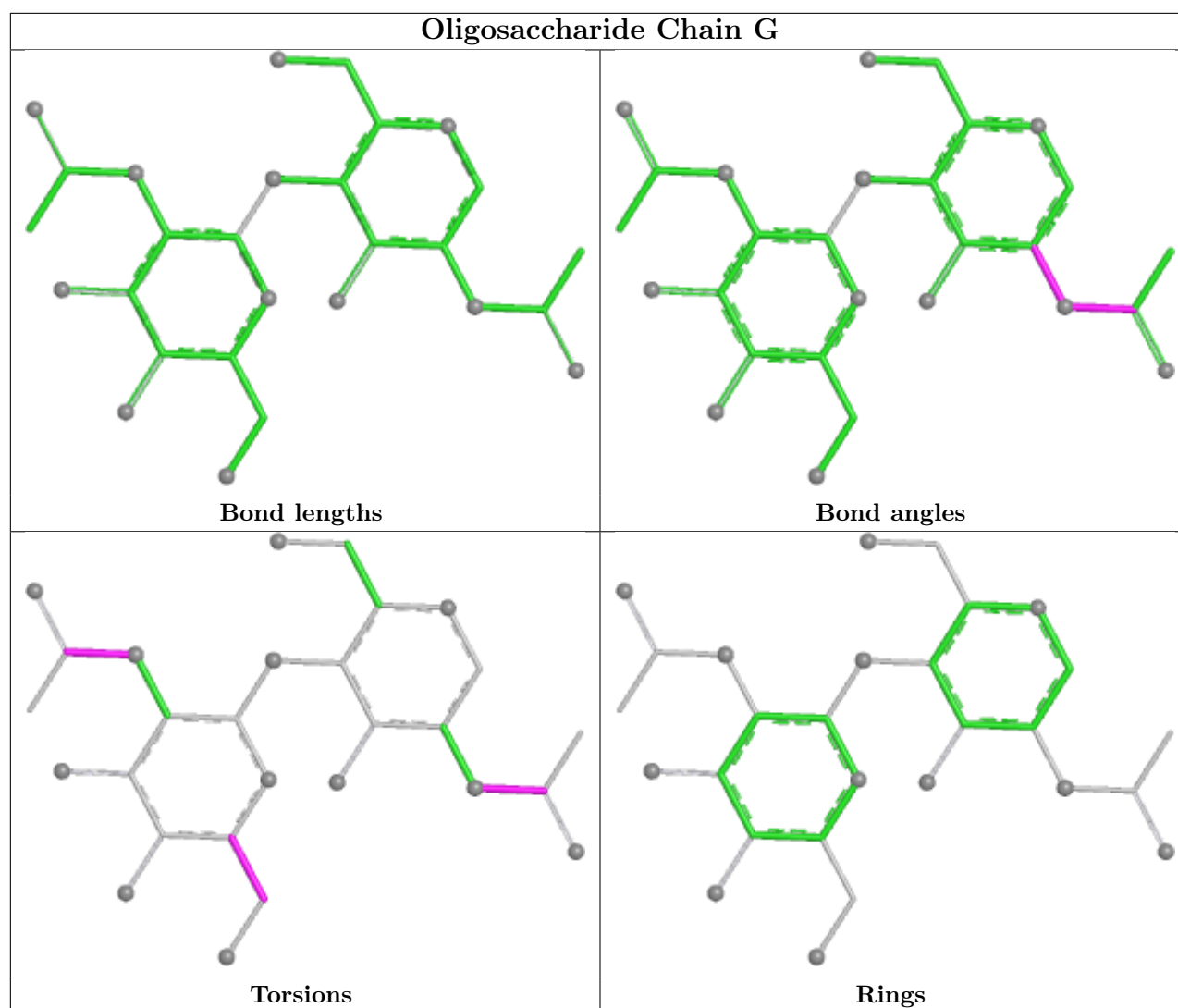
7 monomers are involved in 16 short contacts:

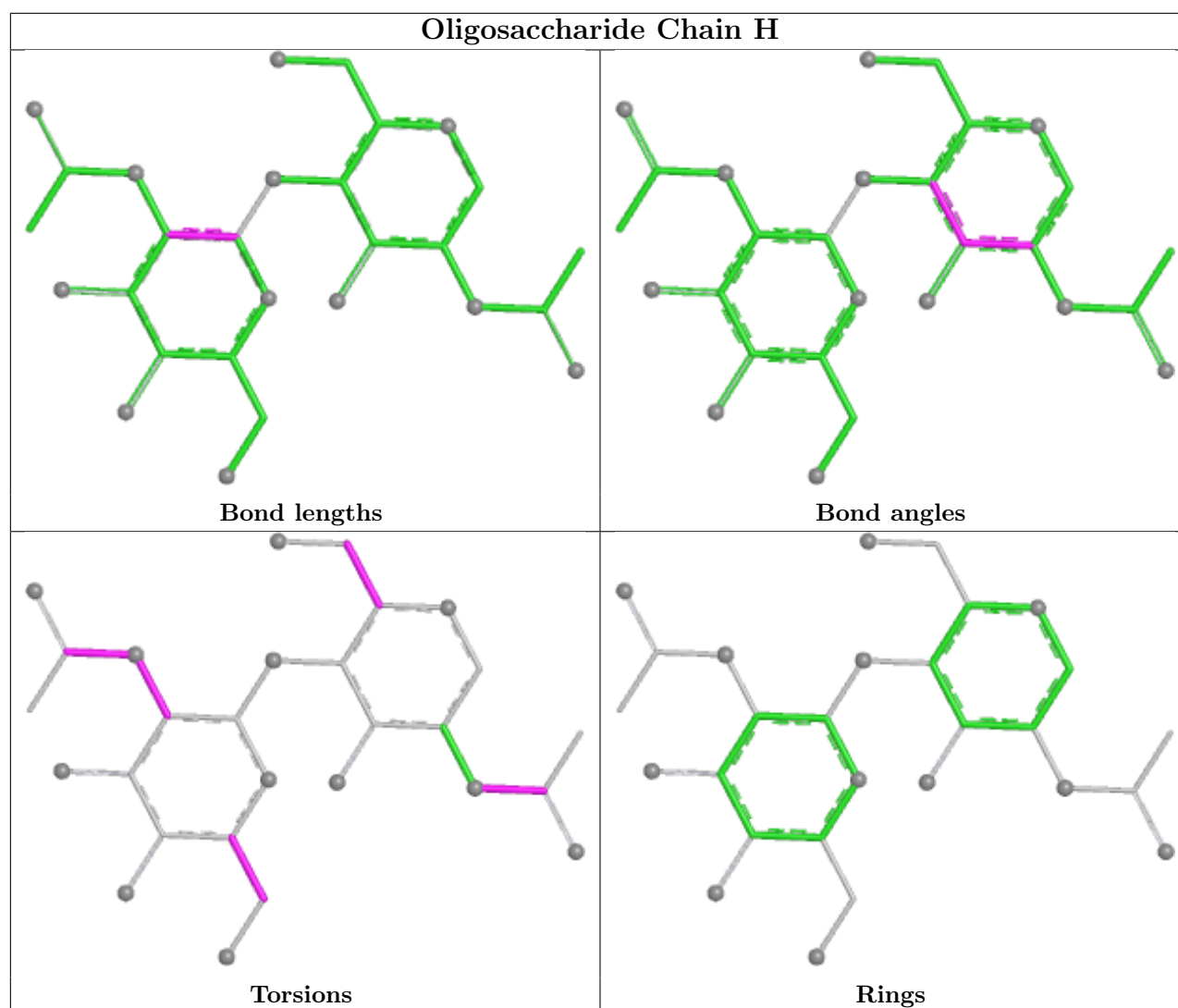
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	5	0
3	F	1	NAG	1	0
3	E	2	NAG	6	0
3	H	1	NAG	1	0
3	E	1	NAG	7	0
3	G	1	NAG	5	0
3	F	2	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	404	1	14,14,15	0.70	1 (7%)	17,19,21	0.55	0
4	NAG	C	410	1	14,14,15	0.62	0	17,19,21	0.64	0
4	NAG	C	407	1	14,14,15	0.58	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	401	1	14,14,15	0.60	0	17,19,21	0.71	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	A	404	1	-	5/6/23/26	0/1/1/1
4	NAG	C	410	1	-	5/6/23/26	0/1/1/1
4	NAG	C	407	1	-	3/6/23/26	0/1/1/1
4	NAG	A	401	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	NAG	C1-C2	2.14	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	407	NAG	C2-N2-C7	-2.11	120.07	122.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	A	404	NAG	C1-C2-N2-C7
4	A	404	NAG	C8-C7-N2-C2
4	A	404	NAG	O7-C7-N2-C2
4	C	407	NAG	C8-C7-N2-C2
4	C	407	NAG	O7-C7-N2-C2
4	C	410	NAG	C1-C2-N2-C7
4	C	410	NAG	C8-C7-N2-C2
4	C	410	NAG	O7-C7-N2-C2
4	C	410	NAG	C4-C5-C6-O6
4	A	404	NAG	C4-C5-C6-O6
4	A	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	401	NAG	C4-C5-C6-O6
4	C	410	NAG	O5-C5-C6-O6
4	A	404	NAG	O5-C5-C6-O6
4	C	407	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/291 (63%)	-1.50	0 100 100	11, 53, 97, 99	0
1	C	184/291 (63%)	-1.52	0 100 100	11, 53, 97, 99	0
2	B	177/177 (100%)	-1.44	0 100 100	19, 83, 100, 104	6 (3%)
2	D	177/177 (100%)	-1.49	0 100 100	19, 81, 100, 104	7 (3%)
All	All	722/936 (77%)	-1.49	0 100 100	11, 68, 99, 104	13 (1%)

There are no RSRZ outliers to report.

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

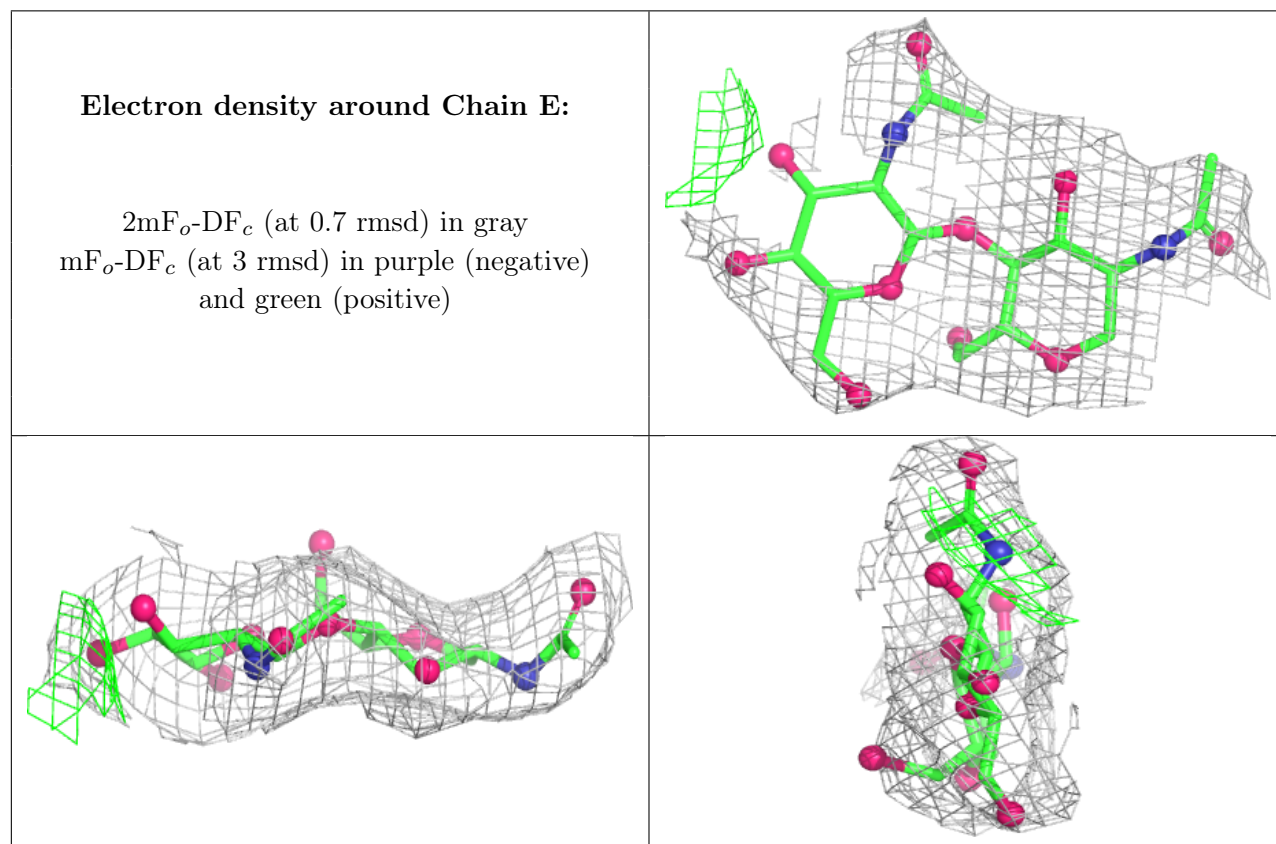
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

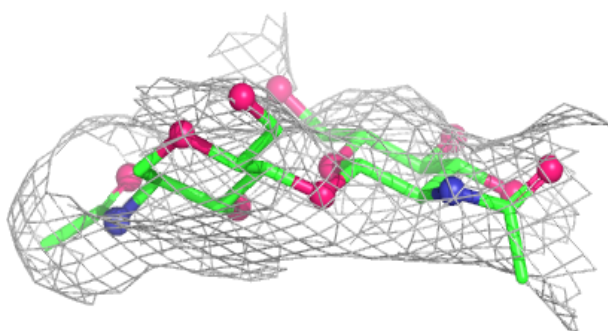
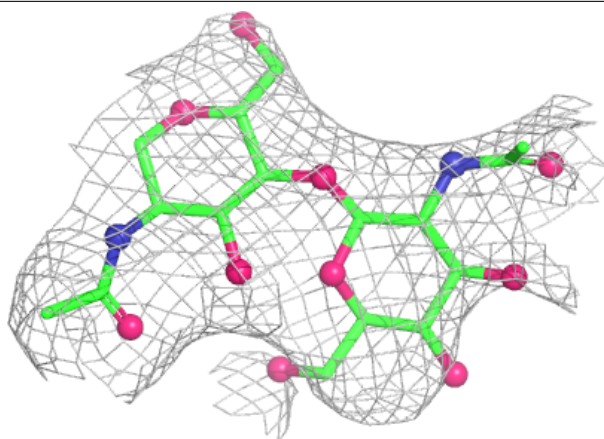
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.97	0.04	81,81,81,81	0
3	NAG	F	2	14/15	0.97	0.04	96,96,96,96	0
3	NAG	G	2	14/15	0.97	0.03	78,78,78,78	0
3	NAG	H	2	14/15	0.98	0.07	96,96,96,96	0
3	NAG	G	1	14/15	0.99	0.03	59,59,59,59	0
3	NAG	F	1	14/15	0.99	0.02	36,36,36,36	0
3	NAG	H	1	14/15	0.99	0.03	30,30,30,30	0
3	NAG	E	1	14/15	0.99	0.04	72,72,72,72	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.



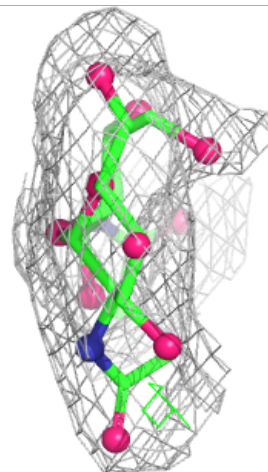
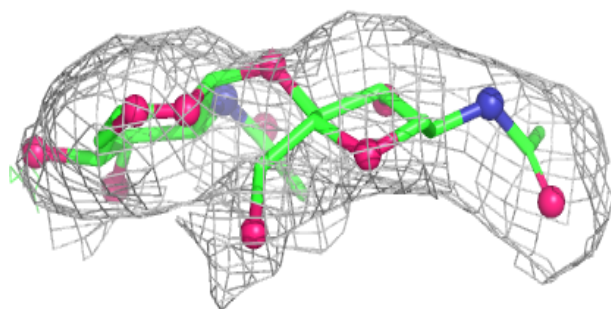
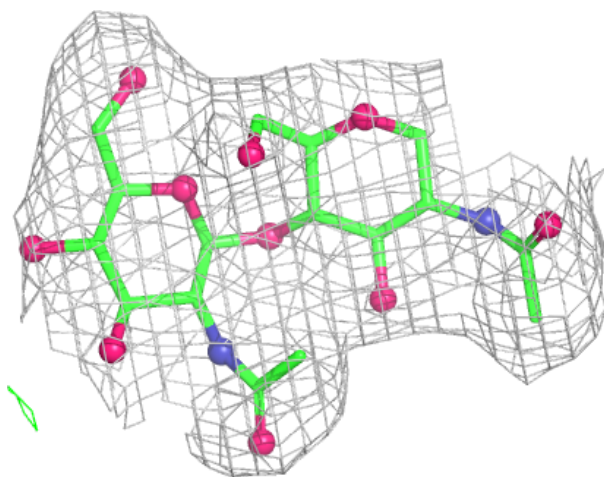
Electron density around Chain F:

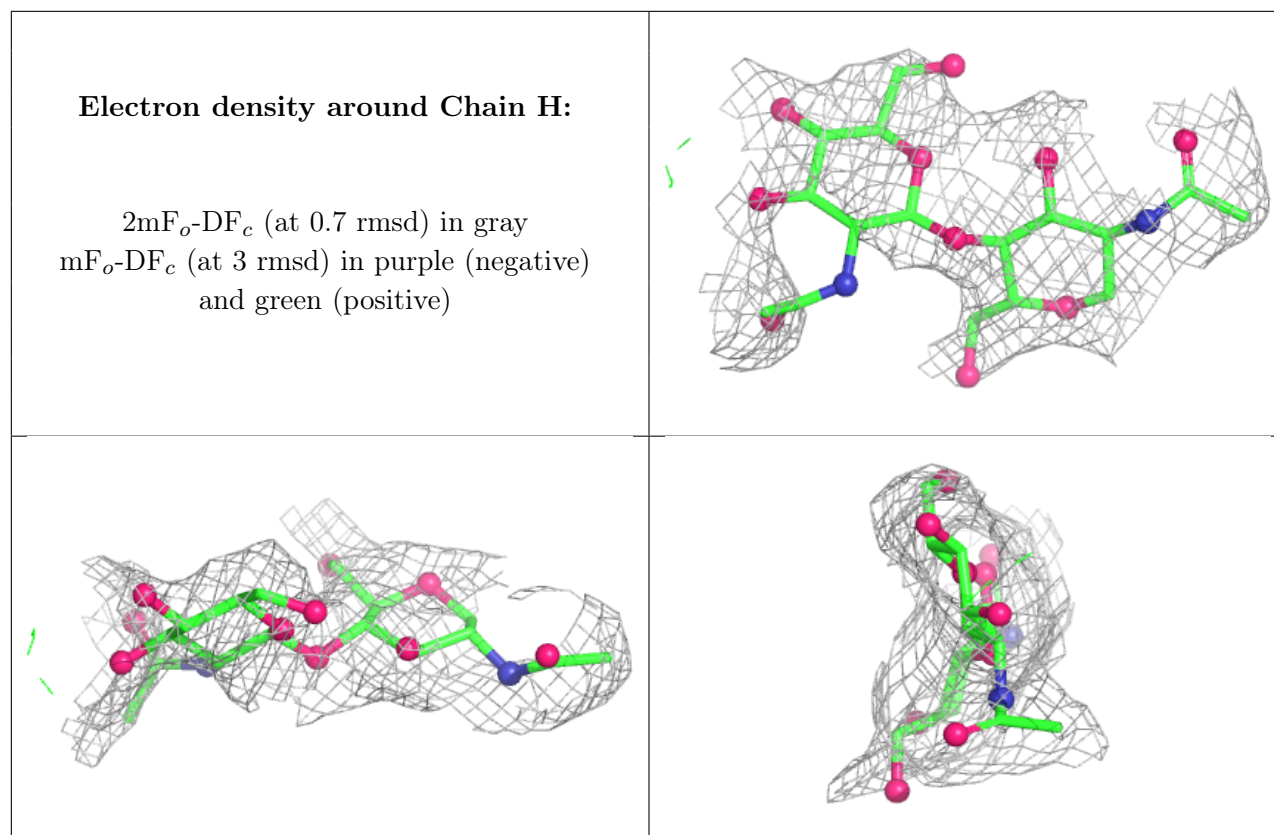
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands [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	NAG	A	401	14/15	0.98	0.03	96,96,96,96	0
4	NAG	C	407	14/15	0.98	0.05	96,96,96,96	0
4	NAG	A	404	14/15	0.99	0.03	95,95,95,95	0
4	NAG	C	410	14/15	0.99	0.03	96,96,96,96	0
5	MG	B	901	1/1	1.00	0.02	95,95,95,95	0
5	MG	D	902	1/1	1.00	0.03	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.