



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:59 PM EDT

PDB ID : 4JM2 / pdb_00004jm2
Title : Crystal Structure of PGT 135 Fab in Complex with gp120 Core Protein from HIV-1 Strain JR-FL Bound to CD4 and 17b Fab
Authors : Kong, L.; Wilson, I.A.
Deposited on : 2013-03-13
Resolution : 3.10 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:

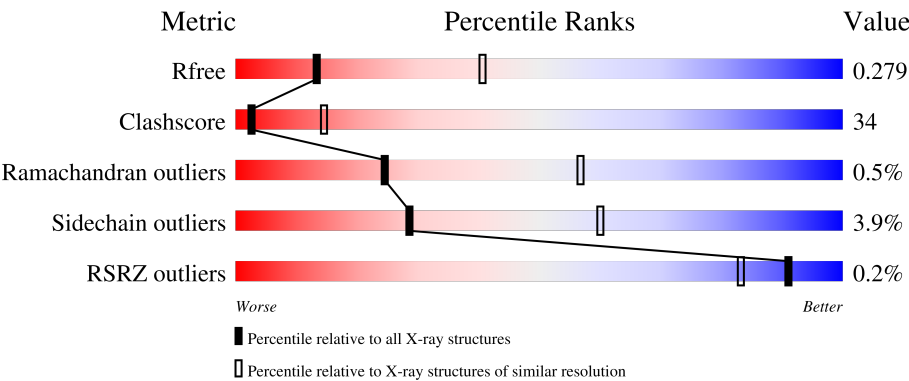
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	236	49%40%7%.
2	B	214	54%44%.
3	C	214	53%44%.
4	D	229	50%41%... .
5	E	321	% 52%41%5%.

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Mol	Chain	Length	Quality of chain
6	F	185	53% 39% • 5%
7	G	8	38% 62%
8	H	10	10% 50% 40%
9	I	3	33% 67%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10907 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 PGT 135 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1744	1106	308	323	7			

- Molecule 2 is a protein called PGT 135 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1672	1050	279	336	7			

- Molecule 3 is a protein called 17b Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1646	1028	282	331	5			

- Molecule 4 is a protein called 17b Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	220	Total	C	N	O	S	0	0	0
			1668	1056	279	328	5			

- Molecule 5 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	315	Total	C	N	O	S	0	0	0
			2467	1539	437	470	21			

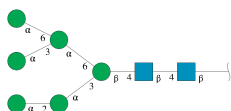
- Molecule 6 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	175	Total	C	N	O	S	0	0	0
			1363	851	239	269	4			

There are 2 discrepancies between the modelled and reference sequences:

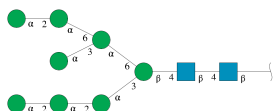
Chain	Residue	Modelled	Actual	Comment	Reference
F	184	ASN	-	expression tag	UNP P01730
F	185	THR	-	expression tag	UNP P01730

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



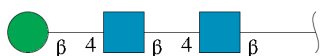
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



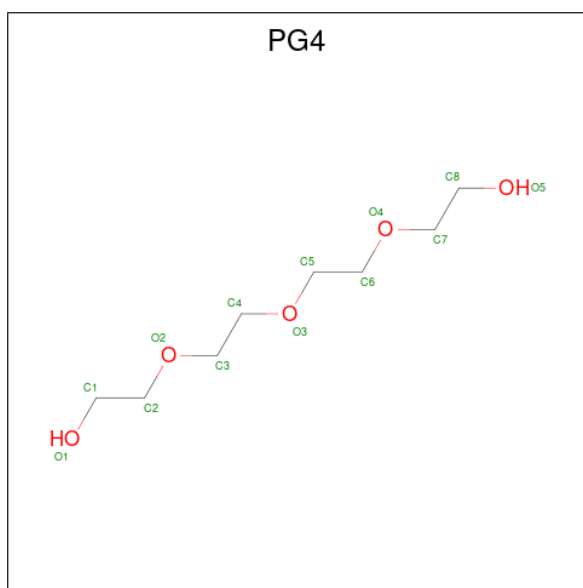
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



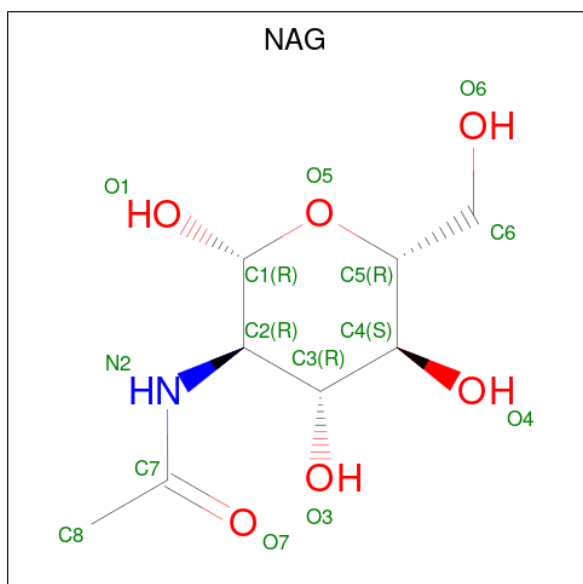
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	E	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		
11	E	1	Total	C	N	O	0	0
			14	8	1	5		

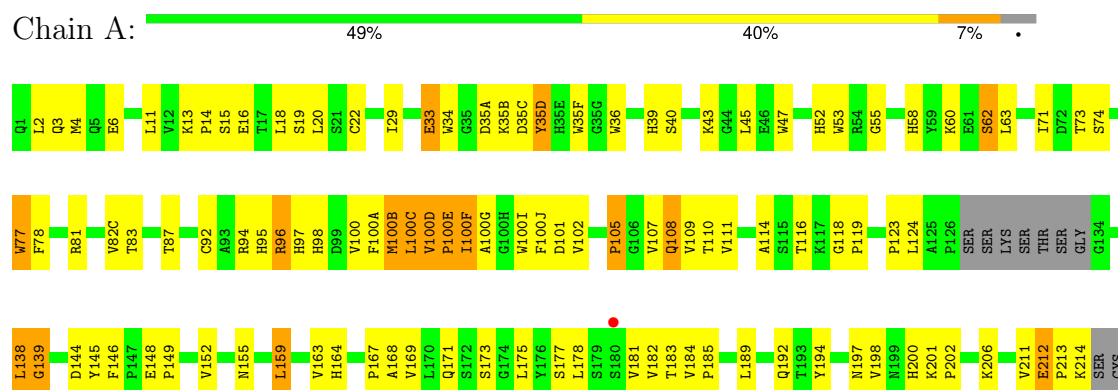
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	O	0	0
			1	1		

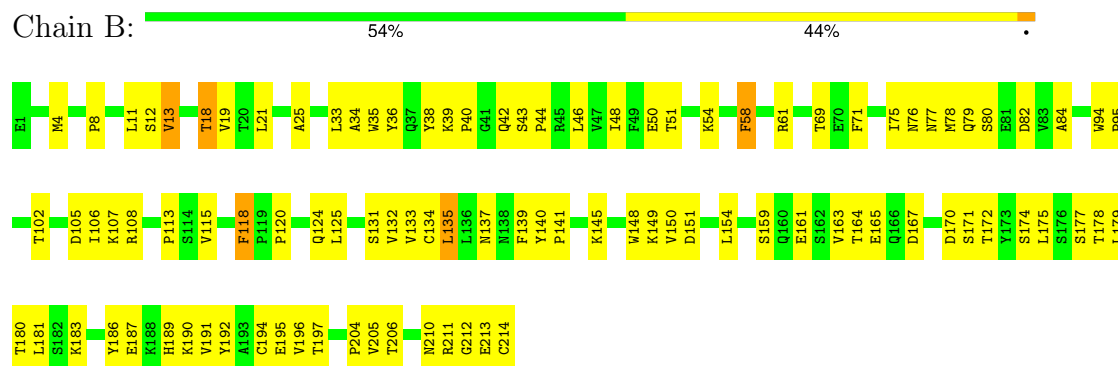
3 Residue-property plots

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.

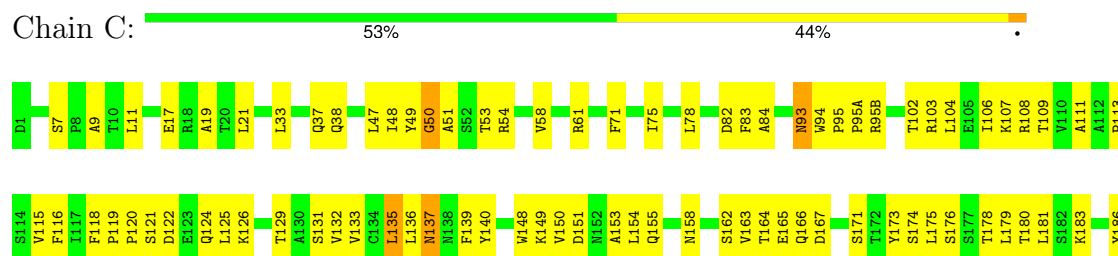
• Molecule 1: PGT 135 Heavy chain



• Molecule 2: PGT 135 Light chain



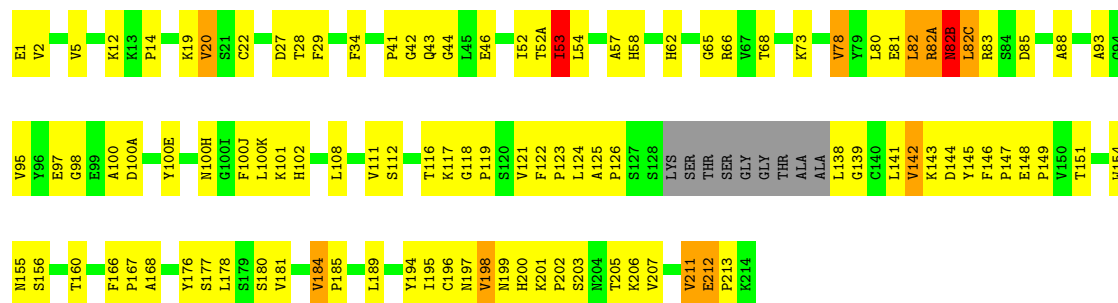
• Molecule 3: 17b Light chain





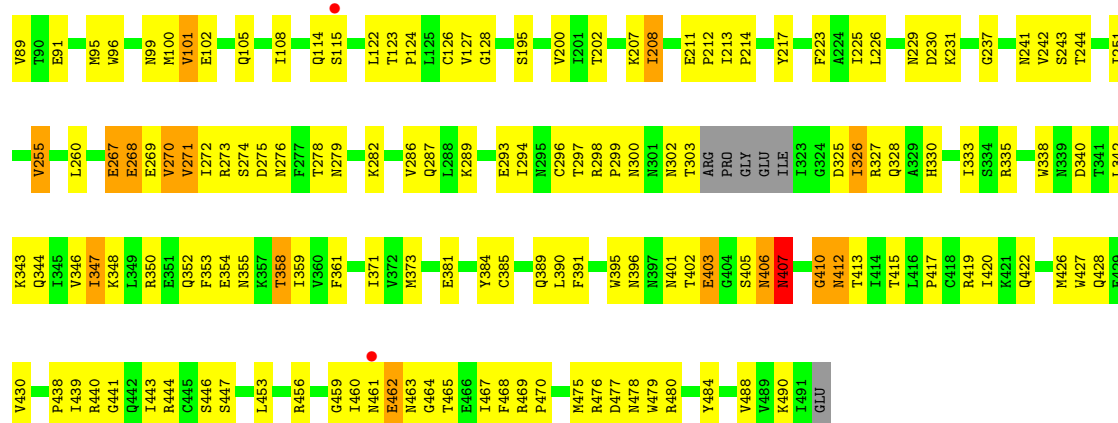
• Molecule 4: 17b Heavy chain

Chain D: 50% 41%



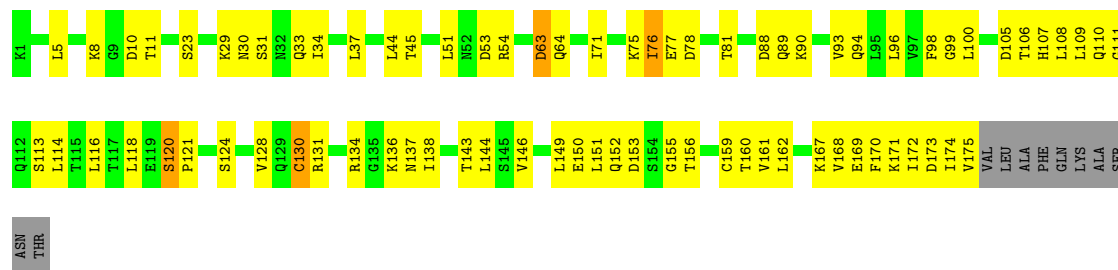
• Molecule 5: gp120

Chain E: 52% 41% 5%



• Molecule 6: T-cell surface glycoprotein CD4

Chain F: 53% 39% 5%



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1

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

Chain G:  38% 62%



• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  10% 50% 40%



• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.41Å 92.15Å 88.19Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	43.58 – 3.10 43.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.58-3.10) 99.6 (43.58-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.238 , 0.285 0.243 , 0.279	Depositor DCC
R_{free} test set	1567 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	104.8	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10907	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: PG4, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/1795	1.01	8/2447 (0.3%)
2	B	0.59	0/1709	1.04	5/2323 (0.2%)
3	C	0.51	0/1683	0.98	5/2288 (0.2%)
4	D	0.66	0/1707	1.11	12/2325 (0.5%)
5	E	0.63	0/2514	1.13	19/3404 (0.6%)
6	F	0.46	0/1382	1.00	7/1863 (0.4%)
All	All	0.58	0/10790	1.05	56/14650 (0.4%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	115	SER	N-CA-C	11.60	123.67	111.14
5	E	406	ASN	N-CA-C	-9.31	96.23	110.10
5	E	237	GLY	CA-C-N	8.26	128.02	119.76
5	E	237	GLY	C-N-CA	8.26	128.02	119.76
4	D	184	VAL	CA-C-N	6.93	126.90	119.76
4	D	184	VAL	C-N-CA	6.93	126.90	119.76
1	A	96	ARG	N-CA-C	6.73	116.87	108.19
5	E	412	ASN	N-CA-C	6.67	119.39	111.33
5	E	267	GLU	N-CA-C	-6.62	100.68	110.48
2	B	118	PHE	CA-C-N	6.59	127.17	120.38
2	B	118	PHE	C-N-CA	6.59	127.17	120.38
5	E	338	TRP	N-CA-C	6.48	118.00	111.07
4	D	125	ALA	CA-C-N	6.35	126.27	119.85
4	D	125	ALA	C-N-CA	6.35	126.27	119.85
4	D	212	GLU	CA-C-N	6.34	127.76	119.84
4	D	212	GLU	C-N-CA	6.34	127.76	119.84
3	C	207	LYS	N-CA-C	-6.27	99.43	109.96
2	B	58	PHE	CA-C-N	6.26	126.23	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	PHE	C-N-CA	6.26	126.23	120.03
5	E	403	GLU	N-CA-C	-6.25	105.43	114.12
5	E	268	GLU	CB-CA-C	-6.17	109.47	116.63
5	E	358	THR	N-CA-C	-6.15	101.31	110.23
5	E	407	ASN	N-CA-C	-6.04	97.93	110.80
1	A	35(D)	TYR	N-CA-C	5.90	118.55	110.24
5	E	270	VAL	N-CA-C	-5.89	101.12	108.89
6	F	113	SER	N-CA-C	-5.86	101.84	110.52
1	A	139	GLY	N-CA-C	5.75	121.66	110.73
1	A	212	GLU	CA-C-N	5.73	125.66	119.76
1	A	212	GLU	C-N-CA	5.73	125.66	119.76
6	F	120	SER	CA-C-N	5.69	126.24	120.38
6	F	120	SER	C-N-CA	5.69	126.24	120.38
4	D	42	GLY	N-CA-C	-5.58	108.03	115.40
6	F	63	ASP	N-CA-C	5.58	119.57	112.87
3	C	93	ASN	N-CA-C	5.54	118.03	110.55
5	E	114	GLN	N-CA-C	5.48	117.05	111.14
6	F	120	SER	N-CA-C	5.45	117.06	108.55
1	A	55	GLY	N-CA-C	5.44	121.22	114.37
5	E	467	ILE	N-CA-C	5.42	115.77	108.17
3	C	50	GLY	N-CA-C	-5.42	106.53	114.61
6	F	172	ILE	N-CA-C	5.39	115.75	107.77
4	D	198	VAL	N-CA-C	5.28	115.46	107.75
4	D	100(H)	ASN	N-CA-C	5.27	118.08	110.28
6	F	111	GLY	N-CA-C	5.26	122.05	115.21
2	B	13	VAL	N-CA-C	5.26	116.30	108.46
5	E	469	ARG	CA-C-N	5.26	125.16	119.85
5	E	469	ARG	C-N-CA	5.26	125.16	119.85
5	E	462	GLU	N-CA-C	-5.24	105.54	112.24
3	C	137	ASN	N-CA-C	5.23	117.49	109.07
4	D	44	GLY	N-CA-C	5.22	120.59	112.60
3	C	199	GLN	N-CA-C	-5.12	105.88	111.82
5	E	410	GLY	N-CA-C	5.12	125.31	113.18
4	D	160	THR	N-CA-C	5.11	121.22	114.12
5	E	101	VAL	N-CA-C	5.03	115.26	110.53
4	D	53	ILE	CB-CA-C	-5.03	105.35	112.14
1	A	118	GLY	CA-C-N	5.01	125.45	120.14
1	A	118	GLY	C-N-CA	5.01	125.45	120.14

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	1744	0	1700	126	0
2	B	1672	0	1619	119	0
3	C	1646	0	1595	126	0
4	D	1668	0	1637	118	0
5	E	2467	0	2412	168	0
6	F	1363	0	1389	96	0
7	G	94	0	79	7	0
8	H	116	0	97	4	0
9	I	39	0	34	0	0
10	C	13	0	18	0	0
11	E	84	0	78	10	0
12	A	1	0	0	0	0
All	All	10907	0	10658	731	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 34.

All (731) 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)
5:E:268:GLU:CG	5:E:269:GLU:H	1.32	1.34
4:D:82(C):LEU:O	4:D:111:VAL:HG11	1.35	1.26
5:E:268:GLU:HG2	5:E:269:GLU:N	1.61	1.11
3:C:151:ASP:OD1	3:C:191:VAL:HG12	1.50	1.10
1:A:33:GLU:HG3	1:A:34:TRP:N	1.37	1.08
5:E:268:GLU:CG	5:E:269:GLU:N	2.09	1.06
1:A:212:GLU:HG3	1:A:213:PRO:HD2	1.39	1.04
5:E:268:GLU:HG2	5:E:269:GLU:H	0.88	1.02
2:B:187:GLU:HA	2:B:211:ARG:HH22	1.21	1.00
6:F:5:LEU:CD1	6:F:98:PHE:CD1	2.46	0.98
5:E:101:VAL:HG13	5:E:102:GLU:OE1	1.63	0.98
5:E:326:ILE:HG13	5:E:327:ARG:H	1.24	0.98
1:A:87:THR:HG22	1:A:111:VAL:H	1.27	0.98
4:D:200:HIS:HB3	4:D:205:THR:OG1	1.63	0.97
5:E:231:LYS:HE3	5:E:267:GLU:OE1	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLU:HG3	1:A:34:TRP:H	0.98	0.96
2:B:150:VAL:HG12	2:B:189:HIS:CG	2.00	0.96
2:B:213:GLU:HG2	2:B:214:CYS:H	1.29	0.96
1:A:100(B):MET:HE3	1:A:100(E):PRO:HA	1.48	0.95
1:A:33:GLU:CG	1:A:34:TRP:N	2.29	0.95
6:F:37:LEU:HD21	6:F:44:LEU:HD11	1.49	0.94
1:A:29:ILE:HG21	1:A:71:ILE:HD11	1.48	0.94
3:C:151:ASP:HA	3:C:191:VAL:CG1	1.98	0.93
5:E:350:ARG:HG2	5:E:355:ASN:HA	1.49	0.93
3:C:201:LEU:HD12	3:C:202:SER:H	1.34	0.92
5:E:268:GLU:HG3	5:E:269:GLU:H	1.33	0.92
4:D:141:LEU:HD21	4:D:143:LYS:HB2	1.50	0.92
6:F:134:ARG:NH2	6:F:152:GLN:HB2	1.86	0.91
2:B:125:LEU:HA	2:B:183:LYS:HZ1	1.33	0.90
3:C:162:SER:HB2	4:D:167:PRO:HG2	1.52	0.90
3:C:201:LEU:HD12	3:C:202:SER:N	1.86	0.90
6:F:161:VAL:O	6:F:167:LYS:HA	1.74	0.88
1:A:171:GLN:HE21	1:A:177:SER:HB2	1.38	0.88
4:D:82(C):LEU:O	4:D:111:VAL:CG1	2.20	0.88
2:B:42:GLN:HG2	2:B:43:SER:H	1.38	0.88
5:E:358:THR:HG22	5:E:465:THR:CB	2.05	0.87
5:E:346:VAL:HG13	5:E:359:ILE:HD11	1.56	0.87
3:C:180:THR:O	3:C:181:LEU:HD23	1.75	0.87
3:C:125:LEU:O	3:C:183:LYS:HE2	1.75	0.86
5:E:327:ARG:HD3	5:E:420:ILE:O	1.76	0.86
2:B:187:GLU:HA	2:B:211:ARG:NH2	1.90	0.85
5:E:325:ASP:O	5:E:326:ILE:HB	1.75	0.84
1:A:171:GLN:NE2	1:A:177:SER:HB2	1.92	0.84
3:C:11:LEU:O	3:C:104:LEU:HD12	1.76	0.83
1:A:33:GLU:CG	1:A:34:TRP:H	1.88	0.83
3:C:120:PRO:HG3	3:C:131:SER:O	1.76	0.83
2:B:118:PHE:HB2	2:B:133:VAL:HG22	1.61	0.82
1:A:212:GLU:CG	1:A:213:PRO:HD2	2.09	0.82
5:E:346:VAL:HA	5:E:359:ILE:CD1	2.10	0.81
2:B:213:GLU:HG2	2:B:214:CYS:N	1.95	0.81
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.63	0.81
5:E:358:THR:HG22	5:E:465:THR:HB	1.62	0.81
7:G:3:BMA:H2	7:G:4:MAN:O6	1.81	0.80
5:E:108:ILE:HG22	5:E:427:TRP:HH2	1.44	0.80
4:D:167:PRO:C	4:D:178:LEU:HD21	2.08	0.79
2:B:80:SER:HA	2:B:106:ILE:CD1	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ILE:HD13	3:C:54:ARG:HA	1.61	0.79
1:A:100(C):LEU:CD1	5:E:415:THR:HG21	2.12	0.79
1:A:34:TRP:CH2	5:E:419:ARG:HG2	2.18	0.79
5:E:326:ILE:HG13	5:E:327:ARG:N	1.97	0.79
6:F:134:ARG:HH22	6:F:152:GLN:HB2	1.45	0.79
6:F:116:LEU:HD11	6:F:144:LEU:HD13	1.65	0.78
2:B:164:THR:HG22	2:B:174:SER:H	1.48	0.78
5:E:346:VAL:HG22	5:E:359:ILE:HD11	1.66	0.78
6:F:108:LEU:HB3	6:F:175:VAL:C	2.08	0.78
1:A:39:HIS:HB2	1:A:45:LEU:CD2	2.13	0.78
4:D:184:VAL:HG13	4:D:185:PRO:HD2	1.66	0.78
4:D:138:LEU:HD11	4:D:211:VAL:HG21	1.65	0.78
2:B:149:LYS:HG2	2:B:154:LEU:HD23	1.66	0.77
4:D:138:LEU:HD11	4:D:211:VAL:CG2	2.14	0.77
6:F:5:LEU:HD21	6:F:168:VAL:HB	1.65	0.77
1:A:29:ILE:CG2	1:A:71:ILE:HD11	2.14	0.77
5:E:270:VAL:O	5:E:348:LYS:HE2	1.85	0.77
5:E:358:THR:CG2	5:E:465:THR:HB	2.14	0.76
3:C:108:ARG:NH2	3:C:140:TYR:HB2	2.00	0.76
1:A:214:LYS:HB3	2:B:214:CYS:SG	2.25	0.76
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.68	0.76
5:E:358:THR:CG2	5:E:465:THR:CB	2.64	0.76
2:B:145:LYS:HB3	2:B:197:THR:OG1	1.86	0.75
1:A:171:GLN:HE21	1:A:177:SER:CB	1.99	0.75
5:E:346:VAL:HA	5:E:359:ILE:HD11	1.67	0.75
4:D:2:VAL:HG12	4:D:102:HIS:ND1	2.02	0.74
5:E:461:ASN:OD1	5:E:462:GLU:N	2.19	0.74
1:A:6:GLU:OE1	1:A:105:PRO:HD2	1.86	0.74
5:E:350:ARG:CG	5:E:355:ASN:HA	2.16	0.74
5:E:126:CYS:HB3	5:E:195:SER:O	1.86	0.74
6:F:160:THR:CG2	6:F:167:LYS:HB2	2.17	0.74
2:B:125:LEU:HA	2:B:183:LYS:NZ	2.01	0.74
6:F:37:LEU:CD2	6:F:44:LEU:HD11	2.18	0.74
4:D:138:LEU:HD21	4:D:211:VAL:HG21	1.67	0.73
6:F:53:ASP:OD1	6:F:54:ARG:HG3	1.89	0.73
1:A:33:GLU:O	1:A:34:TRP:HB2	1.88	0.73
5:E:297:THR:OG1	5:E:444:ARG:HD3	1.88	0.73
5:E:373:MET:HE3	5:E:384:TYR:HB3	1.69	0.73
2:B:151:ASP:CB	2:B:189:HIS:HD2	2.01	0.73
3:C:151:ASP:H	3:C:191:VAL:HG13	1.52	0.72
2:B:125:LEU:HD23	2:B:183:LYS:NZ	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:LYS:CB	4:D:82(C):LEU:HD12	2.19	0.72
5:E:371:ILE:CD1	6:F:45:THR:HG22	2.20	0.71
3:C:108:ARG:HG2	3:C:109:THR:N	2.05	0.71
1:A:2:LEU:C	1:A:2:LEU:HD23	2.16	0.71
5:E:335:ARG:NE	5:E:410:GLY:O	2.22	0.71
6:F:5:LEU:HD11	6:F:98:PHE:CD1	2.25	0.71
2:B:164:THR:CG2	2:B:174:SER:H	2.02	0.71
3:C:158:ASN:HD22	3:C:181:LEU:HD21	1.56	0.71
6:F:30:ASN:HD21	6:F:34:ILE:HD12	1.56	0.71
1:A:2:LEU:HD21	1:A:4:MET:HE3	1.71	0.71
6:F:5:LEU:CD1	6:F:98:PHE:CE1	2.73	0.71
3:C:151:ASP:HA	3:C:191:VAL:HG12	1.73	0.71
5:E:289:LYS:O	5:E:289:LYS:HD3	1.91	0.71
6:F:5:LEU:HD12	6:F:98:PHE:CD1	2.26	0.71
1:A:16:GLU:O	1:A:82(C):VAL:HG23	1.91	0.70
2:B:40:PRO:HG3	2:B:165:GLU:HG2	1.74	0.70
2:B:161:GLU:OE2	2:B:175:LEU:HD22	1.91	0.70
3:C:17:GLU:O	3:C:78:LEU:HD13	1.91	0.70
4:D:156:SER:H	4:D:195:ILE:HD11	1.56	0.70
3:C:47:LEU:HA	3:C:58:VAL:HG21	1.74	0.70
5:E:95:MET:HE2	5:E:96:TRP:NE1	2.06	0.70
5:E:342:LEU:O	5:E:346:VAL:HG23	1.90	0.70
5:E:459:GLY:HA2	6:F:33:GLN:HB2	1.73	0.70
5:E:346:VAL:CG1	5:E:359:ILE:HD11	2.21	0.70
3:C:94:TRP:HA	3:C:95:PRO:C	2.17	0.70
6:F:96:LEU:HD23	6:F:98:PHE:HZ	1.57	0.69
6:F:128:VAL:HB	6:F:144:LEU:HD11	1.75	0.69
1:A:201:LYS:N	1:A:202:PRO:HD2	2.07	0.69
5:E:260:LEU:HD21	5:E:453:LEU:HD11	1.74	0.69
4:D:121:VAL:HG22	4:D:142:VAL:HG13	1.73	0.69
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.73	0.69
5:E:279:ASN:HA	11:E:526:NAG:H83	1.73	0.69
3:C:151:ASP:CA	3:C:191:VAL:CG1	2.69	0.69
3:C:188:LYS:C	3:C:189:HIS:HD2	2.01	0.69
5:E:91:GLU:CD	5:E:242:VAL:HG21	2.18	0.69
6:F:5:LEU:HD13	6:F:98:PHE:CE1	2.27	0.69
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.75	0.69
3:C:158:ASN:ND2	3:C:179:LEU:HD11	2.08	0.69
1:A:2:LEU:HD23	1:A:3:GLN:N	2.08	0.68
6:F:31:SER:HB3	6:F:81:THR:HB	1.74	0.68
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LYS:HE2	2:B:58:PHE:O	1.93	0.68
2:B:135:LEU:HD21	2:B:137:ASN:HB2	1.74	0.68
1:A:100(C):LEU:HD11	5:E:415:THR:HG21	1.76	0.68
3:C:95:PRO:HG3	5:E:202:THR:HG22	1.74	0.68
5:E:335:ARG:HD2	5:E:410:GLY:O	1.94	0.68
2:B:25:ALA:O	2:B:69:THR:HG23	1.94	0.67
3:C:108:ARG:HG2	3:C:109:THR:H	1.59	0.67
5:E:241:ASN:OD1	5:E:241:ASN:C	2.36	0.67
4:D:82(A):ARG:O	4:D:82(B):ASN:HB2	1.95	0.67
5:E:268:GLU:O	5:E:289:LYS:HG3	1.94	0.67
5:E:326:ILE:CG1	5:E:327:ARG:H	1.98	0.67
4:D:139:GLY:HA2	4:D:154:TRP:HH2	1.59	0.67
2:B:150:VAL:HG12	2:B:189:HIS:CD2	2.30	0.66
5:E:335:ARG:CD	5:E:410:GLY:O	2.43	0.66
6:F:110:GLN:HG2	6:F:151:LEU:HB2	1.76	0.66
1:A:100(C):LEU:HD12	5:E:415:THR:HG21	1.78	0.66
4:D:118:GLY:HA3	4:D:205:THR:HG21	1.78	0.66
4:D:148:GLU:OE2	4:D:149:PRO:HA	1.95	0.66
6:F:23:SER:HB2	6:F:63:ASP:HA	1.77	0.66
2:B:205:VAL:HG12	2:B:206:THR:N	2.09	0.66
2:B:125:LEU:HD23	2:B:183:LYS:HZ1	1.60	0.66
3:C:135:LEU:HD12	4:D:181:VAL:HG11	1.77	0.66
4:D:34:PHE:HD2	4:D:52(A):THR:HG21	1.61	0.66
5:E:207:LYS:O	5:E:208:ILE:HD13	1.96	0.66
5:E:346:VAL:CB	5:E:359:ILE:HD11	2.26	0.65
6:F:106:THR:O	6:F:106:THR:HG22	1.94	0.65
3:C:122:ASP:O	3:C:126:LYS:HG3	1.96	0.65
5:E:346:VAL:HG13	5:E:359:ILE:CD1	2.26	0.65
4:D:141:LEU:CD2	4:D:143:LYS:HB2	2.26	0.65
6:F:5:LEU:CD2	6:F:168:VAL:HB	2.26	0.65
5:E:298:ARG:HH11	5:E:443:ILE:HD12	1.62	0.65
1:A:2:LEU:HD22	1:A:102:VAL:HG11	1.79	0.64
1:A:13:LYS:O	1:A:16:GLU:HB2	1.98	0.64
5:E:463:ASN:ND2	5:E:463:ASN:O	2.30	0.64
5:E:108:ILE:HG22	5:E:427:TRP:CH2	2.31	0.64
1:A:82(C):VAL:CG1	1:A:111:VAL:HG21	2.28	0.64
3:C:106:ILE:HD11	3:C:171:SER:OG	1.97	0.64
5:E:346:VAL:CA	5:E:359:ILE:HD11	2.28	0.64
6:F:110:GLN:HA	6:F:149:LEU:HD11	1.80	0.64
1:A:4:MET:HG2	1:A:22:CYS:SG	2.38	0.63
1:A:123:PRO:HB3	1:A:211:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:LEU:HD23	2:B:135:LEU:C	2.23	0.63
3:C:151:ASP:HA	3:C:191:VAL:HG11	1.80	0.63
5:E:358:THR:CG2	5:E:465:THR:OG1	2.46	0.63
4:D:82:LEU:HD12	4:D:82(A):ARG:N	2.14	0.63
3:C:21:LEU:HD23	3:C:102:THR:HG23	1.79	0.63
4:D:34:PHE:CD2	4:D:52(A):THR:HG21	2.33	0.63
4:D:65:GLY:O	4:D:82(A):ARG:NH1	2.30	0.63
8:H:8:MAN:C1	8:H:9:MAN:H5	2.28	0.63
3:C:148:TRP:CE3	3:C:179:LEU:HD22	2.34	0.63
4:D:143:LYS:HG2	4:D:144:ASP:OD2	1.99	0.63
6:F:160:THR:HG22	6:F:167:LYS:HB2	1.79	0.63
2:B:124:GLN:NE2	2:B:131:SER:H	1.97	0.63
5:E:346:VAL:CG2	5:E:359:ILE:HD11	2.28	0.63
6:F:156:THR:HG21	6:F:171:LYS:HE2	1.80	0.63
6:F:143:THR:C	6:F:144:LEU:HD12	2.23	0.63
1:A:184:VAL:HG13	1:A:185:PRO:HD2	1.81	0.62
4:D:1:GLU:OE1	4:D:1:GLU:N	2.30	0.62
2:B:150:VAL:HG12	2:B:189:HIS:CB	2.30	0.62
3:C:151:ASP:CG	3:C:191:VAL:HG12	2.24	0.62
1:A:2:LEU:HD21	1:A:4:MET:CE	2.29	0.62
1:A:124:LEU:HB3	2:B:118:PHE:CD1	2.34	0.62
1:A:212:GLU:CG	1:A:213:PRO:CD	2.76	0.62
2:B:190:LYS:HD3	2:B:211:ARG:HB3	1.81	0.62
2:B:150:VAL:CG1	2:B:189:HIS:CG	2.79	0.62
1:A:87:THR:CG2	1:A:111:VAL:H	2.08	0.62
1:A:14:PRO:O	1:A:15:SER:CB	2.45	0.62
5:E:279:ASN:HB2	11:E:526:NAG:HN2	1.65	0.62
3:C:21:LEU:HD23	3:C:102:THR:CG2	2.29	0.62
4:D:12:LYS:HB2	4:D:82(C):LEU:HD12	1.82	0.62
2:B:151:ASP:HB3	2:B:189:HIS:HD2	1.64	0.61
4:D:194:TYR:HB2	4:D:211:VAL:HG11	1.82	0.61
2:B:39:LYS:HB3	2:B:40:PRO:HD2	1.82	0.61
4:D:203:SER:HB2	4:D:205:THR:HG23	1.82	0.61
2:B:190:LYS:CD	2:B:211:ARG:HB3	2.30	0.61
1:A:123:PRO:CB	1:A:211:VAL:HG12	2.31	0.61
1:A:35(B):LYS:HD2	1:A:35(B):LYS:N	2.16	0.61
1:A:144:ASP:OD1	1:A:171:GLN:NE2	2.33	0.61
2:B:42:GLN:HG2	2:B:43:SER:N	2.13	0.61
3:C:189:HIS:O	3:C:211:ARG:HD2	2.01	0.61
1:A:189:LEU:HD11	1:A:213:PRO:HG3	1.83	0.61
2:B:118:PHE:HB2	2:B:133:VAL:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ASP:HB2	2:B:189:HIS:HD2	1.64	0.61
4:D:119:PRO:HB3	4:D:145:TYR:HB3	1.81	0.61
6:F:96:LEU:HD23	6:F:98:PHE:CZ	2.35	0.61
4:D:82(C):LEU:HB3	4:D:111:VAL:HG21	1.83	0.60
3:C:107:LYS:HA	3:C:140:TYR:OH	2.01	0.60
4:D:53:ILE:HG23	4:D:54:LEU:N	2.15	0.60
2:B:205:VAL:CG1	2:B:206:THR:N	2.64	0.60
4:D:68:THR:HG23	4:D:82(A):ARG:NH2	2.15	0.60
1:A:108:GLN:HB3	1:A:149:PRO:HD3	1.84	0.60
3:C:164:THR:HG22	3:C:174:SER:H	1.65	0.60
3:C:175:LEU:C	4:D:166:PHE:CE2	2.80	0.60
6:F:105:ASP:O	6:F:106:THR:HB	2.02	0.60
3:C:150:VAL:HG11	3:C:155:GLN:NE2	2.17	0.60
6:F:136:LYS:HG3	6:F:138:ILE:HD11	1.83	0.60
5:E:344:GLN:O	5:E:347:ILE:HB	2.01	0.60
2:B:124:GLN:HE22	2:B:131:SER:CB	2.15	0.60
7:G:3:BMA:H2	7:G:4:MAN:C5	2.32	0.60
3:C:93:ASN:ND2	3:C:95(B):ARG:HB2	2.17	0.59
1:A:35(C):ASP:O	1:A:52:HIS:CD2	2.55	0.59
2:B:187:GLU:CA	2:B:211:ARG:HH22	2.05	0.59
5:E:278:THR:HG22	11:E:526:NAG:H82	1.84	0.59
5:E:475:MET:O	5:E:478:ASN:HB2	2.02	0.59
2:B:11:LEU:HD23	2:B:19:VAL:CG2	2.32	0.59
1:A:82(C):VAL:HG12	1:A:111:VAL:HG21	1.84	0.59
2:B:120:PRO:HD3	2:B:132:VAL:CG2	2.32	0.59
4:D:168:ALA:HA	4:D:178:LEU:CD2	2.32	0.59
1:A:11:LEU:HD23	1:A:11:LEU:H	1.68	0.59
2:B:21:LEU:CD2	2:B:102:THR:HG21	2.33	0.59
3:C:19:ALA:HB3	3:C:75:ILE:HG23	1.85	0.59
1:A:97:HIS:ND1	1:A:98:HIS:N	2.43	0.59
1:A:114:ALA:HB3	1:A:146:PHE:CE2	2.38	0.59
3:C:49:TYR:CZ	3:C:53:THR:HG21	2.38	0.58
4:D:168:ALA:HA	4:D:178:LEU:HD21	1.84	0.58
6:F:5:LEU:CD1	6:F:98:PHE:HD1	2.11	0.58
3:C:151:ASP:CA	3:C:191:VAL:HG12	2.34	0.58
3:C:188:LYS:C	3:C:189:HIS:CD2	2.80	0.58
4:D:19:LYS:HA	4:D:80:LEU:O	2.04	0.58
6:F:106:THR:O	6:F:107:HIS:ND1	2.36	0.58
1:A:138:LEU:HD23	1:A:139:GLY:H	1.68	0.58
4:D:82(C):LEU:HB3	4:D:111:VAL:CG2	2.34	0.58
1:A:87:THR:HG22	1:A:111:VAL:N	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:GLN:HB3	3:C:158:ASN:HD21	1.69	0.58
6:F:109:LEU:HD12	6:F:110:GLN:H	1.68	0.58
3:C:19:ALA:HB3	3:C:75:ILE:CG2	2.34	0.57
3:C:187:GLU:HA	3:C:211:ARG:NH2	2.19	0.57
5:E:358:THR:CG2	5:E:358:THR:O	2.50	0.57
6:F:120:SER:HB3	6:F:121:PRO:HD2	1.84	0.57
2:B:61:ARG:HD2	2:B:76:ASN:O	2.03	0.57
3:C:120:PRO:HG3	3:C:131:SER:C	2.29	0.57
3:C:131:SER:OG	3:C:180:THR:HG22	2.04	0.57
5:E:353:PHE:O	5:E:354:GLU:HG2	2.04	0.57
1:A:105:PRO:HA	2:B:43:SER:OG	2.04	0.57
3:C:135:LEU:C	3:C:135:LEU:HD23	2.29	0.57
3:C:187:GLU:HA	3:C:211:ARG:CZ	2.35	0.57
6:F:114:LEU:O	6:F:146:VAL:HG12	2.05	0.57
4:D:58:HIS:HE1	5:E:202:THR:HG21	1.68	0.57
4:D:66:ARG:O	4:D:82:LEU:HD12	2.05	0.57
6:F:150:GLU:CD	6:F:150:GLU:H	2.13	0.57
3:C:54:ARG:HG2	3:C:58:VAL:HB	1.85	0.57
4:D:154:TRP:NE1	4:D:180:SER:OG	2.34	0.57
1:A:95:HIS:ND1	1:A:100(G):ALA:HB1	2.20	0.56
4:D:58:HIS:CE1	5:E:202:THR:HG21	2.40	0.56
2:B:178:THR:O	2:B:178:THR:HG23	2.05	0.56
2:B:78:MET:SD	2:B:82:ASP:HB2	2.45	0.56
3:C:33:LEU:HD13	3:C:71:PHE:CD1	2.40	0.56
6:F:96:LEU:HB3	6:F:98:PHE:HE1	1.71	0.56
6:F:160:THR:HA	6:F:168:VAL:O	2.05	0.56
3:C:151:ASP:N	3:C:191:VAL:HG13	2.21	0.56
5:E:420:ILE:HG21	5:E:438:PRO:HG3	1.87	0.56
5:E:223:PHE:CE1	5:E:490:LYS:HB2	2.41	0.56
5:E:350:ARG:HG2	5:E:355:ASN:OD1	2.05	0.56
5:E:446:SER:O	11:E:524:NAG:H83	2.06	0.56
2:B:180:THR:O	2:B:181:LEU:HD23	2.05	0.56
5:E:95:MET:HE2	5:E:96:TRP:CE2	2.41	0.56
5:E:326:ILE:HG23	5:E:327:ARG:N	2.21	0.56
5:E:477:ASP:HA	5:E:480:ARG:HG3	1.88	0.56
6:F:100:LEU:HD11	6:F:118:LEU:HD12	1.87	0.56
4:D:29:PHE:CD2	4:D:73:LYS:HA	2.41	0.56
6:F:109:LEU:O	6:F:149:LEU:HD11	2.06	0.56
6:F:89:GLN:HG3	6:F:90:LYS:N	2.22	0.55
4:D:167:PRO:O	4:D:178:LEU:HD21	2.05	0.55
3:C:116:PHE:HD2	3:C:135:LEU:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LEU:CA	4:D:166:PHE:HE2	2.19	0.55
3:C:133:VAL:HG12	3:C:178:THR:OG1	2.07	0.55
1:A:163:VAL:C	1:A:164:HIS:HD2	2.14	0.55
3:C:150:VAL:HG23	3:C:192:TYR:CE1	2.42	0.55
6:F:131:ARG:HA	6:F:136:LYS:O	2.07	0.55
6:F:149:LEU:C	6:F:149:LEU:HD12	2.31	0.55
6:F:108:LEU:HD22	6:F:174:ILE:HG13	1.89	0.55
2:B:8:PRO:CG	2:B:11:LEU:HD13	2.37	0.55
3:C:150:VAL:O	3:C:151:ASP:HB2	2.07	0.55
4:D:68:THR:OG1	4:D:81:GLU:HB3	2.07	0.55
3:C:164:THR:HG23	3:C:165:GLU:O	2.07	0.54
1:A:18:LEU:O	1:A:81:ARG:HA	2.07	0.54
3:C:94:TRP:CE3	3:C:95(A):PRO:HD3	2.42	0.54
4:D:20:VAL:HG13	4:D:80:LEU:HB3	1.90	0.54
5:E:268:GLU:HG3	5:E:269:GLU:N	1.99	0.54
6:F:5:LEU:HD12	6:F:98:PHE:HD1	1.68	0.54
5:E:406:ASN:O	5:E:407:ASN:HB2	2.07	0.54
6:F:134:ARG:NH1	6:F:150:GLU:HG3	2.22	0.54
2:B:94:TRP:CD1	7:G:7:MAN:H2	2.42	0.54
4:D:95:VAL:HG21	4:D:100(J):PHE:O	2.07	0.54
4:D:112:SER:OG	4:D:146:PHE:CZ	2.61	0.54
6:F:161:VAL:HB	6:F:168:VAL:HG12	1.88	0.54
5:E:102:GLU:O	5:E:105:GLN:HB3	2.08	0.54
6:F:37:LEU:HD21	6:F:44:LEU:CD1	2.32	0.54
1:A:163:VAL:O	1:A:164:HIS:CD2	2.61	0.54
2:B:35:TRP:HD1	2:B:48:ILE:HB	1.73	0.54
2:B:125:LEU:CD2	2:B:183:LYS:HZ1	2.21	0.54
4:D:34:PHE:HD2	4:D:52(A):THR:CG2	2.20	0.54
1:A:212:GLU:HG3	1:A:213:PRO:CD	2.23	0.54
3:C:191:VAL:HG13	3:C:191:VAL:O	2.07	0.54
5:E:327:ARG:NE	5:E:422:GLN:OE1	2.40	0.54
2:B:125:LEU:O	2:B:183:LYS:HE3	2.08	0.54
3:C:106:ILE:HG12	3:C:166:GLN:NE2	2.23	0.54
1:A:189:LEU:HG	1:A:213:PRO:HG2	1.90	0.54
2:B:148:TRP:CD1	2:B:159:SER:HB3	2.43	0.54
3:C:83:PHE:CE1	3:C:106:ILE:HG22	2.42	0.54
2:B:69:THR:HG22	2:B:69:THR:O	2.09	0.53
4:D:12:LYS:HB3	4:D:82(C):LEU:HD12	1.89	0.53
4:D:145:TYR:CZ	4:D:176:TYR:HB2	2.43	0.53
6:F:99:GLY:O	6:F:100:LEU:HD12	2.08	0.53
5:E:241:ASN:OD1	5:E:242:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:HIS:ND1	7:G:8:MAN:H3	2.24	0.53
2:B:139:PHE:CZ	2:B:175:LEU:HD12	2.44	0.53
3:C:75:ILE:HD11	3:C:82:ASP:OD2	2.08	0.53
6:F:120:SER:HB3	6:F:124:SER:OG	2.08	0.53
5:E:214:PRO:HA	5:E:251:ILE:O	2.08	0.53
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.44	0.53
3:C:11:LEU:O	3:C:104:LEU:CD1	2.54	0.53
5:E:346:VAL:HG22	5:E:359:ILE:CD1	2.38	0.53
6:F:51:LEU:HD13	6:F:71:ILE:HD13	1.90	0.53
1:A:35(A):ASP:CG	1:A:35(B):LYS:HD3	2.34	0.52
4:D:116:THR:HG22	4:D:147:PRO:HD3	1.89	0.52
2:B:34:ALA:HA	2:B:48:ILE:O	2.08	0.52
4:D:119:PRO:CB	4:D:145:TYR:HB3	2.39	0.52
2:B:12:SER:HA	2:B:105:ASP:OD1	2.09	0.52
1:A:95:HIS:CE1	1:A:100(G):ALA:HB1	2.44	0.52
2:B:77:ASN:O	2:B:77:ASN:ND2	2.42	0.52
4:D:184:VAL:HG12	4:D:185:PRO:O	2.09	0.52
5:E:99:ASN:O	5:E:100:MET:C	2.51	0.52
5:E:462:GLU:HG3	5:E:462:GLU:O	2.09	0.52
2:B:125:LEU:CA	2:B:183:LYS:HZ1	2.14	0.52
3:C:148:TRP:CE2	3:C:179:LEU:HB2	2.45	0.52
4:D:139:GLY:HA3	4:D:180:SER:O	2.09	0.52
5:E:124:PRO:HD2	5:E:430:VAL:O	2.09	0.52
6:F:93:VAL:HG12	6:F:94:GLN:N	2.25	0.52
3:C:50:GLY:O	3:C:51:ALA:HB3	2.10	0.52
3:C:175:LEU:HD23	3:C:176:SER:N	2.25	0.52
3:C:203:SER:OG	3:C:205:VAL:HG23	2.10	0.52
1:A:138:LEU:HD21	1:A:211:VAL:HB	1.92	0.51
1:A:200:HIS:NE2	1:A:202:PRO:HG2	2.25	0.51
3:C:48:ILE:HG21	3:C:51:ALA:O	2.09	0.51
3:C:108:ARG:HH12	3:C:111:ALA:HB2	1.74	0.51
4:D:194:TYR:HB2	4:D:211:VAL:CG1	2.40	0.51
1:A:97:HIS:HB2	1:A:100(F):ILE:O	2.10	0.51
2:B:124:GLN:NE2	2:B:131:SER:N	2.58	0.51
1:A:18:LEU:HD12	1:A:19:SER:N	2.26	0.51
1:A:184:VAL:HG11	1:A:194:TYR:OH	2.10	0.51
2:B:80:SER:HA	2:B:106:ILE:HD11	1.92	0.51
3:C:83:PHE:CZ	3:C:106:ILE:HG22	2.45	0.51
4:D:139:GLY:HA2	4:D:154:TRP:CH2	2.44	0.51
6:F:118:LEU:HD21	6:F:120:SER:OG	2.10	0.51
1:A:35(A):ASP:OD1	1:A:35(B):LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:GLN:HE22	2:B:131:SER:H	1.58	0.51
2:B:167:ASP:HB3	2:B:170:ASP:OD1	2.09	0.51
5:E:95:MET:SD	5:E:484:TYR:HB2	2.50	0.51
5:E:100:MET:HE3	5:E:217:TYR:CD2	2.45	0.51
3:C:186:TYR:CE1	3:C:192:TYR:HE2	2.28	0.51
5:E:373:MET:HB3	5:E:385:CYS:O	2.09	0.51
3:C:113:PRO:HB3	3:C:139:PHE:HB3	1.92	0.51
3:C:124:GLN:HG2	3:C:129:THR:O	2.10	0.51
6:F:108:LEU:HG	6:F:109:LEU:N	2.25	0.51
2:B:11:LEU:HD23	2:B:19:VAL:HG21	1.92	0.51
2:B:124:GLN:HE22	2:B:131:SER:N	2.08	0.51
2:B:131:SER:HA	2:B:179:LEU:O	2.10	0.51
4:D:124:LEU:HD11	4:D:138:LEU:HA	1.93	0.51
1:A:39:HIS:HB2	1:A:45:LEU:HD23	1.88	0.51
6:F:106:THR:O	6:F:106:THR:CG2	2.58	0.51
3:C:21:LEU:HD12	3:C:21:LEU:N	2.25	0.51
2:B:19:VAL:CG1	2:B:75:ILE:HB	2.41	0.51
2:B:190:LYS:HD3	2:B:211:ARG:HD2	1.93	0.51
6:F:159:CYS:O	6:F:169:GLU:HA	2.11	0.51
1:A:167:PRO:HG2	2:B:163:VAL:O	2.11	0.50
2:B:150:VAL:CG1	2:B:189:HIS:HB2	2.40	0.50
1:A:107:VAL:HG13	1:A:107:VAL:O	2.11	0.50
1:A:163:VAL:C	1:A:164:HIS:CD2	2.90	0.50
2:B:108:ARG:HD2	2:B:171:SER:HG	1.77	0.50
1:A:13:LYS:HD3	1:A:13:LYS:N	2.27	0.50
2:B:150:VAL:CG1	2:B:189:HIS:CB	2.89	0.50
6:F:5:LEU:HD21	6:F:168:VAL:CB	2.40	0.50
3:C:149:LYS:HA	3:C:153:ALA:O	2.11	0.50
3:C:186:TYR:CD1	3:C:192:TYR:HE2	2.29	0.50
4:D:168:ALA:N	4:D:178:LEU:HD21	2.26	0.50
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.47	0.50
4:D:58:HIS:HE1	5:E:202:THR:CG2	2.23	0.50
5:E:396:ASN:OD1	5:E:402:THR:O	2.30	0.50
1:A:40:SER:O	1:A:43:LYS:O	2.30	0.50
2:B:50:GLU:O	2:B:51:THR:HB	2.12	0.50
5:E:275:ASP:HB3	5:E:282:LYS:HD2	1.93	0.50
5:E:276:ASN:ND2	5:E:279:ASN:HB2	2.25	0.50
5:E:293:GLU:OE1	11:E:527:NAG:H4	2.12	0.50
3:C:94:TRP:CZ3	3:C:95(A):PRO:HD3	2.46	0.50
5:E:381:GLU:HG3	5:E:443:ILE:HD13	1.94	0.50
2:B:18:THR:O	2:B:18:THR:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:403:GLU:O	5:E:403:GLU:OE1	2.30	0.50
2:B:124:GLN:HE22	2:B:131:SER:HB2	1.77	0.49
5:E:272:ILE:HD11	5:E:352:GLN:HG3	1.94	0.49
2:B:164:THR:HG23	2:B:165:GLU:O	2.12	0.49
3:C:125:LEU:HD23	3:C:183:LYS:HD3	1.95	0.49
5:E:333:ILE:HD12	5:E:390:LEU:HD21	1.93	0.49
3:C:150:VAL:O	3:C:150:VAL:HG13	2.12	0.49
5:E:294:ILE:HG23	5:E:294:ILE:O	2.12	0.49
5:E:358:THR:HG22	5:E:465:THR:CA	2.42	0.49
6:F:100:LEU:HD22	6:F:170:PHE:CD1	2.47	0.49
6:F:96:LEU:HB3	6:F:98:PHE:CE1	2.47	0.49
4:D:82:LEU:HD12	4:D:82(A):ARG:H	1.77	0.49
2:B:140:TYR:CD1	2:B:141:PRO:HA	2.47	0.49
3:C:132:VAL:O	3:C:132:VAL:HG13	2.13	0.49
4:D:57:ALA:C	4:D:58:HIS:HD2	2.20	0.49
5:E:126:CYS:CB	5:E:195:SER:O	2.59	0.49
5:E:340:ASP:O	5:E:343:LYS:HB3	2.12	0.49
5:E:462:GLU:OE1	5:E:462:GLU:HA	2.13	0.49
1:A:14:PRO:O	1:A:15:SER:OG	2.30	0.49
2:B:191:VAL:HG22	2:B:210:ASN:OD1	2.12	0.49
5:E:226:LEU:CD2	5:E:244:THR:HG22	2.43	0.49
3:C:135:LEU:HD21	3:C:137:ASN:HB2	1.95	0.49
4:D:14:PRO:HD3	4:D:112:SER:C	2.38	0.49
5:E:358:THR:HG23	5:E:465:THR:OG1	2.12	0.48
1:A:77:TRP:CE3	1:A:77:TRP:C	2.90	0.48
3:C:115:VAL:HG12	3:C:116:PHE:N	2.28	0.48
3:C:198:HIS:CD2	3:C:200:GLY:H	2.30	0.48
1:A:34:TRP:HE3	5:E:417:PRO:HB2	1.78	0.48
1:A:35(B):LYS:HG3	1:A:35(D):TYR:CE2	2.48	0.48
1:A:87:THR:HA	1:A:109:VAL:O	2.13	0.48
4:D:97:GLU:HG3	4:D:100(E):TYR:CZ	2.49	0.48
5:E:100:MET:HE3	5:E:217:TYR:HD2	1.78	0.48
6:F:138:ILE:N	6:F:138:ILE:HD12	2.28	0.48
2:B:13:VAL:O	2:B:106:ILE:HA	2.14	0.48
5:E:346:VAL:HG21	5:E:395:TRP:CD2	2.48	0.48
5:E:371:ILE:HD13	6:F:45:THR:HG22	1.94	0.48
6:F:75:LYS:HD2	6:F:77:GLU:OE1	2.13	0.48
3:C:135:LEU:C	3:C:136:LEU:HD12	2.38	0.48
4:D:27:ASP:OD1	4:D:28:THR:N	2.42	0.48
2:B:21:LEU:HD23	2:B:102:THR:HG21	1.95	0.48
4:D:82(C):LEU:C	4:D:111:VAL:HG11	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LYS:HG3	4:D:177:SER:HB3	1.95	0.48
6:F:53:ASP:OD1	6:F:53:ASP:C	2.56	0.48
1:A:4:MET:CE	1:A:35(F):TRP:HZ3	2.27	0.48
6:F:30:ASN:ND2	6:F:34:ILE:HB	2.28	0.48
1:A:169:VAL:HG22	1:A:177:SER:O	2.13	0.48
4:D:93:ALA:HA	4:D:102:HIS:O	2.13	0.48
4:D:124:LEU:HG	4:D:139:GLY:O	2.14	0.48
5:E:476:ARG:HA	5:E:479:TRP:CD1	2.49	0.48
1:A:35(C):ASP:O	1:A:52:HIS:NE2	2.47	0.47
2:B:35:TRP:CD1	2:B:48:ILE:HB	2.49	0.47
2:B:151:ASP:HB3	2:B:189:HIS:CD2	2.47	0.47
4:D:22:CYS:HB3	4:D:78:VAL:HG13	1.96	0.47
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.49	0.47
4:D:168:ALA:CA	4:D:178:LEU:HD21	2.44	0.47
1:A:163:VAL:O	1:A:164:HIS:HD2	1.98	0.47
1:A:183:THR:O	1:A:183:THR:HG22	2.13	0.47
4:D:145:TYR:CZ	4:D:176:TYR:CB	2.98	0.47
4:D:200:HIS:HB3	4:D:205:THR:HG1	1.72	0.47
5:E:96:TRP:CE3	5:E:275:ASP:HB2	2.49	0.47
6:F:64:GLN:O	6:F:64:GLN:HG3	2.15	0.47
6:F:120:SER:CB	6:F:121:PRO:HD2	2.44	0.47
1:A:35(B):LYS:N	1:A:35(B):LYS:CD	2.77	0.47
1:A:100(D):VAL:HG22	7:G:2:NAG:C7	2.45	0.47
5:E:89:VAL:HG22	5:E:89:VAL:O	2.13	0.47
5:E:95:MET:HE2	5:E:96:TRP:HE1	1.77	0.47
5:E:282:LYS:HA	5:E:282:LYS:HD3	1.68	0.47
5:E:412:ASN:OD1	5:E:412:ASN:O	2.33	0.47
6:F:155:GLY:O	6:F:173:ASP:HA	2.14	0.47
2:B:125:LEU:CD2	2:B:183:LYS:NZ	2.75	0.47
2:B:194:CYS:O	2:B:206:THR:HA	2.14	0.47
5:E:271:VAL:HG13	5:E:287:GLN:HB3	1.97	0.47
1:A:35(C):ASP:HA	1:A:53:TRP:HE1	1.80	0.47
1:A:82(C):VAL:HG11	1:A:111:VAL:HG21	1.96	0.47
1:A:163:VAL:HG22	1:A:182:VAL:HG13	1.95	0.47
3:C:125:LEU:HD23	3:C:183:LYS:CD	2.45	0.47
3:C:194:CYS:O	3:C:206:THR:HB	2.15	0.47
4:D:201:LYS:N	4:D:202:PRO:CD	2.78	0.47
5:E:391:PHE:CE2	5:E:470:PRO:HB3	2.50	0.47
6:F:116:LEU:HD11	6:F:144:LEU:CD1	2.40	0.47
1:A:36:TRP:CZ3	1:A:92:CYS:HB3	2.50	0.47
1:A:212:GLU:HG2	1:A:213:PRO:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HD22	1:A:159:LEU:HD13	1.80	0.47
2:B:196:VAL:HG13	2:B:196:VAL:O	2.13	0.47
3:C:106:ILE:O	3:C:106:ILE:HG13	2.13	0.47
6:F:8:LYS:HD2	6:F:76:ILE:CD1	2.45	0.47
3:C:150:VAL:CG2	3:C:192:TYR:HE1	2.28	0.46
5:E:300:ASN:HB2	5:E:441:GLY:O	2.15	0.46
1:A:96:ARG:HD3	1:A:101:ASP:CG	2.39	0.46
5:E:350:ARG:HH21	5:E:350:ARG:HG3	1.80	0.46
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.97	0.46
3:C:210:ASN:O	3:C:211:ARG:C	2.58	0.46
5:E:412:ASN:OD1	5:E:412:ASN:C	2.58	0.46
1:A:35(A):ASP:O	1:A:35(B):LYS:HB2	2.15	0.46
2:B:11:LEU:CD2	2:B:19:VAL:HG23	2.45	0.46
2:B:38:TYR:CD1	2:B:44:PRO:HG3	2.51	0.46
1:A:100(D):VAL:HG22	7:G:2:NAG:O7	2.15	0.46
2:B:8:PRO:HG3	2:B:11:LEU:HD13	1.97	0.46
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.98	0.46
2:B:149:LYS:NZ	2:B:195:GLU:HB2	2.30	0.46
3:C:119:PRO:HG2	3:C:209:PHE:CD1	2.50	0.46
4:D:155:ASN:HD21	4:D:194:TYR:HD1	1.60	0.46
5:E:271:VAL:HG11	5:E:273:ARG:NH2	2.30	0.46
5:E:298:ARG:O	5:E:298:ARG:HG2	2.15	0.46
5:E:462:GLU:C	5:E:464:GLY:H	2.23	0.46
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.98	0.46
5:E:213:ILE:HG23	5:E:214:PRO:HD2	1.98	0.46
4:D:54:LEU:HD23	4:D:54:LEU:HA	1.55	0.46
3:C:11:LEU:O	3:C:104:LEU:HA	2.16	0.46
5:E:358:THR:HG22	5:E:465:THR:HA	1.98	0.46
4:D:124:LEU:HG	4:D:139:GLY:H	1.81	0.46
1:A:200:HIS:CE1	1:A:202:PRO:HG2	2.52	0.45
3:C:108:ARG:CG	3:C:109:THR:H	2.28	0.45
3:C:108:ARG:CG	3:C:109:THR:N	2.77	0.45
4:D:122:PHE:HA	4:D:123:PRO:HD3	1.82	0.45
6:F:100:LEU:HD13	6:F:170:PHE:CZ	2.51	0.45
3:C:151:ASP:N	3:C:191:VAL:CG1	2.78	0.45
4:D:12:LYS:HB2	4:D:82(C):LEU:CD1	2.46	0.45
5:E:211:GLU:O	5:E:212:PRO:C	2.56	0.45
5:E:242:VAL:HG12	5:E:243:SER:N	2.30	0.45
1:A:96:ARG:NH2	8:H:10:MAN:H4	2.32	0.45
1:A:178:LEU:HD12	1:A:178:LEU:C	2.42	0.45
4:D:138:LEU:CD1	4:D:211:VAL:HG21	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:353:PHE:C	5:E:354:GLU:HG2	2.42	0.45
6:F:77:GLU:CD	6:F:77:GLU:H	2.24	0.45
1:A:100(D):VAL:HG23	1:A:100(D):VAL:O	2.15	0.45
3:C:9:ALA:O	3:C:102:THR:HA	2.17	0.45
3:C:54:ARG:HD2	3:C:58:VAL:HG12	1.99	0.45
4:D:145:TYR:CE1	4:D:176:TYR:HB2	2.51	0.45
4:D:195:ILE:CD1	4:D:197:ASN:HB2	2.47	0.45
5:E:447:SER:HA	11:E:524:NAG:C8	2.46	0.45
6:F:110:GLN:OE1	6:F:150:GLU:HA	2.17	0.45
2:B:205:VAL:CG1	2:B:206:THR:H	2.29	0.45
4:D:95:VAL:CG2	4:D:101:LYS:H	2.30	0.45
4:D:151:THR:OG1	4:D:199:ASN:HB3	2.17	0.45
4:D:203:SER:HB2	4:D:205:THR:CG2	2.44	0.45
6:F:144:LEU:HD12	6:F:144:LEU:N	2.31	0.45
4:D:82(C):LEU:O	4:D:83:ARG:C	2.56	0.45
1:A:34:TRP:CE3	5:E:417:PRO:HB2	2.52	0.45
1:A:155:ASN:ND2	1:A:159:LEU:HD13	2.32	0.45
2:B:148:TRP:HD1	2:B:159:SER:HB3	1.82	0.45
5:E:358:THR:O	5:E:358:THR:HG23	2.15	0.45
5:E:447:SER:HA	11:E:524:NAG:H82	1.99	0.45
6:F:131:ARG:HD3	6:F:137:ASN:HD21	1.81	0.45
4:D:178:LEU:HD23	4:D:178:LEU:HA	1.68	0.45
5:E:456:ARG:HB2	5:E:468:PHE:CE1	2.52	0.45
2:B:115:VAL:HG21	2:B:196:VAL:HG11	1.99	0.45
2:B:145:LYS:HB3	2:B:197:THR:HG1	1.81	0.45
3:C:113:PRO:O	3:C:115:VAL:HG23	2.16	0.45
3:C:174:SER:O	3:C:175:LEU:HB2	2.17	0.45
5:E:389:GLN:HG2	8:H:1:NAG:H81	1.99	0.45
6:F:106:THR:O	6:F:107:HIS:CG	2.70	0.45
6:F:150:GLU:OE2	6:F:153:ASP:OD2	2.34	0.45
5:E:326:ILE:HG12	5:E:419:ARG:HH22	1.81	0.44
3:C:116:PHE:CD2	3:C:135:LEU:HD22	2.50	0.44
4:D:138:LEU:CD2	4:D:211:VAL:HG21	2.42	0.44
4:D:212:GLU:HA	4:D:213:PRO:HD3	1.86	0.44
5:E:298:ARG:HH11	5:E:443:ILE:CD1	2.29	0.44
1:A:184:VAL:HG12	1:A:185:PRO:O	2.18	0.44
3:C:93:ASN:OD1	3:C:93:ASN:N	2.41	0.44
3:C:150:VAL:HG13	3:C:153:ALA:HB3	2.00	0.44
3:C:209:PHE:CE1	3:C:210:ASN:O	2.71	0.44
4:D:95:VAL:HG23	4:D:100(K):LEU:HA	1.99	0.44
4:D:196:CYS:O	4:D:198:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:122:LEU:HD22	5:E:200:VAL:HG22	1.98	0.44
6:F:10:ASP:CG	6:F:11:THR:H	2.25	0.44
2:B:80:SER:HA	2:B:106:ILE:HD12	1.96	0.44
1:A:2:LEU:C	1:A:2:LEU:CD2	2.87	0.44
4:D:41:PRO:C	4:D:43:GLN:H	2.26	0.44
5:E:358:THR:OG1	5:E:395:TRP:O	2.24	0.44
5:E:459:GLY:O	5:E:460:ILE:CG1	2.66	0.44
6:F:75:LYS:O	6:F:78:ASP:HB2	2.17	0.44
6:F:134:ARG:HH12	6:F:150:GLU:HG3	1.83	0.44
6:F:137:ASN:C	6:F:138:ILE:HD12	2.43	0.44
1:A:192:GLN:HG2	1:A:194:TYR:CZ	2.53	0.44
5:E:350:ARG:HG3	5:E:350:ARG:NH2	2.33	0.44
1:A:144:ASP:HB3	1:A:175:LEU:CD1	2.47	0.44
3:C:119:PRO:HA	3:C:120:PRO:HD3	1.80	0.44
5:E:255:VAL:O	5:E:255:VAL:HG12	2.16	0.44
1:A:78:PHE:CZ	1:A:92:CYS:HB2	2.52	0.43
3:C:121:SER:O	3:C:125:LEU:HD12	2.18	0.43
5:E:91:GLU:OE2	5:E:242:VAL:HG21	2.18	0.43
4:D:12:LYS:CB	4:D:82(C):LEU:CD1	2.92	0.43
4:D:57:ALA:C	4:D:58:HIS:CD2	2.97	0.43
4:D:184:VAL:HG13	4:D:185:PRO:CD	2.45	0.43
6:F:131:ARG:HB2	6:F:137:ASN:HD22	1.82	0.43
1:A:94:ARG:NH2	1:A:101:ASP:OD2	2.36	0.43
2:B:178:THR:O	2:B:178:THR:CG2	2.66	0.43
3:C:103:ARG:CG	3:C:104:LEU:N	2.82	0.43
3:C:106:ILE:HG12	3:C:166:GLN:CD	2.43	0.43
4:D:29:PHE:CE2	4:D:73:LYS:HA	2.54	0.43
3:C:61:ARG:NH1	3:C:82:ASP:OD1	2.52	0.43
3:C:38:GLN:O	3:C:84:ALA:HB1	2.18	0.43
5:E:361:PHE:O	5:E:391:PHE:C	2.62	0.43
5:E:405:SER:HB3	11:E:525:NAG:C7	2.48	0.43
5:E:439:ILE:H	5:E:439:ILE:HG13	1.56	0.43
4:D:194:TYR:O	4:D:211:VAL:HG12	2.18	0.43
5:E:358:THR:HG21	5:E:465:THR:HB	1.97	0.43
6:F:110:GLN:HA	6:F:149:LEU:CD1	2.47	0.43
1:A:47:TRP:O	1:A:60:LYS:HD2	2.18	0.43
1:A:82(C):VAL:HG12	1:A:83:THR:N	2.34	0.43
5:E:439:ILE:C	5:E:439:ILE:HD12	2.44	0.43
1:A:148:GLU:OE1	1:A:149:PRO:HA	2.19	0.43
4:D:46:GLU:OE2	4:D:62:HIS:NE2	2.37	0.43
4:D:146:PHE:HA	4:D:147:PRO:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:VAL:HG22	5:E:128:GLY:N	2.33	0.43
5:E:225:ILE:HG12	5:E:488:VAL:HG22	1.99	0.43
1:A:6:GLU:HG3	1:A:92:CYS:SG	2.59	0.43
3:C:49:TYR:CZ	3:C:53:THR:CG2	3.01	0.43
1:A:198:VAL:O	1:A:206:LYS:HD2	2.19	0.43
3:C:103:ARG:HG2	3:C:104:LEU:N	2.34	0.43
3:C:163:VAL:HG12	3:C:164:THR:O	2.19	0.43
4:D:189:LEU:N	4:D:189:LEU:HD12	2.34	0.43
1:A:60:LYS:HG3	2:B:95:PRO:HB2	2.00	0.42
1:A:152:VAL:HA	1:A:197:ASN:O	2.19	0.42
2:B:69:THR:O	2:B:69:THR:CG2	2.67	0.42
4:D:119:PRO:HB2	4:D:142:VAL:HG12	2.01	0.42
3:C:108:ARG:HH22	3:C:140:TYR:HB2	1.81	0.42
4:D:82(A):ARG:O	4:D:82(B):ASN:CB	2.66	0.42
4:D:100(A):ASP:N	4:D:100(A):ASP:OD1	2.51	0.42
4:D:206:LYS:O	4:D:207:VAL:HG13	2.19	0.42
5:E:279:ASN:HA	11:E:526:NAG:C8	2.45	0.42
3:C:175:LEU:C	3:C:175:LEU:HD23	2.43	0.42
4:D:141:LEU:O	4:D:141:LEU:HD23	2.19	0.42
6:F:108:LEU:HD12	6:F:109:LEU:H	1.84	0.42
1:A:14:PRO:O	1:A:15:SER:HB3	2.18	0.42
2:B:43:SER:HA	2:B:44:PRO:HD3	1.96	0.42
3:C:150:VAL:HG21	3:C:189:HIS:ND1	2.35	0.42
4:D:98:GLY:O	4:D:100:ALA:N	2.50	0.42
5:E:459:GLY:C	5:E:460:ILE:HG13	2.45	0.42
2:B:186:TYR:O	2:B:192:TYR:OH	2.38	0.42
4:D:2:VAL:HG12	4:D:102:HIS:CE1	2.55	0.42
6:F:93:VAL:CG1	6:F:94:GLN:N	2.82	0.42
1:A:100(D):VAL:HG21	7:G:2:NAG:O3	2.20	0.42
2:B:4:MET:HE2	2:B:33:LEU:HD11	2.02	0.42
3:C:191:VAL:HG23	3:C:210:ASN:OD1	2.20	0.42
4:D:101:LYS:HG3	4:D:102:HIS:CD2	2.55	0.42
5:E:213:ILE:HD13	5:E:213:ILE:HA	1.91	0.42
5:E:296:CYS:HA	5:E:330:HIS:O	2.19	0.42
1:A:201:LYS:N	1:A:202:PRO:CD	2.79	0.42
2:B:38:TYR:HD1	2:B:44:PRO:HG3	1.85	0.42
3:C:106:ILE:HD11	3:C:171:SER:CB	2.49	0.42
1:A:2:LEU:CD2	1:A:4:MET:HE3	2.45	0.42
3:C:118:PHE:CD2	4:D:124:LEU:HD13	2.55	0.42
5:E:123:THR:HG23	5:E:124:PRO:HD2	2.01	0.42
6:F:156:THR:CG2	6:F:171:LYS:HE2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:CB	1:A:45:LEU:HD23	2.49	0.41
2:B:19:VAL:HG12	2:B:75:ILE:HB	2.02	0.41
4:D:126:PRO:HG2	4:D:213:PRO:HA	2.02	0.41
2:B:11:LEU:CD2	2:B:19:VAL:CG2	2.98	0.41
2:B:135:LEU:CD2	2:B:137:ASN:HB2	2.49	0.41
4:D:83:ARG:HG3	4:D:85:ASP:CG	2.45	0.41
6:F:128:VAL:CB	6:F:144:LEU:HD11	2.47	0.41
2:B:11:LEU:HA	2:B:11:LEU:HD12	1.81	0.41
2:B:211:ARG:HG2	2:B:212:GLY:N	2.35	0.41
3:C:125:LEU:HD21	3:C:186:TYR:CD2	2.54	0.41
4:D:68:THR:CG2	4:D:82(A):ARG:NH2	2.81	0.41
5:E:272:ILE:HG22	5:E:286:VAL:HG22	2.02	0.41
3:C:124:GLN:HG3	4:D:122:PHE:CE2	2.55	0.41
4:D:88:ALA:O	4:D:108:LEU:HD12	2.20	0.41
4:D:121:VAL:CG2	4:D:142:VAL:HG13	2.47	0.41
6:F:109:LEU:O	6:F:149:LEU:HD21	2.20	0.41
5:E:96:TRP:CH2	5:E:274:SER:HA	2.55	0.41
5:E:302:ASN:HA	5:E:303:THR:HA	1.68	0.41
6:F:150:GLU:CD	6:F:150:GLU:N	2.77	0.41
1:A:192:GLN:HA	1:A:192:GLN:OE1	2.21	0.41
4:D:52:ILE:HG23	4:D:100(E):TYR:CZ	2.55	0.41
2:B:77:ASN:HD22	2:B:79:GLN:NE2	2.18	0.41
5:E:229:ASN:O	5:E:230:ASP:C	2.63	0.41
5:E:267:GLU:O	5:E:268:GLU:HB3	2.20	0.41
5:E:395:TRP:CZ3	11:E:525:NAG:H82	2.56	0.41
2:B:107:LYS:HA	2:B:140:TYR:OH	2.21	0.41
5:E:279:ASN:OD1	6:F:29:LYS:NZ	2.47	0.41
1:A:184:VAL:CG1	1:A:185:PRO:N	2.83	0.41
3:C:33:LEU:HD13	3:C:71:PHE:CG	2.56	0.41
6:F:149:LEU:HD12	6:F:149:LEU:O	2.21	0.41
6:F:151:LEU:C	6:F:151:LEU:HD23	2.46	0.41
1:A:62:SER:C	1:A:63:LEU:HD12	2.45	0.41
5:E:101:VAL:HG13	5:E:102:GLU:N	2.36	0.41
5:E:462:GLU:C	5:E:464:GLY:N	2.77	0.41
6:F:130:CYS:O	6:F:137:ASN:HA	2.20	0.41
1:A:87:THR:HG22	1:A:110:THR:HA	2.03	0.40
1:A:184:VAL:HG13	1:A:185:PRO:CD	2.50	0.40
2:B:135:LEU:C	2:B:135:LEU:CD2	2.93	0.40
3:C:132:VAL:CG1	3:C:179:LEU:HB3	2.50	0.40
3:C:166:GLN:HB2	3:C:173:TYR:CZ	2.56	0.40
5:E:426:MET:HB3	5:E:428:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:459:GLY:O	5:E:460:ILE:HG13	2.21	0.40
2:B:170:ASP:OD1	2:B:170:ASP:C	2.64	0.40
3:C:150:VAL:CG2	3:C:192:TYR:CE1	3.01	0.40
3:C:167:ASP:O	3:C:171:SER:HA	2.20	0.40
5:E:268:GLU:HG3	5:E:269:GLU:HG3	2.03	0.40
5:E:326:ILE:HG23	5:E:328:GLN:N	2.36	0.40
5:E:420:ILE:CG2	5:E:438:PRO:HG3	2.50	0.40
8:H:7:MAN:O4	8:H:8:MAN:H5	2.20	0.40
1:A:212:GLU:CG	1:A:213:PRO:N	2.85	0.40
2:B:108:ARG:NH1	2:B:172:THR:CG2	2.85	0.40
5:E:208:ILE:HD13	5:E:208:ILE:HA	1.72	0.40
5:E:242:VAL:CG1	5:E:243:SER:N	2.83	0.40
5:E:371:ILE:HD12	6:F:45:THR:HG22	2.01	0.40
1:A:14:PRO:HG3	1:A:111:VAL:HG12	2.04	0.40
3:C:148:TRP:CD2	3:C:179:LEU:HD22	2.56	0.40
5:E:298:ARG:HD3	5:E:443:ILE:HD12	2.04	0.40
5:E:440:ARG:HG2	5:E:441:GLY:H	1.87	0.40
4:D:66:ARG:O	4:D:82:LEU:CD1	2.70	0.40
6:F:146:VAL:HG13	6:F:146:VAL:O	2.22	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	223/236 (94%)	201 (90%)	20 (9%)	2 (1%)	14	44
2	B	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
4	D	216/229 (94%)	213 (99%)	2 (1%)	1 (0%)	24	57
5	E	311/321 (97%)	291 (94%)	16 (5%)	4 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	173/185 (94%)	165 (95%)	8 (5%)	0	100	100
All	All	1347/1399 (96%)	1273 (94%)	67 (5%)	7 (0%)	24	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	326	ILE
5	E	407	ASN
1	A	62	SER
5	E	299	PRO
4	D	82(B)	ASN
1	A	105	PRO
5	E	347	ILE

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	193/201 (96%)	173 (90%)	20 (10%)	7	27
2	B	190/190 (100%)	187 (98%)	3 (2%)	55	75
3	C	184/184 (100%)	180 (98%)	4 (2%)	45	71
4	D	188/193 (97%)	177 (94%)	11 (6%)	18	48
5	E	282/287 (98%)	277 (98%)	5 (2%)	51	73
6	F	159/167 (95%)	155 (98%)	4 (2%)	42	69
All	All	1196/1222 (98%)	1149 (96%)	47 (4%)	28	60

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	33	GLU
1	A	73	THR
1	A	74	SER

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Mol	Chain	Res	Type
1	A	77	TRP
1	A	100	VAL
1	A	100(A)	PHE
1	A	100(B)	MET
1	A	100(C)	LEU
1	A	100(D)	VAL
1	A	100(E)	PRO
1	A	100(F)	ILE
1	A	100(I)	TRP
1	A	100(J)	PHE
1	A	108	GLN
1	A	116	THR
1	A	138	LEU
1	A	159	LEU
1	A	173	SER
1	A	181	VAL
2	B	18	THR
2	B	135	LEU
2	B	177	SER
3	C	7	SER
3	C	135	LEU
3	C	154	LEU
3	C	201	LEU
4	D	5	VAL
4	D	20	VAL
4	D	53	ILE
4	D	78	VAL
4	D	82	LEU
4	D	82(A)	ARG
4	D	82(B)	ASN
4	D	82(C)	LEU
4	D	117	LYS
4	D	142	VAL
4	D	211	VAL
5	E	208	ILE
5	E	255	VAL
5	E	271	VAL
5	E	401	ASN
5	E	413	THR
6	F	76	ILE
6	F	88	ASP
6	F	130	CYS

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Mol	Chain	Res	Type
6	F	162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	52	HIS
1	A	108	GLN
1	A	164	HIS
1	A	171	GLN
2	B	77	ASN
2	B	124	GLN
2	B	189	HIS
2	B	199	GLN
3	C	92	ASN
3	C	138	ASN
3	C	198	HIS
4	D	43	GLN
4	D	58	HIS
4	D	164	HIS
4	D	192	GLN
5	E	103	GLN
5	E	114	GLN
5	E	216	HIS
5	E	229	ASN
5	E	249	HIS
5	E	302	ASN
5	E	328	GLN
5	E	407	ASN
5	E	463	ASN
6	F	89	GLN
6	F	129	GLN
6	F	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

21 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$
7	NAG	G	1	5,7	14,14,15	1.07	1 (7%)	17,19,21	1.87	4 (23%)
7	NAG	G	2	7	14,14,15	1.32	2 (14%)	17,19,21	3.04	6 (35%)
7	BMA	G	3	7	11,11,12	1.47	1 (9%)	15,15,17	3.22	9 (60%)
7	MAN	G	4	7	11,11,12	1.54	3 (27%)	15,15,17	1.54	2 (13%)
7	MAN	G	5	7	11,11,12	1.53	3 (27%)	15,15,17	1.57	1 (6%)
7	MAN	G	6	7	11,11,12	1.01	0	15,15,17	2.39	4 (26%)
7	MAN	G	7	7	11,11,12	1.25	1 (9%)	15,15,17	1.00	1 (6%)
7	MAN	G	8	7	11,11,12	0.69	0	15,15,17	1.57	2 (13%)
8	NAG	H	1	8,5	14,14,15	0.54	0	17,19,21	1.10	1 (5%)
8	MAN	H	10	8	11,11,12	0.65	0	15,15,17	0.70	0
8	NAG	H	2	8	14,14,15	1.00	1 (7%)	17,19,21	3.16	8 (47%)
8	BMA	H	3	8	11,11,12	1.45	2 (18%)	15,15,17	0.84	1 (6%)
8	MAN	H	4	8	11,11,12	0.59	0	15,15,17	0.71	0
8	MAN	H	5	8	11,11,12	0.69	0	15,15,17	1.46	3 (20%)
8	MAN	H	6	8	11,11,12	0.70	0	15,15,17	1.10	1 (6%)
8	MAN	H	7	8	11,11,12	1.53	3 (27%)	15,15,17	1.20	2 (13%)
8	MAN	H	8	8	11,11,12	1.51	3 (27%)	15,15,17	1.35	1 (6%)
8	MAN	H	9	8	11,11,12	1.29	1 (9%)	15,15,17	2.35	4 (26%)
9	NAG	I	1	9,5	14,14,15	1.42	3 (21%)	17,19,21	1.13	1 (5%)
9	NAG	I	2	9	14,14,15	0.53	0	17,19,21	1.17	2 (11%)
9	BMA	I	3	9	11,11,12	0.64	0	15,15,17	0.57	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
7	NAG	G	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	3/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	0/2/19/22	0/1/1/1
7	MAN	G	6	7	-	0/2/19/22	0/1/1/1
7	MAN	G	7	7	-	0/2/19/22	0/1/1/1
7	MAN	G	8	7	-	0/2/19/22	0/1/1/1
8	NAG	H	1	8,5	-	1/6/23/26	0/1/1/1
8	MAN	H	10	8	-	0/2/19/22	0/1/1/1
8	NAG	H	2	8	-	2/6/23/26	0/1/1/1
8	BMA	H	3	8	-	0/2/19/22	0/1/1/1
8	MAN	H	4	8	-	0/2/19/22	0/1/1/1
8	MAN	H	5	8	-	2/2/19/22	0/1/1/1
8	MAN	H	6	8	-	0/2/19/22	0/1/1/1
8	MAN	H	7	8	-	0/2/19/22	0/1/1/1
8	MAN	H	8	8	-	0/2/19/22	0/1/1/1
8	MAN	H	9	8	-	2/2/19/22	0/1/1/1
9	NAG	I	1	9,5	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	7	MAN	O5-C1	-3.69	1.37	1.43
7	G	3	BMA	O5-C5	-3.15	1.37	1.43
8	H	9	MAN	O5-C1	3.10	1.48	1.43
8	H	7	MAN	O5-C1	3.06	1.48	1.43
7	G	5	MAN	O5-C1	2.97	1.48	1.43
7	G	2	NAG	C4-C5	-2.95	1.46	1.53
8	H	3	BMA	O5-C1	2.93	1.48	1.43
7	G	4	MAN	O5-C1	2.88	1.48	1.43
8	H	8	MAN	O5-C1	2.82	1.48	1.43
7	G	4	MAN	O5-C5	2.80	1.48	1.43
7	G	5	MAN	O5-C5	2.75	1.48	1.43
8	H	3	BMA	O5-C5	2.75	1.48	1.43
9	I	1	NAG	O5-C1	2.73	1.48	1.43
9	I	1	NAG	O5-C5	2.67	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	8	MAN	O5-C5	2.62	1.48	1.43
8	H	7	MAN	O5-C5	2.50	1.48	1.43
7	G	4	MAN	O2-C2	2.41	1.48	1.43
8	H	8	MAN	O2-C2	2.40	1.48	1.43
7	G	5	MAN	O2-C2	2.22	1.48	1.43
8	H	2	NAG	O5-C1	-2.16	1.40	1.43
7	G	2	NAG	O4-C4	-2.16	1.37	1.43
8	H	7	MAN	O3-C3	2.13	1.48	1.43
7	G	1	NAG	O4-C4	2.04	1.48	1.43
9	I	1	NAG	O4-C4	2.03	1.48	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	2	NAG	C2-N2-C7	-8.31	111.77	122.90
8	H	2	NAG	O5-C1-C2	-7.46	99.75	111.29
8	H	9	MAN	C1-O5-C5	-7.37	102.31	112.19
7	G	3	BMA	C1-O5-C5	-6.93	102.90	112.19
7	G	2	NAG	O5-C5-C6	6.17	119.68	107.66
7	G	6	MAN	C1-O5-C5	6.07	120.32	112.19
8	H	2	NAG	C4-C3-C2	-5.82	102.48	111.02
8	H	2	NAG	C1-O5-C5	-5.74	104.49	112.19
7	G	3	BMA	C2-C3-C4	-5.25	101.63	110.86
7	G	5	MAN	C1-O5-C5	5.20	119.15	112.19
7	G	3	BMA	O2-C2-C3	5.00	120.50	110.15
7	G	4	MAN	C1-O5-C5	4.84	118.67	112.19
7	G	1	NAG	C4-C3-C2	-4.57	104.33	111.02
7	G	6	MAN	O4-C4-C5	4.38	120.12	109.32
7	G	8	MAN	C1-O5-C5	4.34	118.00	112.19
8	H	8	MAN	C1-O5-C5	3.79	117.26	112.19
7	G	1	NAG	O5-C1-C2	-3.69	105.58	111.29
8	H	2	NAG	O5-C5-C4	-3.59	102.09	110.83
7	G	2	NAG	O4-C4-C5	-3.47	100.78	109.32
9	I	1	NAG	C1-O5-C5	3.42	116.77	112.19
8	H	5	MAN	C2-C3-C4	-3.31	105.03	110.86
7	G	2	NAG	O6-C6-C5	-3.18	100.50	111.33
7	G	3	BMA	O3-C3-C4	-3.09	103.08	110.38
8	H	9	MAN	C1-C2-C3	-3.00	105.28	109.64
8	H	2	NAG	C3-C4-C5	-2.98	104.83	110.23
7	G	1	NAG	C2-N2-C7	-2.97	118.92	122.90
7	G	3	BMA	O3-C3-C2	2.89	115.95	110.05
8	H	2	NAG	O4-C4-C5	2.88	116.41	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	7	MAN	C1-O5-C5	2.81	115.95	112.19
7	G	6	MAN	C1-C2-C3	2.80	113.72	109.64
8	H	2	NAG	C2-N2-C7	-2.79	119.16	122.90
7	G	8	MAN	O2-C2-C3	-2.74	104.47	110.15
7	G	1	NAG	C1-O5-C5	2.73	115.84	112.19
8	H	1	NAG	O5-C1-C2	-2.69	107.13	111.29
7	G	3	BMA	O6-C6-C5	-2.63	102.39	111.33
7	G	3	BMA	O2-C2-C1	-2.57	103.35	109.22
7	G	3	BMA	C3-C4-C5	2.33	114.45	110.23
8	H	5	MAN	O2-C2-C1	-2.31	103.93	109.22
7	G	3	BMA	O5-C1-C2	2.26	116.18	110.79
8	H	5	MAN	O2-C2-C3	-2.23	105.53	110.15
8	H	7	MAN	C1-C2-C3	2.22	112.88	109.64
7	G	2	NAG	O4-C4-C3	-2.21	105.16	110.38
9	I	2	NAG	C2-N2-C7	-2.17	119.99	122.90
7	G	6	MAN	O3-C3-C4	2.16	115.48	110.38
8	H	3	BMA	C1-O5-C5	2.13	115.04	112.19
8	H	2	NAG	O3-C3-C4	-2.10	105.43	110.38
8	H	9	MAN	O5-C5-C4	-2.09	105.75	110.83
8	H	9	MAN	C2-C3-C4	-2.08	107.20	110.86
9	I	2	NAG	C1-O5-C5	2.08	114.97	112.19
8	H	6	MAN	O5-C1-C2	-2.07	105.86	110.79
7	G	4	MAN	C1-C2-C3	2.05	112.64	109.64
7	G	7	MAN	C1-O5-C5	-2.01	109.49	112.19
7	G	2	NAG	C8-C7-N2	2.01	119.45	116.12

There are no chirality outliers.

All (12) torsion outliers are listed below:

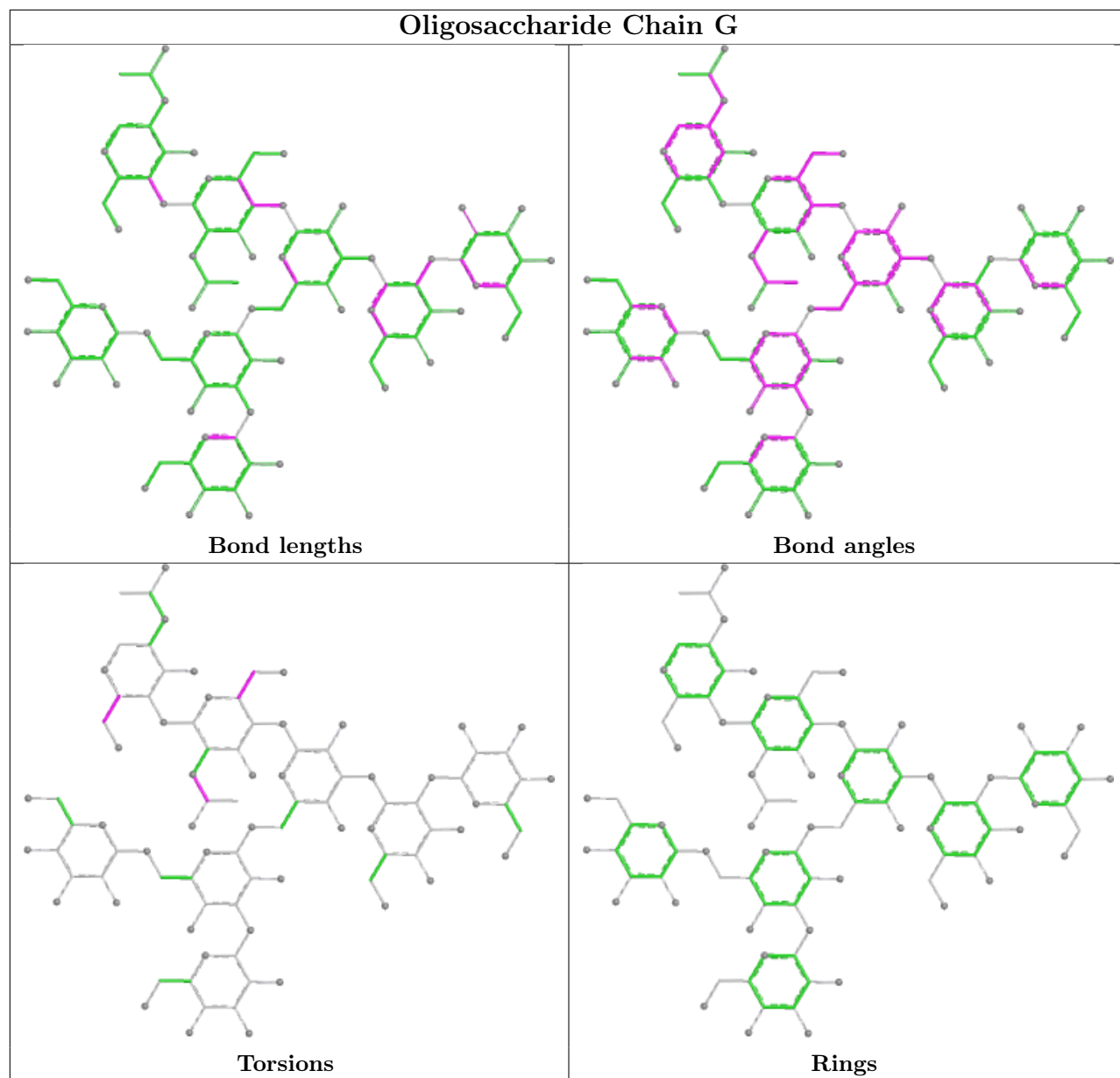
Mol	Chain	Res	Type	Atoms
8	H	2	NAG	O5-C5-C6-O6
8	H	5	MAN	C4-C5-C6-O6
8	H	9	MAN	O5-C5-C6-O6
8	H	5	MAN	O5-C5-C6-O6
8	H	9	MAN	C4-C5-C6-O6
8	H	2	NAG	C4-C5-C6-O6
7	G	2	NAG	O7-C7-N2-C2
7	G	1	NAG	C4-C5-C6-O6
7	G	1	NAG	O5-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
8	H	1	NAG	C4-C5-C6-O6
7	G	2	NAG	C8-C7-N2-C2

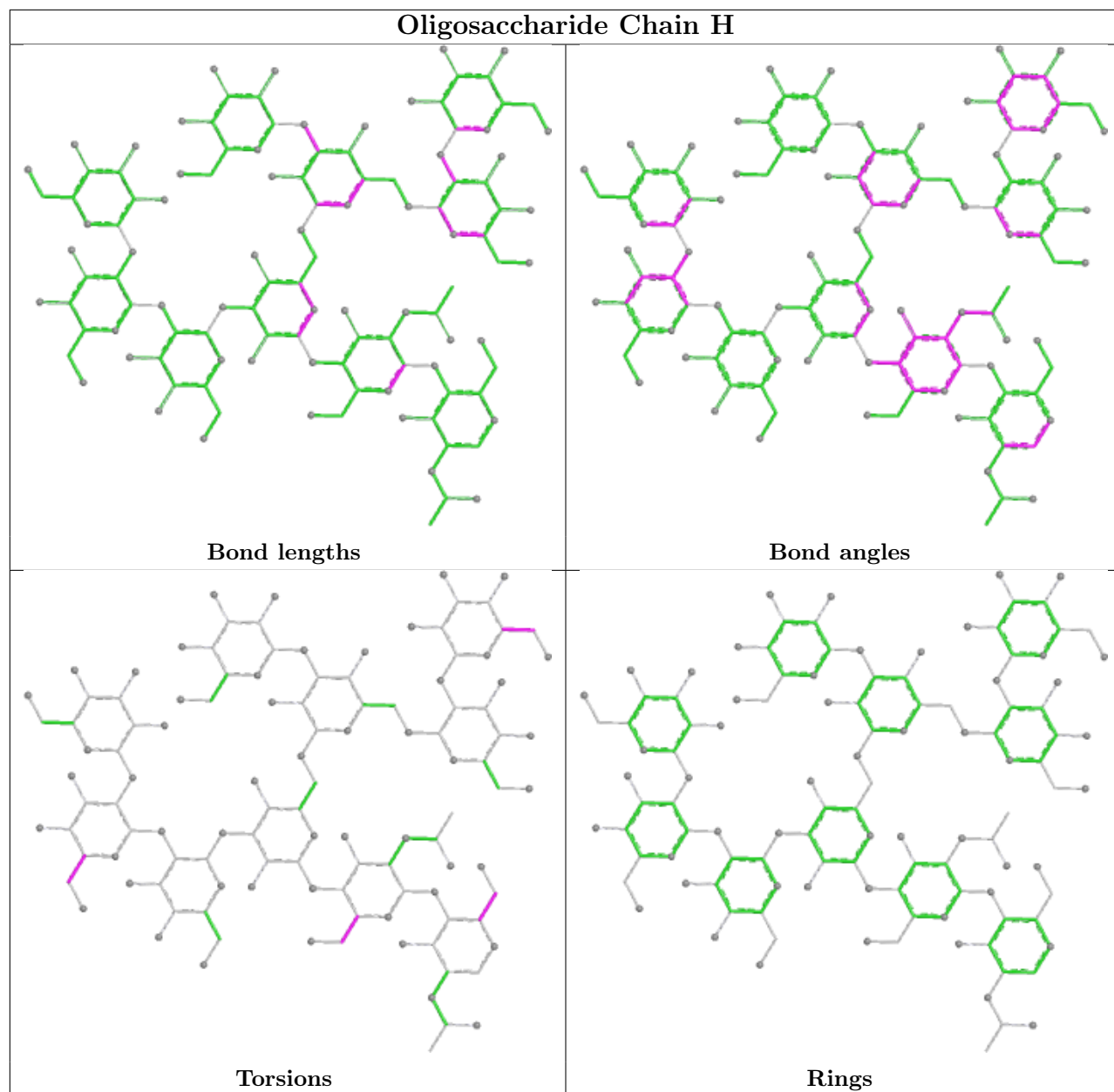
There are no ring outliers.

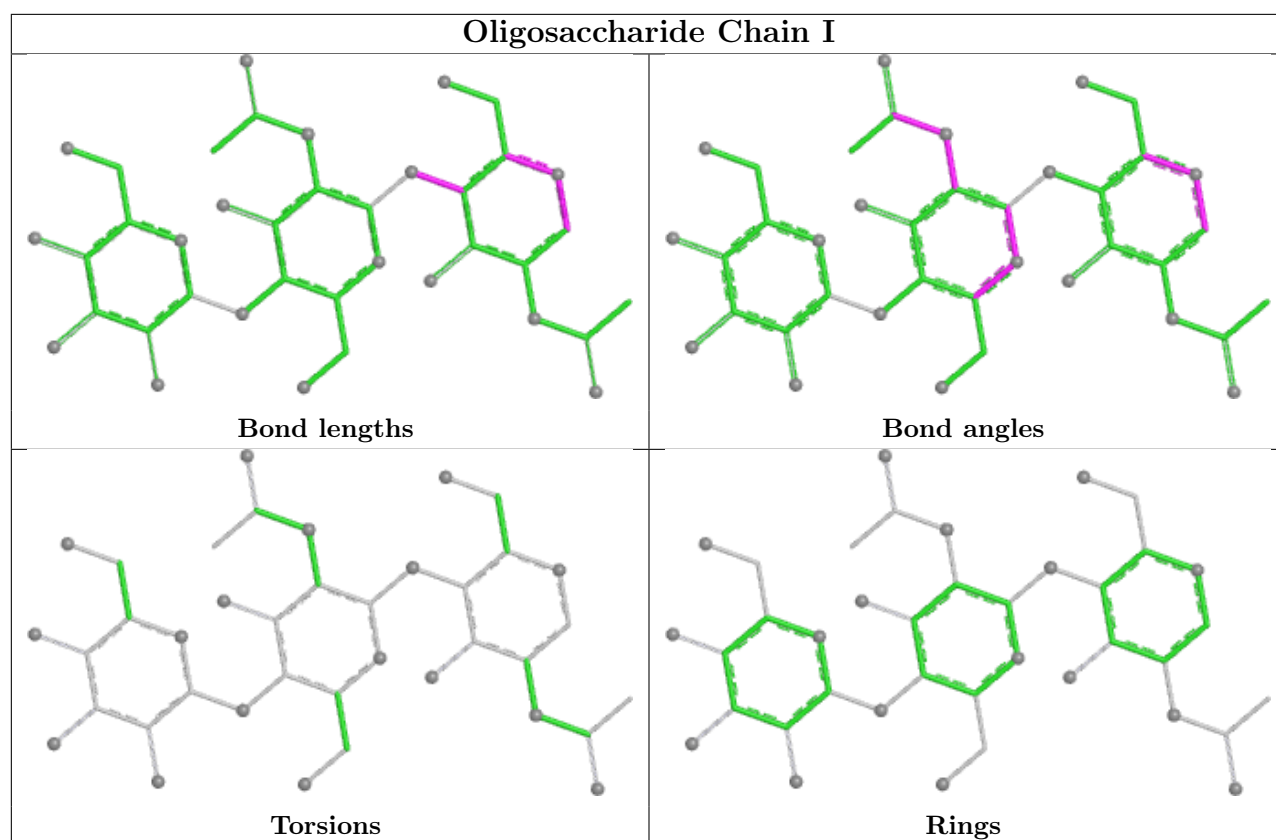
10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	9	MAN	1	0
7	G	7	MAN	1	0
7	G	3	BMA	2	0
8	H	1	NAG	1	0
8	H	8	MAN	2	0
7	G	2	NAG	3	0
8	H	7	MAN	1	0
8	H	10	MAN	1	0
7	G	8	MAN	1	0
7	G	4	MAN	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](#)

7 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$
11	NAG	E	525	5	14,14,15	0.55	0	17,19,21	0.70	0
11	NAG	E	527	5	14,14,15	0.62	0	17,19,21	0.55	0
11	NAG	E	523	5	14,14,15	0.51	0	17,19,21	0.94	1 (5%)
11	NAG	E	522	5	14,14,15	0.54	0	17,19,21	0.78	0
10	PG4	C	301	-	12,12,12	0.68	0	11,11,11	0.81	0
11	NAG	E	526	5	14,14,15	0.64	0	17,19,21	0.70	0
11	NAG	E	524	5	14,14,15	0.51	0	17,19,21	1.31	2 (11%)

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
11	NAG	E	525	5	-	4/6/23/26	0/1/1/1
11	NAG	E	527	5	-	2/6/23/26	0/1/1/1
11	NAG	E	523	5	-	4/6/23/26	0/1/1/1
11	NAG	E	522	5	-	2/6/23/26	0/1/1/1
10	PG4	C	301	-	-	4/10/10/10	-
11	NAG	E	526	5	-	3/6/23/26	0/1/1/1
11	NAG	E	524	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	524	NAG	C2-N2-C7	-2.85	119.08	122.90
11	E	523	NAG	C1-O5-C5	2.81	115.95	112.19
11	E	524	NAG	O5-C1-C2	-2.56	107.33	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	E	522	NAG	C8-C7-N2-C2
11	E	522	NAG	O7-C7-N2-C2
11	E	525	NAG	O7-C7-N2-C2
11	E	526	NAG	C8-C7-N2-C2
11	E	526	NAG	O7-C7-N2-C2
11	E	525	NAG	C8-C7-N2-C2
11	E	527	NAG	C8-C7-N2-C2
11	E	527	NAG	O7-C7-N2-C2
11	E	523	NAG	O5-C5-C6-O6
11	E	523	NAG	C4-C5-C6-O6
10	C	301	PG4	O2-C3-C4-O3
11	E	525	NAG	O5-C5-C6-O6
11	E	523	NAG	C8-C7-N2-C2
11	E	523	NAG	O7-C7-N2-C2
10	C	301	PG4	C8-C7-O4-C6
10	C	301	PG4	C6-C5-O3-C4
11	E	526	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
11	E	524	NAG	O5-C5-C6-O6
11	E	525	NAG	C4-C5-C6-O6
10	C	301	PG4	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	525	NAG	2	0
11	E	527	NAG	1	0
11	E	526	NAG	4	0
11	E	524	NAG	3	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	227/236 (96%)	-0.34	1 (0%) 88 76	75, 122, 168, 178	0
2	B	214/214 (100%)	-0.32	0 100 100	72, 121, 182, 197	0
3	C	214/214 (100%)	-0.25	0 100 100	81, 145, 187, 197	0
4	D	220/229 (96%)	-0.34	0 100 100	49, 96, 210, 242	0
5	E	315/321 (98%)	-0.34	2 (0%) 85 70	27, 110, 174, 204	0
6	F	175/185 (94%)	-0.12	0 100 100	79, 143, 214, 222	0
All	All	1365/1399 (97%)	-0.29	3 (0%) 91 83	27, 122, 194, 242	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	115	SER	3.4
1	A	180	SER	2.1
5	E	461	ASN	2.0

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
9	BMA	I	3	11/12	0.49	0.08	131,140,144,146	0

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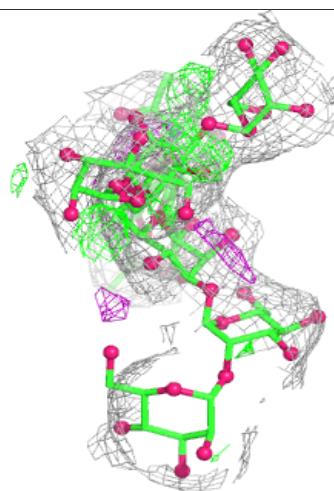
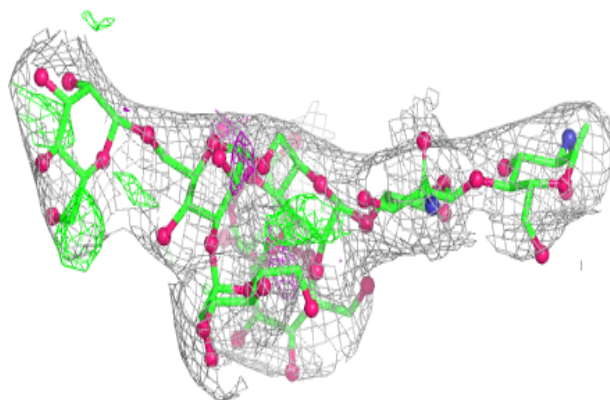
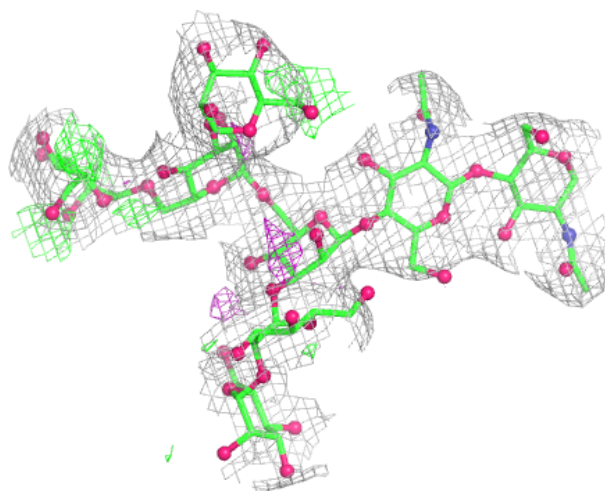
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MAN	H	9	11/12	0.55	0.11	135,140,144,152	0
7	MAN	G	8	11/12	0.68	0.13	94,97,103,110	0
7	MAN	G	4	11/12	0.69	0.11	121,125,134,144	0
8	MAN	H	6	11/12	0.69	0.14	100,107,114,114	0
7	MAN	G	5	11/12	0.74	0.09	148,152,157,159	0
7	MAN	G	7	11/12	0.79	0.11	86,92,103,104	0
9	NAG	I	2	14/15	0.82	0.10	116,125,135,139	0
8	MAN	H	8	11/12	0.82	0.13	116,121,127,128	0
9	NAG	I	1	14/15	0.84	0.14	104,113,123,136	0
8	MAN	H	4	11/12	0.85	0.10	86,88,97,97	0
7	BMA	G	3	11/12	0.86	0.10	88,94,105,110	0
8	MAN	H	7	11/12	0.87	0.12	89,93,101,107	0
7	MAN	G	6	11/12	0.87	0.12	85,91,95,101	0
8	MAN	H	10	11/12	0.89	0.12	87,88,90,93	0
8	NAG	H	2	14/15	0.89	0.08	94,102,105,118	0
8	MAN	H	5	11/12	0.90	0.10	80,86,94,100	0
8	BMA	H	3	11/12	0.90	0.08	83,89,96,96	0
7	NAG	G	2	14/15	0.90	0.09	77,87,100,110	0
8	NAG	H	1	14/15	0.93	0.09	87,96,99,101	0
7	NAG	G	1	14/15	0.95	0.06	75,86,100,106	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.

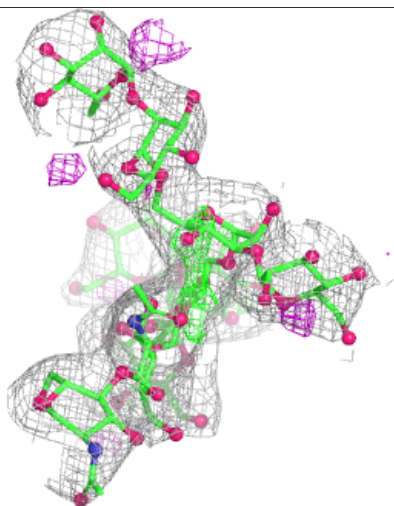
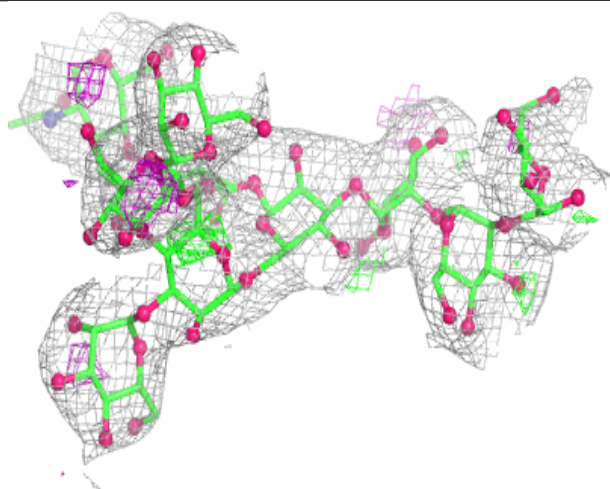
Electron density around Chain G:

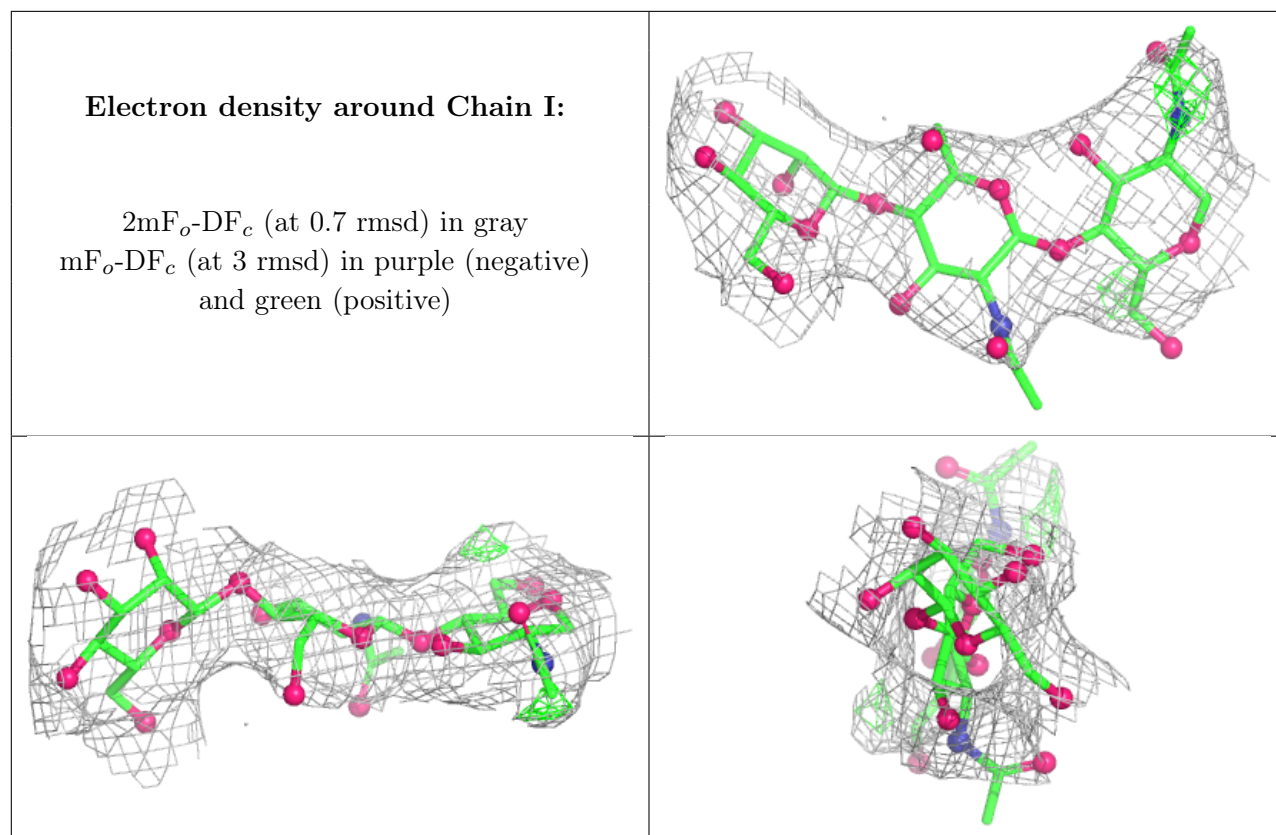
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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
11	NAG	E	525	14/15	0.58	0.11	148,154,164,165	0
11	NAG	E	526	14/15	0.63	0.09	114,126,132,132	0
11	NAG	E	524	14/15	0.68	0.09	120,142,156,156	0
11	NAG	E	527	14/15	0.81	0.08	115,135,142,144	0
10	PG4	C	301	13/13	0.87	0.13	85,107,121,123	0
11	NAG	E	523	14/15	0.88	0.07	86,91,97,100	0
11	NAG	E	522	14/15	0.92	0.07	100,107,112,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.