



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:02 PM UTC

PDB ID : 3H32 / pdb_00003h32
Title : Crystal structure of D-dimer from human fibrin complexed with Gly-His-Arg-Pro-Tyr-amide
Authors : Doolittle, R.F.; Pandi, L.
Deposited on : 2009-04-15
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

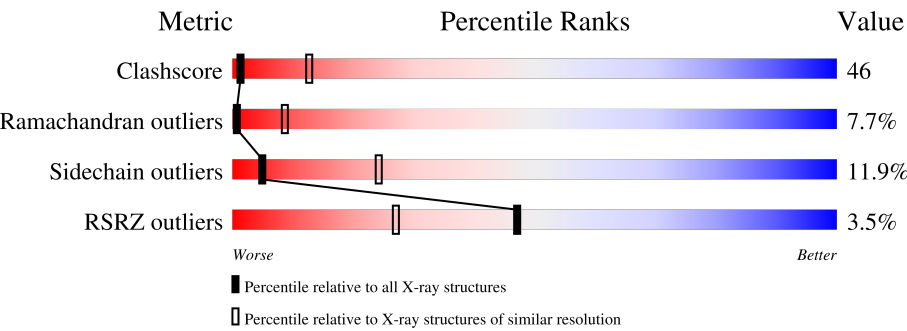
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	197	
1	D	197	
2	B	458	
2	E	458	
3	C	317	
3	F	317	
4	M	5	

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Mol	Chain	Length	Quality of chain
4	N	5	 60%40%
5	G	8	 75%25%
5	H	8	 50%50%

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
5	NAG	G	2	X	-	-	-
5	NAG	G	5	X	-	-	-
5	MAN	G	8	X	-	-	-
5	NAG	H	2	X	-	-	-
5	NAG	H	5	X	-	-	-
5	SIA	H	7	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11246 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	308	Total	C	N	O	S	0	0	0
			2474	1544	434	474	22			
2	E	308	Total	C	N	O	S	0	0	0
			2474	1544	434	474	22			

- Molecule 3 is a protein called Fibrinogen gamma chain, isoform gamma-A.

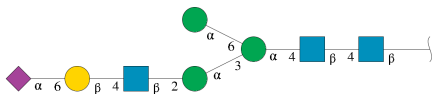
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	301	Total	C	N	O	S	0	0	0
			2404	1523	405	465	11			
3	F	296	Total	C	N	O	S	0	0	0
			2372	1504	400	457	11			

- Molecule 4 is a protein called Fibrin B knob pentapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	0
			45	28	10	7			
4	N	5	Total	C	N	O	0	0	0
			45	28	10	7			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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
5	G	8	Total	C	N	O	0	0	0
			106	59	4	43			
5	H	8	Total	C	N	O	0	0	0
			106	59	4	43			

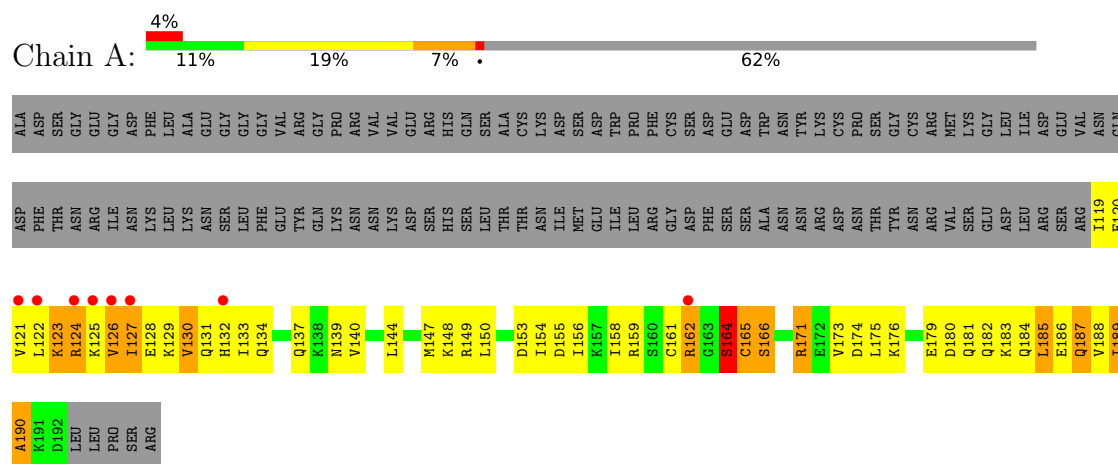
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

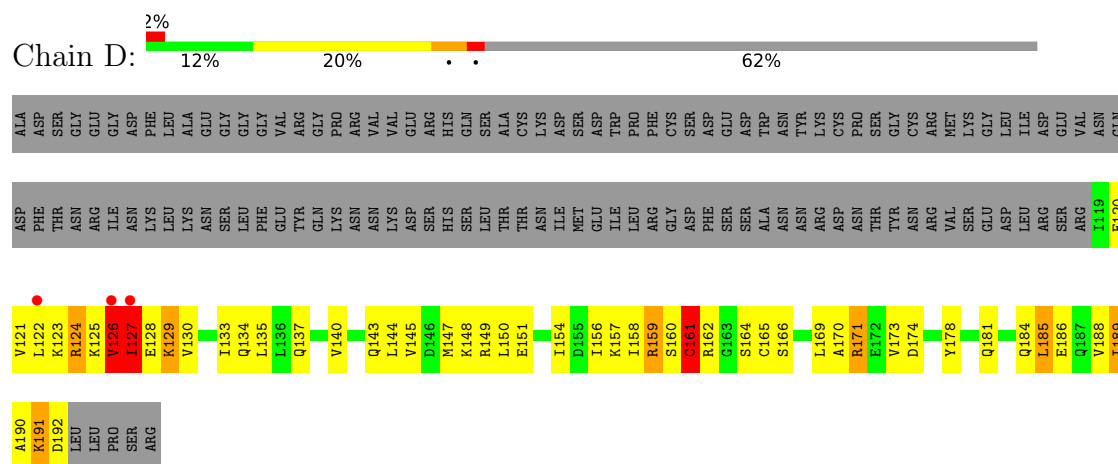
3 Residue-property plots

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.

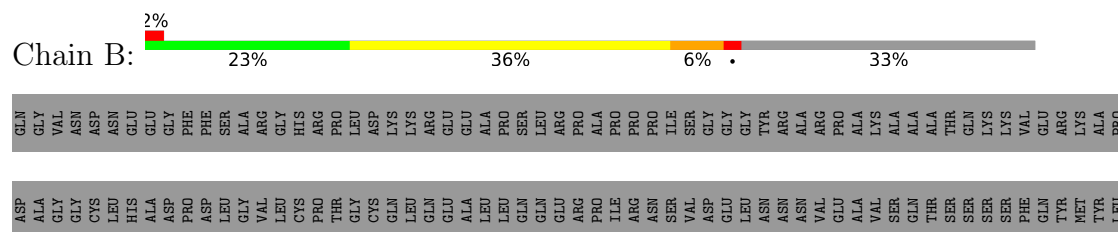
• Molecule 1: Fibrinogen alpha chain

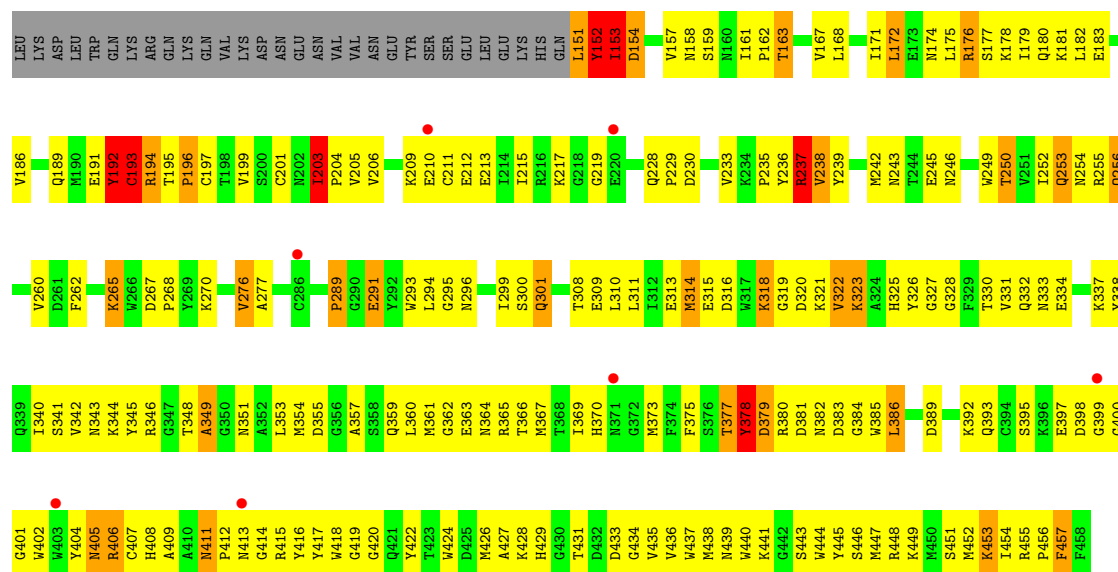


• Molecule 1: Fibrinogen alpha chain

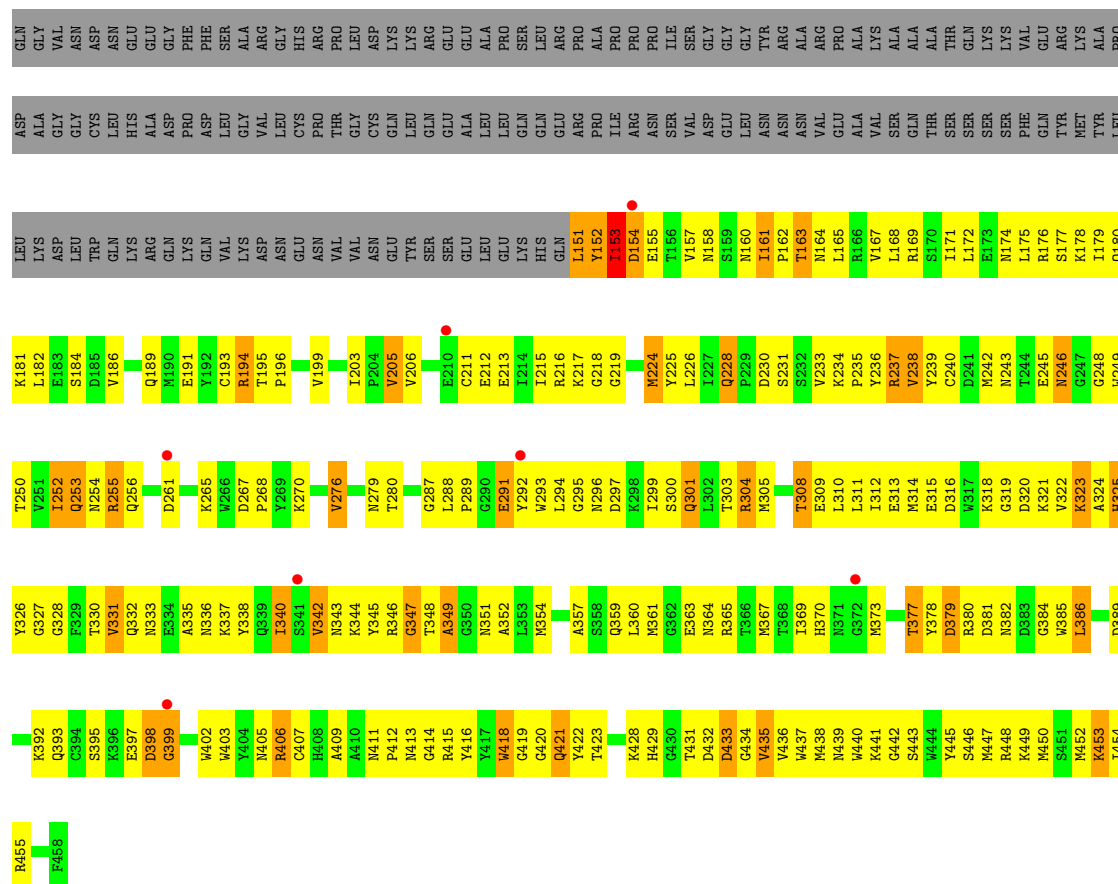
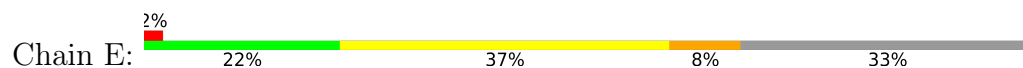


• Molecule 2: Fibrinogen beta chain



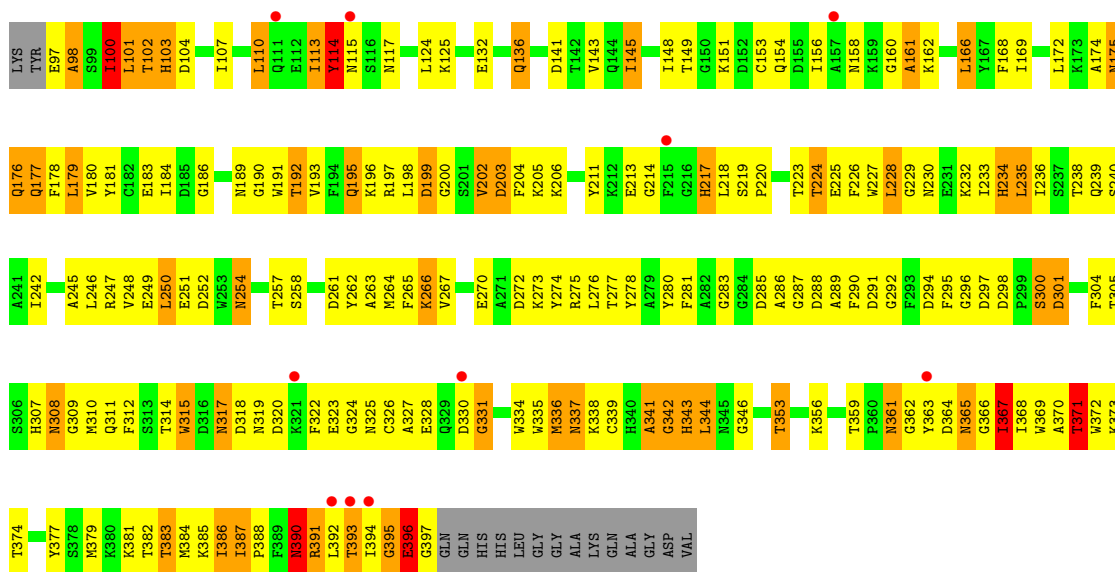


• Molecule 2: Fibrinogen beta chain

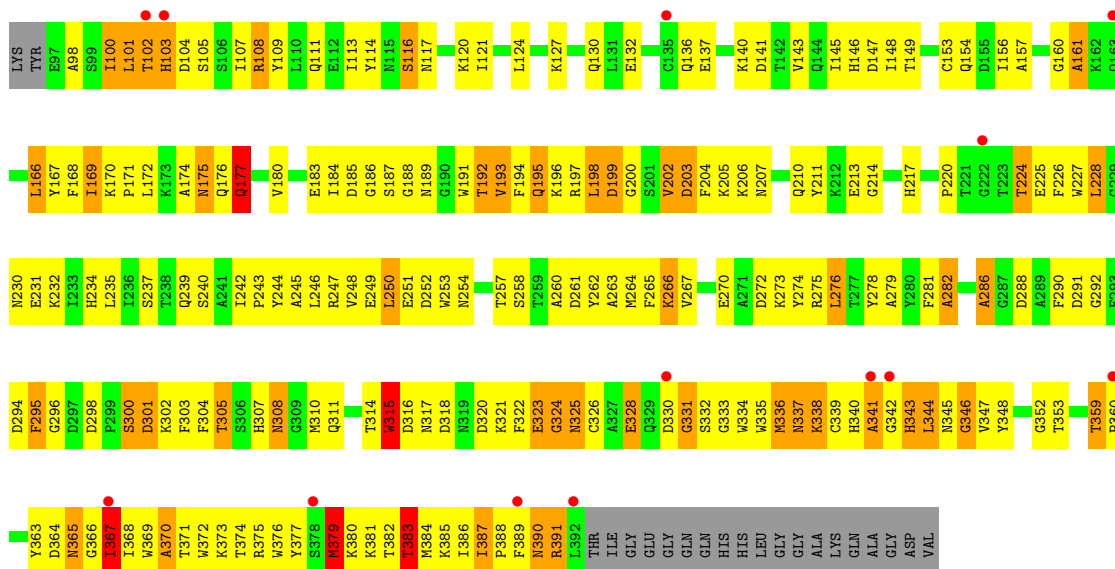


• Molecule 3: Fibrinogen gamma chain, isoform gamma-A





• Molecule 3: Fibrinogen gamma chain, isoform gamma-A



• Molecule 4: Fibrin B knob pentapeptide



• Molecule 4: Fibrin B knob pentapeptide



● Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  75% 25%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	ST17	MAN8
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● Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)] alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 50%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	ST17	MAN8
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.72Å 97.32Å 132.49Å 90.00° 122.78° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	75.5 (50.00-3.60) 75.6 (50.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	30.66 (at 3.55Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.320 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 12.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11246	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, GAL, MAN, SIA

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	1.04	4/609 (0.7%)	1.29	5/811 (0.6%)
1	D	0.91	2/609 (0.3%)	1.27	5/811 (0.6%)
2	B	0.73	1/2536 (0.0%)	1.08	13/3425 (0.4%)
2	E	0.78	2/2536 (0.1%)	1.07	16/3425 (0.5%)
3	C	0.73	2/2469 (0.1%)	1.01	7/3339 (0.2%)
3	F	0.68	1/2437 (0.0%)	1.02	10/3296 (0.3%)
4	M	0.58	0/47	0.95	0/61
4	N	0.65	0/47	0.88	0/61
All	All	0.76	12/11290 (0.1%)	1.07	56/15229 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	359	THR	CA-CB	7.34	1.63	1.53
1	D	126	VAL	CA-CB	7.30	1.64	1.54
1	A	127	ILE	CA-CB	6.99	1.64	1.54
1	A	126	VAL	CA-CB	6.91	1.63	1.54
2	E	361	MET	SD-CE	6.18	1.95	1.79
1	D	127	ILE	CA-CB	5.93	1.62	1.54
2	E	153	ILE	CA-CB	5.75	1.62	1.54
3	C	394	ILE	CA-CB	5.59	1.62	1.54
1	A	127	ILE	CA-C	5.32	1.59	1.52
2	B	153	ILE	CA-CB	5.27	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	102	THR	CA-CB	5.23	1.61	1.53
1	A	121	VAL	CA-CB	5.13	1.61	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	N-CA-C	12.84	124.81	111.07
1	D	124	ARG	N-CA-C	11.65	123.67	110.97
1	A	121	VAL	N-CA-C	10.45	121.27	110.72
2	B	154	ASP	N-CA-C	9.60	122.75	111.71
2	E	409	ALA	N-CA-C	-9.33	102.27	114.31
2	E	152	TYR	N-CA-C	8.70	125.37	113.37
3	C	102	THR	N-CA-C	8.57	122.23	111.69
2	B	409	ALA	N-CA-C	-7.98	101.28	113.89
2	E	154	ASP	N-CA-C	7.90	120.89	111.33
3	C	254	ASN	N-CA-C	-7.89	102.18	112.68
1	A	165	CYS	CA-CB-SG	-7.76	96.56	114.40
3	F	341	ALA	N-CA-C	-7.75	102.08	114.09
2	B	152	TYR	N-CA-C	7.53	122.66	113.17
2	E	228	GLN	CA-C-N	7.48	128.43	120.12
2	E	228	GLN	C-N-CA	7.48	128.43	120.12
2	E	194	ARG	N-CA-C	-7.21	104.23	113.16
3	C	156	ILE	N-CA-C	-7.09	103.61	110.42
2	E	406	ARG	N-CA-C	6.96	121.00	111.39
2	B	194	ARG	N-CA-C	-6.77	105.03	113.28
1	D	121	VAL	N-CA-C	6.69	119.46	111.09
3	F	359	THR	CA-C-N	6.52	126.29	119.05
3	F	359	THR	C-N-CA	6.52	126.29	119.05
3	F	380	LYS	N-CA-C	-6.49	104.55	113.18
3	F	286	ALA	N-CA-C	-6.33	106.15	114.31
2	B	318	LYS	N-CA-C	-6.32	105.89	113.97
1	D	127	ILE	N-CA-C	6.27	117.83	111.00
2	B	411	ASN	N-CA-C	6.14	120.95	110.02
2	B	406	ARG	N-CA-C	6.09	119.80	111.39
3	F	328	GLU	N-CA-C	-6.04	104.33	111.03
1	D	129	LYS	N-CA-C	6.01	119.81	112.23
2	E	155	GLU	N-CA-C	6.01	119.44	111.75
2	B	448	ARG	N-CA-C	-5.96	106.14	113.41
2	E	153	ILE	N-CA-C	5.90	121.61	109.34
2	B	192	TYR	N-CA-C	5.85	117.45	111.14
2	E	379	ASP	N-CA-C	-5.71	106.67	113.97
1	A	127	ILE	N-CA-C	5.67	117.59	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	341	ALA	N-CA-C	-5.63	104.99	113.89
3	F	338	LYS	N-CA-C	5.56	121.95	113.61
2	E	205	VAL	CB-CA-C	-5.48	104.65	112.22
3	C	100	ILE	N-CA-C	5.46	119.69	112.76
3	C	113	ILE	CB-CA-C	-5.41	104.99	112.24
2	E	448	ARG	N-CA-C	-5.41	106.84	113.50
1	A	130	VAL	N-CA-C	5.38	119.64	111.89
2	B	203	ILE	CA-C-N	5.27	125.03	119.76
2	B	203	ILE	C-N-CA	5.27	125.03	119.76
2	E	161	ILE	CB-CA-C	-5.24	108.72	113.70
2	B	153	ILE	N-CA-C	5.22	120.20	109.34
3	C	114	TYR	N-CA-C	-5.22	105.59	111.28
2	E	384	GLY	N-CA-C	-5.20	106.66	115.34
2	E	160	ASN	N-CA-C	5.19	117.93	111.24
3	F	193	VAL	N-CA-C	5.11	115.63	108.89
2	E	252	ILE	CB-CA-C	-5.06	106.61	111.06
3	F	116	SER	N-CA-C	-5.04	105.78	111.28
1	D	161	CYS	CA-CB-SG	5.03	125.98	114.40
2	B	379	ASP	N-CA-C	-5.03	107.69	113.88
3	F	323	GLU	N-CA-C	-5.01	105.33	111.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	192	TYR	Sidechain

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	608	0	649	66	0
1	D	608	0	649	63	0
2	B	2474	0	2336	211	0
2	E	2474	0	2336	243	0
3	C	2404	0	2249	245	0
3	F	2372	0	2219	260	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	45	0	41	5	0
4	N	45	0	41	5	0
5	G	106	0	89	5	0
5	H	106	0	89	6	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	11246	0	10698	1006	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 46.

All (1006) 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)
3:F:228:LEU:HG	3:F:232:LYS:HD2	1.22	1.15
2:E:415:ARG:H	2:E:434:GLY:HA2	0.98	1.14
3:F:338:LYS:N	3:F:339:CYS:HA	1.70	1.07
3:C:166:LEU:HD12	3:C:166:LEU:H	1.20	1.07
3:C:305:THR:HB	3:C:341:ALA:HB2	1.37	1.07
2:B:415:ARG:H	2:B:434:GLY:HA2	1.20	1.05
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.37	1.02
3:C:338:LYS:N	3:C:339:CYS:HA	1.78	0.98
2:E:300:SER:HA	2:E:331:VAL:HG23	1.44	0.98
3:F:196:LYS:HD2	3:F:383:THR:HB	1.47	0.97
2:B:203:ILE:H	2:B:203:ILE:HD12	1.29	0.94
2:E:415:ARG:N	2:E:434:GLY:HA2	1.82	0.94
3:F:197:ARG:HA	3:F:225:GLU:HG2	1.50	0.93
1:A:123:LYS:HZ2	2:B:151:LEU:HB3	1.34	0.92
1:A:123:LYS:NZ	2:B:151:LEU:HB3	1.84	0.92
5:G:6:GAL:H4	5:G:7:SIA:H8	1.51	0.92
5:H:6:GAL:H4	5:H:7:SIA:H6	1.51	0.92
3:C:174:ALA:HB2	3:C:235:LEU:HD22	1.49	0.92
2:B:309:GLU:HB3	2:B:327:GLY:HA2	1.52	0.91
2:E:203:ILE:HD12	2:E:203:ILE:H	1.34	0.91
3:F:305:THR:HB	3:F:341:ALA:HB2	1.53	0.91
2:E:228:GLN:HE22	3:F:177:GLN:HE22	1.19	0.89
2:B:380:ARG:NH2	2:B:382:ASN:HD21	1.70	0.89
1:D:147:MET:HE1	2:E:179:ILE:HD11	1.53	0.88
1:D:181:GLN:NE2	2:E:171:ILE:HA	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:SER:HA	2:B:331:VAL:HG23	1.53	0.88
1:D:154:ILE:O	1:D:158:ILE:HG12	1.73	0.87
1:D:169:LEU:H	2:E:189:GLN:HE22	1.20	0.87
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.55	0.87
3:C:334:TRP:CD1	3:C:335:TRP:H	1.92	0.86
2:B:252:ILE:HD11	2:B:299:ILE:HG12	1.57	0.86
3:C:325:ASN:HD21	3:C:328:GLU:HB2	1.40	0.86
1:D:186:GLU:HA	1:D:189:ILE:HD11	1.57	0.86
2:B:158:ASN:O	2:B:162:PRO:HG2	1.75	0.85
3:C:191:TRP:HA	3:C:387:ILE:HD13	1.60	0.84
2:B:359:GLN:C	2:B:360:LEU:HD12	2.02	0.84
3:F:249:GLU:HB3	3:F:383:THR:HG23	1.60	0.84
3:C:264:MET:HE3	3:C:266:LYS:NZ	1.92	0.83
5:H:3:MAN:H4	5:H:8:MAN:H2	1.61	0.83
1:D:169:LEU:H	2:E:189:GLN:NE2	1.76	0.83
3:F:367:ILE:HD13	3:F:367:ILE:H	1.44	0.83
3:C:107:ILE:HA	3:C:110:LEU:HD23	1.62	0.82
3:C:287:GLY:HA3	3:C:371:THR:HB	1.59	0.82
1:D:120:GLU:HG2	1:D:124:ARG:HD2	1.58	0.82
2:B:293:TRP:HE1	2:B:296:ASN:ND2	1.77	0.82
3:F:251:GLU:HB2	3:F:257:THR:HG22	1.61	0.82
2:E:191:GLU:O	2:E:194:ARG:HG2	1.79	0.82
3:C:166:LEU:HD12	3:C:166:LEU:N	1.95	0.82
2:E:386:LEU:HD23	2:E:386:LEU:H	1.43	0.81
3:C:288:ASP:OD2	3:C:291:ASP:HB2	1.79	0.81
3:F:240:SER:HB2	3:F:242:ILE:HG12	1.62	0.81
3:C:110:LEU:HD22	3:C:110:LEU:H	1.43	0.81
1:D:181:GLN:HE21	2:E:171:ILE:HA	1.43	0.80
3:F:166:LEU:N	3:F:166:LEU:HD12	1.95	0.80
2:E:436:VAL:HG12	2:E:445:TYR:O	1.80	0.80
2:B:315:GLU:HB3	2:B:321:LYS:HG2	1.64	0.80
1:A:186:GLU:HA	1:A:189:ILE:HD11	1.64	0.80
3:C:192:THR:HG23	3:C:386:ILE:HG23	1.61	0.80
2:B:370:HIS:CE1	2:B:402:TRP:HE1	1.99	0.79
1:D:151:GLU:HG3	1:D:173:VAL:HG13	1.63	0.79
3:C:338:LYS:H	3:C:339:CYS:HA	1.45	0.79
2:B:386:LEU:H	2:B:386:LEU:HD23	1.47	0.79
2:B:318:LYS:HD2	2:B:320:ASP:OD2	1.83	0.78
1:D:159:ARG:HG2	1:D:159:ARG:HH11	1.48	0.78
2:E:252:ILE:HD11	2:E:299:ILE:HG12	1.66	0.78
3:F:192:THR:HG23	3:F:386:ILE:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:GLN:HA	2:B:183:GLU:OE2	1.85	0.77
3:C:367:ILE:HD13	3:C:367:ILE:H	1.49	0.77
3:C:110:LEU:HD22	3:C:110:LEU:N	1.99	0.77
2:B:295:GLY:O	2:B:299:ILE:HG13	1.85	0.76
2:E:295:GLY:O	2:E:299:ILE:HG13	1.84	0.76
3:F:334:TRP:CD1	3:F:335:TRP:H	2.04	0.76
2:B:201:CYS:O	3:C:143:VAL:HG21	1.86	0.76
3:C:98:ALA:O	3:C:101:LEU:HG	1.85	0.76
3:C:286:ALA:O	3:C:372:TRP:HB2	1.86	0.76
3:F:171:PRO:HA	3:F:239:GLN:HE22	1.50	0.75
3:F:338:LYS:H	3:F:339:CYS:HA	1.48	0.75
2:E:309:GLU:HB3	2:E:327:GLY:HA2	1.67	0.75
2:B:438:MET:HE1	4:M:1:GLY:H2	1.52	0.75
3:C:264:MET:HE3	3:C:266:LYS:CE	2.16	0.75
3:F:264:MET:HE3	3:F:266:LYS:HE2	1.66	0.75
2:E:415:ARG:H	2:E:434:GLY:CA	1.90	0.75
2:E:313:GLU:HA	2:E:323:LYS:HB3	1.69	0.75
3:C:310:MET:HE3	3:C:337:ASN:ND2	2.02	0.74
2:E:406:ARG:HG3	4:N:3:ARG:HB2	1.69	0.74
2:B:389:ASP:OD2	2:B:392:LYS:HG3	1.86	0.74
1:A:149:ARG:HD3	2:B:427:ALA:O	1.88	0.74
2:E:238:VAL:HG22	2:E:239:TYR:H	1.52	0.74
2:E:270:LYS:HG3	2:E:338:TYR:OH	1.88	0.73
2:B:440:TRP:O	2:B:441:LYS:HE2	1.88	0.73
3:C:97:GLU:OE1	3:C:100:ILE:HG12	1.89	0.73
2:E:414:GLY:H	2:E:435:VAL:HG23	1.54	0.73
2:E:242:MET:SD	2:E:248:GLY:HA2	2.28	0.72
2:E:406:ARG:N	2:E:407:CYS:HA	2.03	0.72
2:B:230:ASP:HB3	2:B:233:VAL:HG12	1.71	0.72
3:C:228:LEU:HG	3:C:232:LYS:HD2	1.70	0.72
2:E:343:ASN:ND2	2:E:344:LYS:HG2	2.05	0.72
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.04	0.72
3:F:166:LEU:HD12	3:F:166:LEU:H	1.52	0.72
3:C:251:GLU:HB2	3:C:257:THR:HG22	1.72	0.72
3:F:382:THR:HG22	3:F:383:THR:H	1.54	0.72
2:E:315:GLU:HB3	2:E:321:LYS:HG2	1.71	0.72
3:F:311:GLN:O	3:F:335:TRP:HA	1.90	0.71
3:C:367:ILE:HG12	3:C:379:MET:H	1.55	0.71
1:A:147:MET:HE1	2:B:179:ILE:HD11	1.71	0.71
2:B:203:ILE:H	2:B:203:ILE:CD1	2.02	0.71
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PRO:O	2:B:413:ASN:HB2	1.88	0.71
2:E:359:GLN:C	2:E:360:LEU:HD12	2.13	0.71
3:F:156:ILE:HG22	3:F:161:ALA:CB	2.19	0.71
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.72	0.71
2:B:406:ARG:N	2:B:407:CYS:HA	2.04	0.71
2:B:203:ILE:HD12	2:B:203:ILE:N	2.04	0.71
3:C:214:GLY:HA3	3:C:228:LEU:O	1.90	0.71
2:B:308:THR:HG22	2:B:309:GLU:N	2.06	0.70
2:B:351:ASN:ND2	2:B:354:MET:HG2	2.07	0.70
3:F:321:LYS:HB2	3:F:337:ASN:OD1	1.90	0.70
2:E:389:ASP:OD2	2:E:392:LYS:HG3	1.90	0.70
3:F:308:ASN:C	3:F:308:ASN:HD22	1.99	0.70
5:G:3:MAN:H2	5:G:4:MAN:O6	1.91	0.70
3:C:132:GLU:O	3:C:136:GLN:HB2	1.92	0.70
3:F:244:TYR:HA	3:F:388:PRO:HA	1.72	0.69
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.72	0.69
2:B:424:TRP:CH2	5:G:7:SIA:H92	2.27	0.69
2:E:182:LEU:O	2:E:186:VAL:HG23	1.92	0.69
1:A:123:LYS:HZ2	2:B:151:LEU:HD13	1.56	0.69
3:C:169:ILE:O	3:C:177:GLN:HB3	1.92	0.69
2:E:316:ASP:OD1	2:E:318:LYS:HB3	1.92	0.69
3:C:264:MET:HE3	3:C:266:LYS:HE2	1.73	0.69
3:F:171:PRO:HA	3:F:239:GLN:NE2	2.08	0.69
3:F:276:LEU:HD23	3:F:276:LEU:O	1.92	0.69
5:H:2:NAG:H3	5:H:2:NAG:H83	1.73	0.69
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.74	0.69
3:C:195:GLN:OE1	3:C:197:ARG:HG3	1.93	0.68
2:B:191:GLU:HG3	2:B:194:ARG:NH2	2.08	0.68
1:D:150:LEU:HD11	3:F:121:ILE:HG23	1.76	0.68
3:F:180:VAL:HG12	3:F:228:LEU:HD11	1.75	0.68
1:A:128:GLU:HG3	1:A:129:LYS:HD3	1.74	0.68
1:A:129:LYS:O	1:A:132:HIS:ND1	2.27	0.68
3:C:145:ILE:HD12	3:C:145:ILE:O	1.94	0.68
5:H:6:GAL:H4	5:H:7:SIA:C6	2.21	0.68
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.76	0.68
3:F:305:THR:HB	3:F:341:ALA:CB	2.24	0.68
3:F:192:THR:HG23	3:F:386:ILE:HG23	1.75	0.68
3:F:294:ASP:HA	3:F:301:ASP:HB3	1.76	0.68
2:E:454:ILE:C	2:E:454:ILE:HD12	2.19	0.68
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.29	0.68
3:C:373:LYS:HB3	3:C:377:TYR:HD2	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ARG:CG	4:N:3:ARG:HB2	2.24	0.67
2:E:414:GLY:H	2:E:435:VAL:CG2	2.07	0.67
3:F:325:ASN:HD21	3:F:328:GLU:HB2	1.59	0.67
5:G:7:SIA:H112	5:G:7:SIA:H6	1.76	0.67
2:E:412:PRO:O	2:E:413:ASN:HB2	1.93	0.67
3:F:109:TYR:O	3:F:113:ILE:HG23	1.95	0.67
1:D:140:VAL:HG21	1:D:185:LEU:HD21	1.77	0.67
2:B:189:GLN:OE1	2:B:192:TYR:HB2	1.94	0.67
2:B:343:ASN:ND2	2:B:344:LYS:HG2	2.10	0.67
2:E:324:ALA:HB1	2:E:326:TYR:HE1	1.59	0.67
2:E:237:ARG:HD3	2:E:276:VAL:HG21	1.77	0.67
3:C:190:GLY:O	3:C:387:ILE:HD11	1.95	0.67
3:C:276:LEU:HB2	3:C:335:TRP:NE1	2.09	0.67
2:E:176:ARG:HG2	3:F:120:LYS:NZ	2.10	0.67
2:E:255:ARG:HA	2:E:291:GLU:HG2	1.77	0.66
3:C:304:PHE:O	3:C:338:LYS:HB2	1.96	0.66
2:B:277:ALA:HA	2:B:289:PRO:O	1.95	0.66
2:B:447:MET:N	2:B:447:MET:HE2	2.11	0.66
2:E:238:VAL:HG22	2:E:239:TYR:N	2.08	0.66
3:F:246:LEU:HD12	3:F:247:ARG:N	2.10	0.66
3:C:326:CYS:HB2	3:C:336:MET:HG3	1.77	0.66
2:E:228:GLN:HB2	2:E:235:PRO:HG3	1.78	0.66
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.31	0.65
3:F:338:LYS:N	3:F:339:CYS:CA	2.56	0.65
3:F:343:HIS:O	3:F:343:HIS:ND1	2.29	0.65
3:F:387:ILE:HG13	3:F:388:PRO:HD2	1.78	0.65
3:F:195:GLN:NE2	3:F:384:MET:HG3	2.11	0.65
2:B:296:ASN:HA	2:B:299:ILE:HD12	1.78	0.65
3:C:110:LEU:H	3:C:110:LEU:CD2	2.10	0.65
3:C:149:THR:HG23	3:C:168:PHE:C	2.22	0.65
3:C:166:LEU:H	3:C:166:LEU:CD1	2.02	0.65
2:E:203:ILE:HG21	2:E:226:LEU:HD22	1.79	0.65
3:F:336:MET:HB3	3:F:339:CYS:HB3	1.77	0.65
2:E:333:ASN:HD21	2:E:335:ALA:HB3	1.62	0.65
3:F:251:GLU:CB	3:F:257:THR:HG22	2.27	0.65
2:B:238:VAL:HG22	2:B:239:TYR:N	2.12	0.64
3:C:211:TYR:HB3	3:C:230:ASN:HD21	1.61	0.64
1:D:189:ILE:H	1:D:191:LYS:NZ	1.93	0.64
3:C:153:CYS:HB2	3:C:192:THR:HB	1.77	0.64
2:B:415:ARG:N	2:B:434:GLY:HA2	2.04	0.64
3:C:334:TRP:CH2	3:C:344:LEU:HG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:324:GLY:O	3:F:326:CYS:N	2.29	0.64
2:B:377:THR:C	2:B:379:ASP:H	2.04	0.64
1:A:128:GLU:HG3	1:A:129:LYS:CD	2.28	0.64
2:B:211:CYS:SG	2:B:250:THR:HA	2.38	0.64
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.80	0.64
2:E:380:ARG:NH2	2:E:382:ASN:HD21	1.96	0.64
1:A:186:GLU:O	1:A:189:ILE:HG12	1.97	0.64
3:F:192:THR:O	3:F:386:ILE:HG22	1.98	0.64
3:F:153:CYS:SG	3:F:192:THR:HB	2.37	0.64
1:D:147:MET:HE3	2:E:175:LEU:HD22	1.80	0.63
3:F:107:ILE:HB	3:F:108:ARG:HH12	1.63	0.63
1:D:123:LYS:HD3	2:E:151:LEU:N	2.13	0.63
2:E:310:LEU:HD12	2:E:453:LYS:O	1.97	0.63
3:C:310:MET:HE3	3:C:337:ASN:HD21	1.63	0.63
3:C:356:LYS:HG3	3:C:362:GLY:O	1.98	0.63
1:A:189:ILE:HG22	1:A:190:ALA:N	2.12	0.63
3:C:174:ALA:HB2	3:C:235:LEU:CD2	2.25	0.63
3:C:392:LEU:HD13	3:C:397:GLY:HA2	1.81	0.63
1:D:169:LEU:HD12	1:D:171:ARG:HG2	1.80	0.63
3:C:346:GLY:HA3	3:C:366:GLY:H	1.64	0.62
2:B:252:ILE:HD12	2:B:294:LEU:HB3	1.80	0.62
2:B:314:MET:HA	2:B:449:LYS:O	1.99	0.62
2:E:318:LYS:HD2	2:E:320:ASP:OD2	1.99	0.62
1:D:140:VAL:CG2	1:D:185:LEU:HD21	2.29	0.62
3:F:170:LYS:HE3	3:F:175:ASN:HA	1.82	0.62
3:C:198:LEU:O	3:C:199:ASP:C	2.43	0.62
2:E:421:GLN:HG3	2:E:422:TYR:N	2.14	0.62
2:B:386:LEU:HD23	2:B:386:LEU:N	2.13	0.62
3:C:382:THR:HG22	3:C:383:THR:N	2.15	0.62
2:E:415:ARG:HH12	2:E:428:LYS:HB2	1.64	0.62
2:E:213:GLU:O	2:E:217:LYS:HG3	1.99	0.62
3:F:234:HIS:HA	3:F:267:VAL:HG23	1.81	0.62
3:F:365:ASN:C	3:F:365:ASN:HD22	2.06	0.62
3:C:178:PHE:CD2	3:C:232:LYS:HD3	2.35	0.61
2:B:172:LEU:HD22	3:C:113:ILE:HG13	1.79	0.61
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.00	0.61
3:C:166:LEU:HD11	3:C:220:PRO:HG3	1.81	0.61
2:B:415:ARG:HG3	2:B:415:ARG:HH11	1.64	0.61
2:E:351:ASN:ND2	2:E:354:MET:HG2	2.15	0.61
2:B:345:TYR:O	2:B:346:ARG:HG3	2.00	0.61
3:C:263:ALA:O	3:C:278:TYR:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:270:GLU:HB2	3:C:274:TYR:OH	2.00	0.61
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.83	0.61
2:B:296:ASN:HD22	2:B:299:ILE:HD12	1.66	0.61
3:C:258:SER:HA	3:C:285:ASP:OD1	2.00	0.61
3:F:205:LYS:HG2	3:F:331:GLY:O	2.01	0.61
2:B:191:GLU:O	2:B:194:ARG:HG2	2.00	0.61
3:C:265:PHE:O	3:C:266:LYS:HB3	2.00	0.61
3:C:323:GLU:HG2	3:C:324:GLY:H	1.65	0.61
3:F:156:ILE:HG22	3:F:161:ALA:HB2	1.82	0.61
3:C:344:LEU:C	3:C:367:ILE:HG22	2.26	0.61
2:E:163:THR:O	2:E:167:VAL:HG23	2.00	0.61
2:E:246:ASN:HB3	2:E:455:ARG:HH12	1.66	0.61
3:F:368:ILE:HG13	3:F:368:ILE:O	1.99	0.61
3:C:344:LEU:CA	3:C:367:ILE:HG22	2.31	0.60
3:C:143:VAL:HA	3:C:220:PRO:HG2	1.83	0.60
1:D:181:GLN:HE22	2:E:174:ASN:HB3	1.64	0.60
3:F:197:ARG:HG3	3:F:382:THR:HB	1.83	0.60
2:B:237:ARG:HD3	2:B:276:VAL:HG21	1.81	0.60
3:F:156:ILE:O	3:F:161:ALA:HB3	2.01	0.60
3:C:305:THR:HG23	3:C:338:LYS:HD2	1.84	0.60
3:F:196:LYS:CD	3:F:383:THR:HB	2.28	0.60
1:D:185:LEU:HD23	2:E:171:ILE:HD13	1.84	0.60
2:E:158:ASN:O	2:E:162:PRO:HG2	2.02	0.60
3:F:154:GLN:HB2	3:F:387:ILE:HD11	1.83	0.60
1:D:166:SER:HB3	2:E:195:THR:O	2.01	0.59
2:E:393:GLN:O	2:E:397:GLU:HG2	2.00	0.59
2:E:175:LEU:O	2:E:179:ILE:HG13	2.03	0.59
3:F:264:MET:O	3:F:264:MET:HG2	2.01	0.59
4:M:2:HIS:O	4:M:3:ARG:HD3	2.03	0.59
1:A:166:SER:HB3	2:B:195:THR:O	2.03	0.59
3:C:323:GLU:HG2	3:C:324:GLY:N	2.18	0.59
3:F:305:THR:CB	3:F:341:ALA:HB2	2.30	0.59
2:B:345:TYR:CG	2:B:346:ARG:N	2.71	0.59
2:B:357:ALA:HB3	2:B:360:LEU:HD13	1.84	0.59
2:B:385:TRP:CH2	2:B:392:LYS:HB3	2.38	0.59
1:D:140:VAL:HG11	2:E:168:LEU:HD22	1.84	0.59
2:E:326:TYR:HA	2:E:344:LYS:O	2.03	0.59
3:F:252:ASP:HB3	3:F:373:LYS:NZ	2.18	0.59
2:E:340:ILE:HG23	2:E:340:ILE:O	2.02	0.59
1:A:126:VAL:HG22	2:B:154:ASP:HA	1.84	0.59
3:F:108:ARG:HH11	3:F:108:ARG:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HZ2	1:A:179:GLU:HG3	1.68	0.59
2:E:421:GLN:HG3	2:E:422:TYR:H	1.67	0.59
3:F:252:ASP:HB3	3:F:373:LYS:HZ1	1.68	0.59
2:B:293:TRP:NE1	2:B:296:ASN:ND2	2.48	0.59
3:C:234:HIS:HA	3:C:267:VAL:HG23	1.85	0.59
2:B:300:SER:HA	2:B:331:VAL:CG2	2.31	0.58
1:D:169:LEU:N	2:E:189:GLN:HE22	1.96	0.58
1:A:127:ILE:O	1:A:130:VAL:HG22	2.04	0.58
1:A:171:ARG:NH1	1:A:173:VAL:HG22	2.18	0.58
2:E:177:SER:O	2:E:180:GLN:HG3	2.02	0.58
2:B:380:ARG:HG2	2:B:380:ARG:HH11	1.68	0.58
3:C:149:THR:HG23	3:C:168:PHE:O	2.04	0.58
3:C:193:VAL:HG12	3:C:385:LYS:HG2	1.85	0.58
3:F:246:LEU:HD12	3:F:247:ARG:H	1.69	0.58
2:B:326:TYR:C	2:B:328:GLY:H	2.10	0.58
3:C:342:GLY:HA2	3:C:368:ILE:HD12	1.85	0.58
3:C:197:ARG:O	3:C:381:LYS:HA	2.03	0.58
2:E:199:VAL:O	3:F:141:ASP:HA	2.04	0.58
2:E:304:ARG:HD3	2:E:332:GLN:NE2	2.19	0.58
2:E:357:ALA:HB3	2:E:360:LEU:HD13	1.85	0.58
2:B:310:LEU:HD12	2:B:311:LEU:H	1.68	0.58
1:A:123:LYS:NZ	2:B:151:LEU:HD13	2.19	0.58
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.68	0.58
2:B:300:SER:CA	2:B:331:VAL:HG23	2.28	0.58
3:C:338:LYS:O	3:C:338:LYS:HG2	2.04	0.58
2:E:405:ASN:CG	2:E:405:ASN:O	2.43	0.58
1:D:169:LEU:C	1:D:169:LEU:HD13	2.28	0.57
2:B:255:ARG:HE	2:B:435:VAL:HG21	1.69	0.57
3:F:325:ASN:CG	3:F:325:ASN:O	2.47	0.57
3:C:191:TRP:CZ3	3:C:387:ILE:HB	2.38	0.57
2:B:199:VAL:O	3:C:141:ASP:HA	2.03	0.57
2:B:354:MET:HA	2:B:369:ILE:HG23	1.86	0.57
3:C:276:LEU:HB2	3:C:335:TRP:CE2	2.40	0.57
3:F:263:ALA:O	3:F:278:TYR:HB2	2.03	0.57
1:A:123:LYS:HZ2	2:B:151:LEU:CB	2.12	0.57
3:C:334:TRP:CD1	3:C:335:TRP:N	2.71	0.57
2:E:215:ILE:HG23	2:E:216:ARG:N	2.20	0.57
2:B:256:GLN:N	2:B:291:GLU:OE2	2.36	0.57
2:E:351:ASN:HD21	2:E:354:MET:HG2	1.70	0.57
2:E:436:VAL:HG12	2:E:445:TYR:C	2.30	0.57
3:C:246:LEU:O	3:C:261:ASP:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LYS:O	2:B:377:THR:HG21	2.05	0.56
1:D:186:GLU:O	1:D:189:ILE:HG12	2.05	0.56
2:B:172:LEU:HD13	3:C:113:ILE:HD11	1.88	0.56
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.87	0.56
3:F:249:GLU:HB3	3:F:383:THR:CG2	2.34	0.56
2:E:301:GLN:O	2:E:305:MET:HG3	2.05	0.56
2:E:420:GLY:O	2:E:445:TYR:HA	2.06	0.56
2:E:236:TYR:CE2	2:E:294:LEU:HD21	2.41	0.56
3:F:114:TYR:O	3:F:117:ASN:HB2	2.06	0.56
1:D:159:ARG:HG2	1:D:159:ARG:NH1	2.17	0.56
3:F:338:LYS:CG	3:F:338:LYS:O	2.54	0.56
3:C:252:ASP:C	3:C:254:ASN:H	2.14	0.56
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.88	0.56
3:F:197:ARG:O	3:F:381:LYS:HA	2.05	0.56
3:F:288:ASP:CG	3:F:291:ASP:HB2	2.30	0.56
3:C:246:LEU:HD12	3:C:247:ARG:N	2.21	0.56
1:D:164:SER:O	2:E:196:PRO:HA	2.05	0.56
1:D:147:MET:CE	2:E:179:ILE:HD11	2.33	0.56
2:E:377:THR:C	2:E:379:ASP:H	2.14	0.56
3:F:103:HIS:HD2	3:F:104:ASP:H	1.54	0.56
2:B:293:TRP:HE1	2:B:296:ASN:HD21	1.51	0.55
2:B:310:LEU:HD12	2:B:311:LEU:N	2.21	0.55
2:B:331:VAL:HG23	2:B:331:VAL:O	2.06	0.55
2:B:210:GLU:OE1	2:B:456:PRO:HG3	2.06	0.55
3:C:160:GLY:O	3:C:161:ALA:O	2.23	0.55
2:E:310:LEU:CD2	2:E:312:ILE:HD11	2.37	0.55
3:F:300:SER:HB3	3:F:304:PHE:HD2	1.71	0.55
3:F:338:LYS:O	3:F:338:LYS:HG2	2.06	0.55
2:B:230:ASP:HB3	2:B:233:VAL:CG1	2.35	0.55
3:C:240:SER:HB2	3:C:242:ILE:HG12	1.87	0.55
1:D:125:LYS:O	1:D:129:LYS:HG2	2.07	0.55
3:F:325:ASN:ND2	3:F:328:GLU:HB2	2.21	0.55
2:B:385:TRP:CZ2	2:B:392:LYS:HB3	2.41	0.55
3:C:334:TRP:CD2	3:C:343:HIS:HB2	2.41	0.55
3:F:348:TYR:HA	3:F:367:ILE:HD11	1.88	0.55
2:B:250:THR:HB	2:B:454:ILE:HG13	1.87	0.55
3:C:297:ASP:O	3:C:298:ASP:HB2	2.05	0.55
3:C:298:ASP:C	3:C:300:SER:H	2.12	0.55
3:F:367:ILE:HG12	3:F:379:MET:H	1.71	0.55
3:C:318:ASP:OD1	3:C:325:ASN:HA	2.07	0.55
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:246:LEU:O	3:F:261:ASP:HA	2.07	0.55
1:D:127:ILE:O	1:D:130:VAL:HG22	2.06	0.55
2:E:326:TYR:C	2:E:328:GLY:H	2.13	0.55
3:F:174:ALA:HB2	3:F:235:LEU:HD22	1.88	0.55
1:A:175:LEU:HD21	2:B:426:MET:HE1	1.89	0.55
2:B:177:SER:O	2:B:180:GLN:HG3	2.07	0.55
2:B:212:GLU:O	2:B:215:ILE:HG22	2.06	0.55
3:C:100:ILE:O	3:C:102:THR:N	2.40	0.55
3:C:225:GLU:O	3:C:226:PHE:HB3	2.06	0.55
2:E:370:HIS:O	2:E:373:MET:HG2	2.06	0.55
3:C:205:LYS:HG2	3:C:331:GLY:O	2.06	0.55
1:A:133:ILE:HG23	3:C:107:ILE:HD11	1.88	0.55
2:E:217:LYS:HD3	3:F:213:GLU:HG3	1.88	0.55
3:F:270:GLU:HB2	3:F:274:TYR:OH	2.06	0.55
3:C:211:TYR:HB3	3:C:230:ASN:ND2	2.23	0.54
1:D:147:MET:HE1	3:F:121:ILE:HD11	1.89	0.54
2:E:230:ASP:HB3	2:E:233:VAL:HG12	1.87	0.54
2:E:252:ILE:HD11	2:E:299:ILE:CG1	2.36	0.54
3:F:253:TRP:CD1	3:F:352:GLY:HA3	2.42	0.54
2:B:252:ILE:CD1	2:B:294:LEU:HB3	2.37	0.54
3:C:270:GLU:HB2	3:C:274:TYR:CZ	2.43	0.54
3:C:390:ASN:HD22	3:C:391:ARG:N	2.05	0.54
1:D:147:MET:CE	3:F:121:ILE:HD11	2.38	0.54
3:F:207:ASN:HB2	3:F:316:ASP:OD2	2.05	0.54
2:E:250:THR:HB	2:E:454:ILE:HG13	1.89	0.54
2:E:345:TYR:CG	2:E:346:ARG:N	2.75	0.54
3:F:169:ILE:O	3:F:177:GLN:HB3	2.07	0.54
3:F:334:TRP:CD2	3:F:343:HIS:HB2	2.43	0.54
2:E:402:TRP:CG	2:E:403:TRP:N	2.76	0.54
3:F:198:LEU:H	3:F:225:GLU:CG	2.20	0.54
3:F:262:TYR:HD2	3:F:278:TYR:CE1	2.25	0.54
1:D:126:VAL:HG22	2:E:154:ASP:HA	1.88	0.54
2:E:314:MET:SD	2:E:450:MET:HE1	2.47	0.54
1:A:148:LYS:NZ	1:A:182:GLN:HE22	2.06	0.54
2:E:340:ILE:HG12	2:E:342:VAL:HG13	1.90	0.54
2:B:203:ILE:HB	3:C:179:LEU:HD22	1.90	0.54
2:B:360:LEU:HB2	2:B:365:ARG:HB2	1.89	0.54
3:C:184:ILE:HG23	3:C:189:ASN:O	2.07	0.54
3:F:117:ASN:O	3:F:121:ILE:HG13	2.08	0.54
1:A:120:GLU:OE2	1:A:125:LYS:HE3	2.08	0.53
2:E:435:VAL:O	2:E:446:SER:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:SER:HB2	2:B:331:VAL:O	2.09	0.53
3:C:200:GLY:HA2	3:C:225:GLU:OE2	2.07	0.53
2:E:346:ARG:O	2:E:347:GLY:O	2.27	0.53
3:C:387:ILE:HG13	3:C:388:PRO:HD2	1.89	0.53
2:E:438:MET:HG3	2:E:443:SER:N	2.23	0.53
3:F:205:LYS:HE2	3:F:331:GLY:HA2	1.90	0.53
2:E:412:PRO:O	2:E:413:ASN:CB	2.57	0.53
2:B:192:TYR:C	2:B:194:ARG:H	2.15	0.53
2:B:293:TRP:NE1	2:B:296:ASN:HD21	2.06	0.53
3:C:101:LEU:O	3:C:104:ASP:OD1	2.26	0.53
3:F:197:ARG:HB2	3:F:382:THR:OG1	2.08	0.53
1:A:184:GLN:O	1:A:188:VAL:HG22	2.09	0.53
3:C:251:GLU:CB	3:C:257:THR:HG22	2.39	0.53
3:C:252:ASP:OD1	3:C:254:ASN:HB3	2.09	0.53
2:E:234:LYS:HZ3	3:F:145:ILE:HD11	1.73	0.53
3:C:314:THR:OG1	3:C:317:ASN:HB2	2.09	0.53
1:D:157:LYS:HE3	3:F:132:GLU:CD	2.33	0.53
2:E:431:THR:OG1	2:E:432:ASP:N	2.39	0.53
3:F:382:THR:HG22	3:F:383:THR:N	2.21	0.53
3:F:294:ASP:HA	3:F:301:ASP:CB	2.38	0.53
4:N:5:TYR:CD1	4:N:5:TYR:N	2.77	0.53
1:A:123:LYS:HZ3	2:B:151:LEU:HB3	1.69	0.53
2:B:309:GLU:CB	2:B:327:GLY:HA2	2.32	0.53
2:E:224:MET:HG3	2:E:224:MET:O	2.09	0.53
3:F:305:THR:HG23	3:F:338:LYS:HD2	1.90	0.53
2:E:236:TYR:HE2	2:E:294:LEU:HD21	1.74	0.53
2:E:354:MET:HA	2:E:369:ILE:HG23	1.91	0.53
3:F:192:THR:CG2	3:F:386:ILE:O	2.55	0.53
2:B:378:TYR:N	2:B:395:SER:OG	2.41	0.52
2:E:172:LEU:CD2	3:F:114:TYR:HB2	2.40	0.52
3:F:314:THR:O	3:F:316:ASP:N	2.42	0.52
2:B:176:ARG:HG3	2:B:176:ARG:HH11	1.73	0.52
2:B:219:GLY:O	2:B:242:MET:HE3	2.10	0.52
3:C:113:ILE:HG13	3:C:114:TYR:N	2.23	0.52
2:E:176:ARG:HH22	3:F:113:ILE:HG22	1.73	0.52
3:C:166:LEU:HD11	3:C:220:PRO:CG	2.38	0.52
3:F:116:SER:O	3:F:120:LYS:HG3	2.09	0.52
1:A:140:VAL:CG2	1:A:185:LEU:HD21	2.40	0.52
2:B:414:GLY:H	2:B:435:VAL:HG23	1.75	0.52
3:C:365:ASN:HD22	3:C:365:ASN:N	2.07	0.52
1:A:119:ILE:O	1:A:119:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:226:LEU:HD12	2:E:236:TYR:O	2.10	0.52
3:F:214:GLY:HA3	3:F:228:LEU:O	2.10	0.52
3:F:250:LEU:HD13	3:F:379:MET:HE3	1.91	0.52
2:B:360:LEU:HD12	2:B:360:LEU:N	2.25	0.52
3:C:195:GLN:HA	3:C:226:PHE:O	2.10	0.52
3:C:205:LYS:HE2	3:C:331:GLY:HA3	1.92	0.52
3:F:204:PHE:HB3	3:F:211:TYR:OH	2.09	0.52
1:A:126:VAL:HG21	2:B:153:ILE:HG12	1.92	0.52
3:C:114:TYR:CD1	3:C:114:TYR:C	2.88	0.52
3:F:224:THR:HG23	3:F:224:THR:O	2.08	0.52
2:E:308:THR:HG22	2:E:309:GLU:N	2.25	0.51
2:E:311:LEU:HG	2:E:453:LYS:HD3	1.92	0.51
2:E:345:TYR:O	2:E:346:ARG:HG3	2.10	0.51
2:E:357:ALA:O	2:E:365:ARG:HG3	2.10	0.51
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.10	0.51
3:F:252:ASP:OD1	3:F:254:ASN:HB3	2.10	0.51
1:A:123:LYS:HZ2	2:B:151:LEU:CD1	2.22	0.51
3:C:166:LEU:CD1	3:C:220:PRO:HG3	2.40	0.51
3:C:344:LEU:HA	3:C:367:ILE:HA	1.91	0.51
2:E:413:ASN:N	2:E:435:VAL:HG22	2.25	0.51
3:F:334:TRP:CG	3:F:343:HIS:HB2	2.45	0.51
1:A:148:LYS:HZ2	1:A:182:GLN:HE22	1.59	0.51
3:C:238:THR:O	3:C:239:GLN:C	2.53	0.51
2:E:211:CYS:SG	2:E:250:THR:HA	2.51	0.51
3:F:300:SER:O	3:F:302:LYS:N	2.43	0.51
1:A:132:HIS:HD1	1:A:132:HIS:H	1.59	0.51
2:E:203:ILE:HD12	2:E:203:ILE:N	2.15	0.51
3:F:186:GLY:C	3:F:188:GLY:H	2.19	0.51
2:B:373:MET:HE3	2:B:373:MET:HA	1.93	0.51
3:C:276:LEU:C	3:C:276:LEU:HD23	2.35	0.51
2:E:215:ILE:C	2:E:217:LYS:H	2.19	0.51
3:F:292:GLY:O	3:F:302:LYS:HA	2.10	0.51
1:A:126:VAL:HG22	2:B:154:ASP:CA	2.40	0.51
2:B:308:THR:CG2	2:B:309:GLU:N	2.74	0.51
3:C:392:LEU:O	3:C:393:THR:C	2.52	0.51
3:F:252:ASP:C	3:F:254:ASN:H	2.19	0.51
3:F:334:TRP:HE3	3:F:345:ASN:ND2	2.09	0.51
2:E:386:LEU:H	2:E:386:LEU:CD2	2.20	0.51
3:F:166:LEU:HD11	3:F:220:PRO:HG3	1.92	0.51
1:D:184:GLN:O	1:D:188:VAL:HG22	2.11	0.50
2:E:308:THR:HG22	2:E:309:GLU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ILE:HG23	2:B:340:ILE:O	2.11	0.50
3:C:202:VAL:HG11	3:C:225:GLU:HB3	1.93	0.50
3:F:211:TYR:HB3	3:F:230:ASN:HD21	1.75	0.50
2:B:415:ARG:HG3	2:B:415:ARG:NH1	2.25	0.50
3:C:184:ILE:HG22	3:C:186:GLY:H	1.76	0.50
2:E:228:GLN:HE22	3:F:177:GLN:NE2	1.98	0.50
2:E:385:TRP:CE3	4:N:3:ARG:HG3	2.47	0.50
3:F:149:THR:HA	3:F:168:PHE:O	2.11	0.50
5:H:2:NAG:H3	5:H:2:NAG:C8	2.41	0.50
2:B:254:ASN:O	2:B:291:GLU:HA	2.12	0.50
2:B:348:THR:O	2:B:349:ALA:HB2	2.12	0.50
1:D:154:ILE:HD11	3:F:124:LEU:HD21	1.94	0.50
1:D:158:ILE:O	1:D:161:CYS:HB2	2.12	0.50
2:E:224:MET:HB2	2:E:238:VAL:O	2.11	0.50
3:C:174:ALA:CB	3:C:235:LEU:HD13	2.41	0.50
3:C:258:SER:HB2	3:C:286:ALA:HB2	1.93	0.50
3:F:132:GLU:O	3:F:136:GLN:HB2	2.11	0.50
3:F:359:THR:HG21	3:F:363:TYR:O	2.12	0.50
3:F:108:ARG:HH11	3:F:108:ARG:N	2.09	0.50
3:F:320:ASP:OD2	3:F:322:PHE:O	2.29	0.50
3:F:334:TRP:CE3	3:F:345:ASN:ND2	2.79	0.50
3:C:325:ASN:ND2	3:C:328:GLU:HB2	2.20	0.50
3:C:392:LEU:O	3:C:395:GLY:N	2.44	0.50
2:E:176:ARG:HH22	3:F:113:ILE:CG2	2.25	0.50
1:A:181:GLN:HE22	2:B:174:ASN:HB3	1.77	0.49
3:C:346:GLY:C	3:C:366:GLY:HA2	2.37	0.49
2:E:253:GLN:NE2	2:E:452:MET:HG3	2.27	0.49
2:E:360:LEU:HD23	2:E:364:ASN:HB3	1.93	0.49
3:F:198:LEU:O	3:F:199:ASP:C	2.54	0.49
3:F:367:ILE:HD13	3:F:367:ILE:N	2.21	0.49
3:C:154:GLN:O	3:C:158:ASN:HB2	2.12	0.49
3:C:289:ALA:HB3	3:C:369:TRP:CE2	2.48	0.49
2:B:384:GLY:H	2:B:405:ASN:HA	1.77	0.49
3:C:100:ILE:C	3:C:102:THR:H	2.20	0.49
3:C:204:PHE:O	3:C:206:LYS:N	2.40	0.49
3:C:367:ILE:CG1	3:C:379:MET:H	2.25	0.49
3:F:186:GLY:C	3:F:188:GLY:N	2.69	0.49
2:E:380:ARG:HH11	2:E:380:ARG:HG2	1.78	0.49
2:E:418:TRP:HD1	2:E:419:GLY:H	1.60	0.49
3:F:382:THR:C	3:F:383:THR:HG22	2.38	0.49
2:B:310:LEU:HD21	2:B:452:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:VAL:HG12	2:B:446:SER:HA	1.94	0.49
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.13	0.49
2:B:412:PRO:O	2:B:413:ASN:CB	2.57	0.49
3:C:193:VAL:HA	3:C:385:LYS:HA	1.93	0.49
3:C:196:LYS:HD2	3:C:382:THR:O	2.13	0.49
3:C:344:LEU:HD12	3:C:344:LEU:O	2.13	0.49
3:C:365:ASN:N	3:C:365:ASN:ND2	2.60	0.49
1:D:160:SER:OG	2:E:261:ASP:HB2	2.13	0.49
2:E:203:ILE:H	2:E:203:ILE:CD1	2.11	0.49
3:F:346:GLY:HA3	3:F:366:GLY:HA2	1.95	0.49
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.31	0.49
2:E:385:TRP:CZ3	4:N:3:ARG:HG3	2.47	0.49
2:B:422:TYR:O	2:B:444:TRP:HB3	2.13	0.49
3:C:117:ASN:N	3:C:117:ASN:HD22	2.09	0.49
2:E:411:ASN:O	2:E:435:VAL:HA	2.13	0.49
3:F:166:LEU:N	3:F:166:LEU:CD1	2.68	0.49
3:F:300:SER:HB3	3:F:304:PHE:CD2	2.48	0.49
1:A:183:LYS:O	1:A:187:GLN:HB2	2.12	0.49
2:B:205:VAL:HG22	3:C:218:LEU:HD11	1.94	0.49
2:B:411:ASN:O	2:B:435:VAL:HA	2.13	0.49
2:B:418:TRP:O	2:B:420:GLY:N	2.42	0.49
3:F:369:TRP:O	3:F:370:ALA:C	2.56	0.48
2:E:319:GLY:O	2:E:320:ASP:C	2.56	0.48
3:F:166:LEU:HD11	3:F:220:PRO:CA	2.43	0.48
3:F:374:THR:C	3:F:376:TRP:H	2.21	0.48
3:C:251:GLU:HG2	3:C:252:ASP:N	2.27	0.48
3:C:322:PHE:CD2	3:C:323:GLU:N	2.81	0.48
3:C:346:GLY:HA3	3:C:366:GLY:N	2.28	0.48
2:E:437:TRP:O	2:E:439:ASN:N	2.42	0.48
3:F:298:ASP:C	3:F:300:SER:H	2.19	0.48
3:C:249:GLU:HB3	3:C:383:THR:CG2	2.43	0.48
3:C:325:ASN:HD21	3:C:328:GLU:CB	2.20	0.48
2:E:164:ASN:HD22	2:E:164:ASN:N	2.10	0.48
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.95	0.48
3:F:146:HIS:HB2	3:F:167:TYR:CD2	2.48	0.48
3:F:228:LEU:CG	3:F:232:LYS:HD2	2.15	0.48
3:F:366:GLY:O	3:F:368:ILE:HG23	2.13	0.48
1:A:156:ILE:HD13	2:B:415:ARG:HB3	1.96	0.48
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.96	0.48
3:C:166:LEU:HD11	3:C:220:PRO:CA	2.42	0.48
3:C:275:ARG:HA	3:C:311:GLN:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:ASP:HA	2:E:433:ASP:CB	2.27	0.48
3:F:172:LEU:H	3:F:239:GLN:HE21	1.61	0.48
3:F:231:GLU:O	3:F:234:HIS:HB3	2.13	0.48
3:F:275:ARG:HG3	3:F:310:MET:O	2.13	0.48
2:E:212:GLU:O	2:E:215:ILE:HG22	2.14	0.48
2:E:252:ILE:HD11	2:E:299:ILE:CD1	2.43	0.48
2:E:252:ILE:CD1	2:E:299:ILE:HG12	2.41	0.48
2:E:315:GLU:HB3	2:E:321:LYS:CG	2.39	0.48
3:F:141:ASP:CG	3:F:143:VAL:HG22	2.38	0.48
3:F:251:GLU:CG	3:F:257:THR:HG22	2.43	0.48
3:C:265:PHE:O	3:C:266:LYS:CB	2.62	0.48
3:C:304:PHE:O	3:C:338:LYS:CB	2.62	0.48
3:C:365:ASN:HD22	3:C:365:ASN:C	2.21	0.48
2:E:157:VAL:HG13	2:E:161:ILE:HD12	1.96	0.48
3:F:145:ILE:O	3:F:145:ILE:HD12	2.14	0.48
3:F:203:ASP:OD2	3:F:204:PHE:N	2.46	0.48
1:A:144:LEU:HD23	2:B:175:LEU:HD11	1.94	0.48
1:A:164:SER:O	2:B:196:PRO:HA	2.14	0.48
2:B:238:VAL:CG2	2:B:239:TYR:N	2.76	0.48
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.95	0.48
2:E:238:VAL:CG2	2:E:239:TYR:N	2.77	0.48
3:F:191:TRP:CG	3:F:385:LYS:HD3	2.48	0.48
3:F:365:ASN:C	3:F:365:ASN:ND2	2.72	0.48
3:C:197:ARG:HH11	3:C:367:ILE:HG23	1.78	0.48
2:E:215:ILE:HB	2:E:242:MET:CE	2.43	0.48
2:E:437:TRP:H	2:E:447:MET:HE3	1.79	0.48
2:E:381:ASP:HB2	2:E:393:GLN:NE2	2.29	0.47
3:F:326:CYS:O	3:F:330:ASP:N	2.46	0.47
2:B:437:TRP:CD1	2:B:439:ASN:HB2	2.49	0.47
3:C:181:TYR:O	3:C:193:VAL:HG22	2.14	0.47
2:E:311:LEU:HB3	2:E:453:LYS:HG2	1.95	0.47
2:E:380:ARG:HB3	2:E:380:ARG:CZ	2.44	0.47
2:B:253:GLN:NE2	2:B:452:MET:HG3	2.29	0.47
2:B:381:ASP:OD2	2:B:383:ASP:CG	2.57	0.47
3:C:200:GLY:CA	3:C:225:GLU:OE2	2.62	0.47
3:C:224:THR:O	3:C:226:PHE:HD2	1.98	0.47
2:E:309:GLU:CB	2:E:327:GLY:HA2	2.40	0.47
3:C:153:CYS:CB	3:C:192:THR:HB	2.43	0.47
2:E:291:GLU:O	2:E:292:TYR:HB3	2.15	0.47
3:F:169:ILE:HD12	3:F:171:PRO:HD3	1.95	0.47
2:B:377:THR:O	2:B:379:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:LEU:HD11	3:C:220:PRO:N	2.29	0.47
2:E:434:GLY:O	2:E:436:VAL:HG22	2.15	0.47
3:F:149:THR:HG23	3:F:168:PHE:O	2.14	0.47
3:F:258:SER:OG	3:F:286:ALA:HB2	2.14	0.47
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.49	0.47
2:B:406:ARG:HG2	4:M:3:ARG:HB2	1.97	0.47
1:D:169:LEU:CD1	1:D:171:ARG:HG2	2.45	0.47
2:E:402:TRP:CG	2:E:403:TRP:H	2.32	0.47
2:B:360:LEU:CB	2:B:365:ARG:HB2	2.45	0.47
2:B:424:TRP:HA	2:B:444:TRP:CH2	2.50	0.47
3:C:294:ASP:HA	3:C:301:ASP:CB	2.45	0.47
3:C:373:LYS:HZ3	3:C:377:TYR:HE2	1.61	0.47
1:D:185:LEU:HD13	1:D:185:LEU:O	2.15	0.47
2:E:228:GLN:NE2	3:F:177:GLN:HE22	2.00	0.47
2:E:398:ASP:O	2:E:399:GLY:C	2.58	0.47
3:F:308:ASN:C	3:F:308:ASN:ND2	2.72	0.47
3:C:365:ASN:HD22	3:C:365:ASN:H	1.62	0.47
1:D:123:LYS:O	1:D:126:VAL:HG23	2.14	0.47
2:E:238:VAL:CG2	2:E:239:TYR:H	2.25	0.47
3:F:171:PRO:CA	3:F:239:GLN:NE2	2.76	0.47
3:F:261:ASP:HB2	3:F:282:ALA:HB3	1.96	0.47
3:F:334:TRP:CG	3:F:335:TRP:H	2.31	0.47
2:B:348:THR:O	2:B:348:THR:OG1	2.28	0.47
2:B:437:TRP:HD1	2:B:439:ASN:HB2	1.79	0.47
3:C:234:HIS:O	3:C:236:ILE:N	2.48	0.47
3:C:248:VAL:HG12	3:C:250:LEU:HD21	1.96	0.47
3:C:273:LYS:O	3:C:274:TYR:C	2.58	0.47
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.12	0.47
3:F:184:ILE:HG22	3:F:186:GLY:H	1.80	0.47
3:F:248:VAL:HB	3:F:260:ALA:HB3	1.97	0.47
3:F:347:VAL:HG12	3:F:348:TYR:N	2.29	0.47
2:B:313:GLU:HA	2:B:323:LYS:HB3	1.95	0.46
3:C:151:LYS:HD2	3:C:172:LEU:HD21	1.96	0.46
3:C:264:MET:O	3:C:266:LYS:HG2	2.14	0.46
3:F:227:TRP:O	3:F:228:LEU:C	2.59	0.46
3:F:373:LYS:HB3	3:F:377:TYR:HD2	1.80	0.46
3:F:375:ARG:HD2	3:F:376:TRP:CZ3	2.50	0.46
2:B:414:GLY:H	2:B:435:VAL:CG2	2.28	0.46
2:B:428:LYS:HE3	2:B:429:HIS:CD2	2.50	0.46
1:A:161:CYS:HB3	1:A:165:CYS:HB2	1.58	0.46
2:B:315:GLU:HB3	2:B:321:LYS:CG	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:ALA:O	3:C:162:LYS:HD3	2.15	0.46
2:E:191:GLU:HG3	2:E:194:ARG:CZ	2.45	0.46
2:E:296:ASN:O	2:E:297:ASP:C	2.57	0.46
2:E:300:SER:OG	2:E:301:GLN:N	2.47	0.46
2:E:437:TRP:CD1	2:E:439:ASN:HB2	2.50	0.46
2:E:438:MET:SD	2:E:443:SER:HB3	2.54	0.46
1:A:126:VAL:CG2	2:B:154:ASP:HA	2.45	0.46
2:B:238:VAL:HG22	2:B:239:TYR:H	1.79	0.46
2:B:365:ARG:C	2:B:367:MET:H	2.23	0.46
3:F:270:GLU:O	3:F:270:GLU:HG2	2.15	0.46
3:C:203:ASP:HB3	3:C:206:LYS:NZ	2.30	0.46
1:D:159:ARG:NH1	1:D:159:ARG:CG	2.78	0.46
2:E:234:LYS:NZ	3:F:145:ILE:HD11	2.30	0.46
3:F:387:ILE:HG23	3:F:388:PRO:O	2.16	0.46
2:B:172:LEU:HD22	3:C:113:ILE:CG1	2.45	0.46
2:B:265:LYS:C	2:B:377:THR:HG21	2.41	0.46
1:D:140:VAL:O	1:D:143:GLN:HB3	2.15	0.46
1:D:147:MET:HG2	2:E:175:LEU:HD22	1.98	0.46
2:E:364:ASN:HA	2:E:367:MET:HE2	1.97	0.46
3:F:154:GLN:HB2	3:F:387:ILE:CD1	2.46	0.46
2:B:377:THR:C	2:B:379:ASP:N	2.66	0.46
3:C:203:ASP:HB3	3:C:206:LYS:HZ1	1.81	0.46
1:D:169:LEU:HD13	1:D:170:ALA:N	2.30	0.46
3:F:315:TRP:CD1	3:F:315:TRP:C	2.94	0.46
1:A:132:HIS:HB2	3:C:107:ILE:HD13	1.98	0.46
2:B:332:GLN:HA	2:B:332:GLN:NE2	2.31	0.46
2:B:362:GLY:O	2:B:363:GLU:C	2.59	0.46
2:B:397:GLU:HB3	2:B:431:THR:HG21	1.97	0.46
3:C:143:VAL:HG23	3:C:143:VAL:O	2.15	0.46
3:C:262:TYR:CZ	3:C:290:PHE:HD1	2.34	0.46
3:C:390:ASN:ND2	3:C:391:ARG:N	2.63	0.46
2:E:377:THR:HA	2:E:395:SER:OG	2.16	0.46
2:E:454:ILE:O	2:E:455:ARG:HB2	2.16	0.46
3:F:191:TRP:CE3	3:F:385:LYS:HB3	2.51	0.46
1:A:165:CYS:O	1:A:166:SER:C	2.59	0.46
3:C:264:MET:HE3	3:C:266:LYS:HZ3	1.77	0.46
2:E:239:TYR:OH	2:E:287:GLY:O	2.30	0.46
3:F:166:LEU:CD1	3:F:220:PRO:HG3	2.46	0.46
1:D:166:SER:CB	2:E:195:THR:O	2.64	0.46
2:E:172:LEU:HD22	3:F:114:TYR:HB2	1.98	0.46
2:E:314:MET:HE1	2:E:437:TRP:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:LYS:HE3	2:E:429:HIS:CD2	2.51	0.46
3:F:100:ILE:C	3:F:102:THR:H	2.23	0.46
3:F:243:PRO:HB2	3:F:389:PHE:CB	2.46	0.46
3:C:196:LYS:HD2	3:C:383:THR:HB	1.99	0.45
3:C:326:CYS:SG	3:C:336:MET:HB3	2.56	0.45
1:D:161:CYS:O	1:D:165:CYS:HB2	2.16	0.45
3:F:265:PHE:O	3:F:266:LYS:HB3	2.16	0.45
3:F:344:LEU:CB	3:F:367:ILE:HG22	2.46	0.45
1:A:154:ILE:HD12	2:B:182:LEU:HD13	1.96	0.45
2:B:375:PHE:CE2	2:B:402:TRP:N	2.84	0.45
2:E:252:ILE:O	2:E:252:ILE:HG13	2.16	0.45
2:E:452:MET:C	2:E:453:LYS:HD2	2.42	0.45
3:F:343:HIS:O	3:F:343:HIS:CG	2.68	0.45
2:B:393:GLN:O	2:B:397:GLU:HG2	2.17	0.45
2:B:408:HIS:O	4:M:1:GLY:N	2.50	0.45
3:C:224:THR:O	3:C:224:THR:HG23	2.15	0.45
2:E:321:LYS:O	2:E:322:VAL:HG13	2.16	0.45
3:F:197:ARG:HA	3:F:225:GLU:CG	2.35	0.45
3:F:205:LYS:HG2	3:F:331:GLY:C	2.41	0.45
2:B:168:LEU:O	2:B:172:LEU:HB2	2.17	0.45
2:B:203:ILE:O	3:C:218:LEU:HD12	2.16	0.45
3:C:298:ASP:C	3:C:300:SER:N	2.73	0.45
3:C:382:THR:CG2	3:C:383:THR:N	2.79	0.45
3:F:195:GLN:O	3:F:383:THR:HA	2.16	0.45
3:F:276:LEU:CD2	3:F:307:HIS:O	2.65	0.45
3:F:318:ASP:OD1	3:F:320:ASP:OD2	2.35	0.45
3:F:374:THR:C	3:F:376:TRP:N	2.72	0.45
3:C:361:ASN:ND2	3:C:363:TYR:HB2	2.32	0.45
1:D:126:VAL:HG22	2:E:154:ASP:CA	2.47	0.45
2:E:332:GLN:NE2	2:E:332:GLN:HA	2.31	0.45
3:C:110:LEU:O	3:C:113:ILE:HG12	2.17	0.45
3:C:141:ASP:CG	3:C:143:VAL:HG22	2.42	0.45
3:C:195:GLN:HE22	3:C:382:THR:HG22	1.82	0.45
3:C:266:LYS:HG3	3:F:303:PHE:CE2	2.51	0.45
3:C:366:GLY:O	3:C:368:ILE:HG13	2.17	0.45
1:D:156:ILE:HG21	2:E:415:ARG:HE	1.82	0.45
2:E:265:LYS:C	2:E:268:PRO:HD2	2.41	0.45
2:B:406:ARG:CG	4:M:3:ARG:HB2	2.47	0.45
3:C:174:ALA:HB2	3:C:235:LEU:HD13	1.99	0.45
3:C:278:TYR:CE1	3:C:308:ASN:OD1	2.70	0.45
2:E:182:LEU:N	2:E:182:LEU:HD23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:THR:HG23	3:F:169:ILE:HA	1.98	0.45
3:F:375:ARG:HB3	3:F:376:TRP:CE3	2.51	0.45
2:B:361:MET:O	2:B:364:ASN:HB2	2.17	0.45
3:C:373:LYS:HB3	3:C:377:TYR:CD2	2.45	0.45
2:B:316:ASP:OD2	2:B:316:ASP:N	2.50	0.45
2:B:418:TRP:C	2:B:420:GLY:H	2.24	0.45
3:C:229:GLY:O	3:C:230:ASN:C	2.59	0.45
3:C:264:MET:HE3	3:C:266:LYS:HZ1	1.77	0.45
3:C:294:ASP:HA	3:C:301:ASP:HB3	1.97	0.45
1:D:165:CYS:O	1:D:166:SER:C	2.58	0.45
2:E:178:LYS:O	2:E:181:LYS:HB3	2.18	0.45
2:E:316:ASP:HB2	2:E:445:TYR:OH	2.16	0.45
2:E:422:TYR:HE1	2:E:445:TYR:N	2.15	0.45
3:F:127:LYS:O	3:F:130:GLN:HB2	2.17	0.45
3:C:169:ILE:O	3:C:169:ILE:HG13	2.16	0.44
3:C:312:PHE:CE1	3:C:334:TRP:HA	2.52	0.44
3:C:396:GLU:CG	3:C:397:GLY:H	2.30	0.44
3:F:98:ALA:O	3:F:101:LEU:HG	2.17	0.44
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.51	0.44
3:F:322:PHE:O	3:F:323:GLU:C	2.59	0.44
1:A:140:VAL:HG21	1:A:185:LEU:HD21	2.00	0.44
3:C:223:THR:O	3:C:224:THR:HB	2.17	0.44
3:C:334:TRP:CG	3:C:343:HIS:HB2	2.51	0.44
5:G:6:GAL:H5	5:G:7:SIA:O6	2.17	0.44
1:A:125:LYS:O	1:A:129:LYS:HG2	2.17	0.44
1:A:147:MET:CE	2:B:179:ILE:HD11	2.44	0.44
2:B:172:LEU:HD22	3:C:113:ILE:CD1	2.47	0.44
2:E:406:ARG:O	2:E:406:ARG:HG2	2.17	0.44
3:F:205:LYS:HE2	3:F:331:GLY:CA	2.47	0.44
3:F:243:PRO:HB2	3:F:389:PHE:HB2	1.98	0.44
1:A:134:GLN:O	1:A:137:GLN:HB3	2.17	0.44
2:B:262:PHE:O	2:B:400:GLY:HA2	2.18	0.44
3:C:373:LYS:CB	3:C:377:TYR:HD2	2.27	0.44
1:D:130:VAL:O	1:D:133:ILE:HG13	2.18	0.44
2:E:279:ASN:O	2:E:288:LEU:HD12	2.17	0.44
3:F:191:TRP:CD1	3:F:385:LYS:HD3	2.52	0.44
1:A:189:ILE:CG2	1:A:190:ALA:N	2.75	0.44
3:C:149:THR:HA	3:C:168:PHE:O	2.16	0.44
3:C:258:SER:CB	3:C:286:ALA:HB2	2.48	0.44
1:D:144:LEU:O	1:D:147:MET:HB3	2.17	0.44
1:D:189:ILE:HG22	1:D:190:ALA:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:ILE:HB	2:E:242:MET:HE1	2.00	0.44
2:E:231:SER:HB2	3:F:176:GLN:OE1	2.18	0.44
2:E:380:ARG:HH22	2:E:382:ASN:HD21	1.66	0.44
3:F:188:GLY:C	3:F:189:ASN:HD22	2.26	0.44
2:B:175:LEU:O	2:B:179:ILE:HG13	2.17	0.44
2:B:370:HIS:HE1	2:B:408:HIS:HB2	1.82	0.44
3:F:172:LEU:H	3:F:239:GLN:NE2	2.16	0.44
3:F:196:LYS:HD2	3:F:382:THR:O	2.18	0.44
2:E:267:ASP:O	2:E:268:PRO:C	2.61	0.44
3:F:148:ILE:O	3:F:156:ILE:HD12	2.17	0.44
1:A:188:VAL:HG23	1:A:188:VAL:O	2.17	0.44
2:B:217:LYS:HB3	3:C:213:GLU:HG3	2.00	0.44
2:B:417:TYR:HB2	2:B:446:SER:CB	2.48	0.44
3:C:277:THR:HB	3:C:309:GLY:HA2	2.00	0.44
3:F:194:PHE:CZ	3:F:384:MET:HB3	2.53	0.44
3:F:264:MET:SD	3:F:279:ALA:HB2	2.58	0.44
2:B:418:TRP:HD1	2:B:419:GLY:H	1.65	0.43
2:B:457:PHE:CD1	2:B:457:PHE:C	2.96	0.43
3:C:305:THR:CG2	3:C:338:LYS:HD2	2.47	0.43
2:E:377:THR:C	2:E:379:ASP:N	2.75	0.43
2:B:182:LEU:O	2:B:186:VAL:HG23	2.18	0.43
2:B:380:ARG:HH11	2:B:380:ARG:CG	2.30	0.43
3:C:245:ALA:O	3:C:386:ILE:HA	2.17	0.43
3:C:356:LYS:O	3:C:362:GLY:HA2	2.18	0.43
3:F:314:THR:C	3:F:316:ASP:N	2.76	0.43
1:A:159:ARG:HG2	1:A:159:ARG:NH1	2.31	0.43
2:B:163:THR:O	2:B:167:VAL:HG23	2.19	0.43
2:B:308:THR:HG22	2:B:309:GLU:H	1.82	0.43
3:C:219:SER:HB2	3:C:224:THR:HG21	2.00	0.43
1:D:130:VAL:O	1:D:133:ILE:CG1	2.66	0.43
2:E:438:MET:HA	2:E:442:GLY:C	2.44	0.43
3:F:262:TYR:CZ	3:F:290:PHE:HD1	2.37	0.43
1:A:124:ARG:O	1:A:128:GLU:HG2	2.19	0.43
2:B:249:TRP:CZ2	2:B:455:ARG:NH2	2.86	0.43
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.99	0.43
3:C:113:ILE:CG1	3:C:114:TYR:N	2.81	0.43
1:D:134:GLN:O	1:D:137:GLN:HB3	2.18	0.43
1:D:148:LYS:HA	1:D:178:TYR:CE2	2.52	0.43
2:E:309:GLU:HA	2:E:326:TYR:O	2.19	0.43
3:F:136:GLN:O	3:F:136:GLN:HG2	2.18	0.43
3:C:202:VAL:HG11	3:C:225:GLU:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:LYS:HB2	3:C:311:GLN:OE1	2.18	0.43
3:F:137:GLU:OE1	3:F:137:GLU:HA	2.17	0.43
1:A:153:ASP:O	1:A:154:ILE:C	2.59	0.43
2:B:176:ARG:HG3	2:B:176:ARG:NH1	2.34	0.43
2:B:309:GLU:HA	2:B:326:TYR:O	2.18	0.43
3:C:338:LYS:N	3:C:339:CYS:CA	2.65	0.43
2:E:326:TYR:C	2:E:328:GLY:N	2.76	0.43
3:F:206:LYS:HB3	3:F:210:GLN:CD	2.44	0.43
1:A:154:ILE:O	1:A:155:ASP:C	2.61	0.43
2:B:236:TYR:C	2:B:237:ARG:O	2.61	0.43
2:B:326:TYR:C	2:B:328:GLY:N	2.75	0.43
2:B:365:ARG:O	2:B:367:MET:N	2.52	0.43
3:C:100:ILE:C	3:C:102:THR:N	2.77	0.43
3:C:246:LEU:HD12	3:C:247:ARG:H	1.83	0.43
2:E:411:ASN:O	2:E:411:ASN:CG	2.60	0.43
1:A:124:ARG:HG3	1:A:124:ARG:HH11	1.84	0.43
3:C:320:ASP:OD1	3:C:326:CYS:SG	2.77	0.43
3:C:353:THR:HG1	3:C:377:TYR:HD1	1.67	0.43
1:D:166:SER:N	2:E:195:THR:O	2.50	0.43
1:D:188:VAL:HG23	1:D:188:VAL:O	2.19	0.43
2:E:169:ARG:NH1	3:F:109:TYR:CE2	2.86	0.43
2:E:250:THR:O	2:E:453:LYS:HA	2.18	0.43
3:F:206:LYS:HB3	3:F:210:GLN:CB	2.49	0.43
1:A:148:LYS:HZ2	1:A:179:GLU:CG	2.31	0.43
2:B:152:TYR:O	2:B:154:ASP:N	2.52	0.43
2:B:449:LYS:HB2	2:B:449:LYS:HE3	1.74	0.43
3:C:154:GLN:HB2	3:C:387:ILE:HD11	2.00	0.43
1:D:126:VAL:CG2	2:E:154:ASP:HA	2.48	0.43
3:F:141:ASP:OD2	3:F:143:VAL:HG22	2.19	0.43
3:F:174:ALA:CB	3:F:235:LEU:HD13	2.48	0.43
3:F:391:ARG:HD3	3:F:391:ARG:HA	1.41	0.43
1:A:148:LYS:NZ	1:A:179:GLU:HG3	2.34	0.43
1:A:159:ARG:NH2	2:B:418:TRP:CE3	2.87	0.43
3:C:153:CYS:SG	3:C:192:THR:HB	2.59	0.43
3:C:281:PHE:CE2	3:C:288:ASP:HB2	2.54	0.43
1:D:123:LYS:HG2	2:E:151:LEU:O	2.18	0.43
2:E:219:GLY:O	2:E:242:MET:HE3	2.19	0.43
2:E:326:TYR:N	2:E:326:TYR:CD1	2.87	0.43
3:F:102:THR:O	3:F:105:SER:HB2	2.18	0.43
3:F:124:LEU:C	3:F:124:LEU:HD23	2.44	0.43
3:F:382:THR:O	3:F:383:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LEU:N	2:B:182:LEU:HD23	2.33	0.42
2:B:323:LYS:C	2:B:323:LYS:HD2	2.45	0.42
3:C:230:ASN:HA	3:C:233:ILE:HD12	2.00	0.42
2:E:303:THR:C	2:E:305:MET:H	2.27	0.42
3:F:370:ALA:C	3:F:372:TRP:H	2.26	0.42
3:F:390:ASN:N	3:F:390:ASN:HD22	2.17	0.42
1:A:154:ILE:O	1:A:158:ILE:HG12	2.18	0.42
2:B:157:VAL:HG13	2:B:161:ILE:HD12	2.01	0.42
2:B:178:LYS:O	2:B:182:LEU:HG	2.19	0.42
3:C:124:LEU:HD23	3:C:125:LYS:N	2.34	0.42
2:E:215:ILE:CG2	2:E:216:ARG:N	2.81	0.42
3:F:370:ALA:O	3:F:372:TRP:N	2.51	0.42
1:A:165:CYS:HA	2:B:193:CYS:HA	2.02	0.42
2:B:228:GLN:HE22	3:C:177:GLN:HE22	1.67	0.42
2:E:440:TRP:CE3	2:E:441:LYS:HG2	2.54	0.42
2:B:333:ASN:O	2:B:334:GLU:C	2.63	0.42
3:C:325:ASN:O	3:C:325:ASN:CG	2.62	0.42
3:C:327:ALA:O	3:C:328:GLU:C	2.63	0.42
3:C:338:LYS:H	3:C:339:CYS:CA	2.25	0.42
3:C:367:ILE:HG12	3:C:367:ILE:O	2.20	0.42
2:E:365:ARG:C	2:E:367:MET:H	2.28	0.42
2:E:386:LEU:HD23	2:E:386:LEU:N	2.22	0.42
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.54	0.42
3:C:192:THR:O	3:C:192:THR:OG1	2.29	0.42
3:F:111:GLN:O	3:F:114:TYR:HB3	2.19	0.42
3:F:205:LYS:NZ	3:F:205:LYS:HB3	2.35	0.42
3:F:333:GLY:O	3:F:334:TRP:HB2	2.19	0.42
2:B:380:ARG:CZ	2:B:380:ARG:HB3	2.49	0.42
3:C:311:GLN:O	3:C:335:TRP:HA	2.18	0.42
2:E:310:LEU:O	2:E:325:HIS:HA	2.19	0.42
3:F:202:VAL:HG13	3:F:203:ASP:N	2.34	0.42
5:H:3:MAN:H4	5:H:8:MAN:C2	2.43	0.42
1:A:184:GLN:HB2	2:B:171:ILE:HD11	2.01	0.42
3:C:234:HIS:O	3:C:235:LEU:C	2.62	0.42
3:C:307:HIS:HE1	3:C:341:ALA:HB3	1.83	0.42
3:C:344:LEU:HD11	3:C:384:MET:SD	2.60	0.42
2:E:191:GLU:HG3	2:E:194:ARG:NH2	2.35	0.42
2:E:294:LEU:O	2:E:299:ILE:HD11	2.20	0.42
3:F:341:ALA:O	3:F:370:ALA:HB2	2.19	0.42
1:A:140:VAL:HG23	1:A:185:LEU:HD21	2.02	0.42
3:C:315:TRP:N	3:C:327:ALA:HB1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ARG:NH2	2:E:418:TRP:CE3	2.88	0.42
3:F:307:HIS:HE1	3:F:341:ALA:HB3	1.85	0.42
3:F:311:GLN:O	3:F:335:TRP:CD1	2.73	0.42
3:F:347:VAL:N	3:F:366:GLY:HA2	2.34	0.42
1:A:155:ASP:HB2	1:A:173:VAL:HG21	2.02	0.42
3:C:370:ALA:C	3:C:372:TRP:H	2.28	0.42
2:B:204:PRO:HA	3:C:217:HIS:HA	2.01	0.42
3:C:314:THR:O	3:C:315:TRP:C	2.63	0.42
2:E:205:VAL:HG21	3:F:226:PHE:HB2	2.02	0.42
2:E:218:GLY:HA3	3:F:210:GLN:HG2	2.02	0.42
2:E:348:THR:O	2:E:349:ALA:HB2	2.20	0.42
3:F:145:ILE:H	3:F:145:ILE:HG13	1.75	0.42
3:F:166:LEU:HD11	3:F:220:PRO:CG	2.50	0.42
3:F:193:VAL:HG23	3:F:226:PHE:HZ	1.84	0.42
3:C:385:LYS:O	3:C:386:ILE:HB	2.20	0.41
2:E:454:ILE:HD12	2:E:455:ARG:N	2.34	0.41
3:F:239:GLN:O	3:F:240:SER:HB2	2.20	0.41
3:F:264:MET:HE2	3:F:278:TYR:HA	2.02	0.41
3:F:338:LYS:H	3:F:339:CYS:CA	2.25	0.41
3:F:339:CYS:HB2	3:F:340:HIS:H	1.67	0.41
3:F:344:LEU:HD13	3:F:382:THR:HG21	2.02	0.41
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.55	0.41
2:B:418:TRP:CD1	2:B:419:GLY:H	2.38	0.41
2:E:176:ARG:HG2	3:F:120:LYS:HZ2	1.84	0.41
2:E:215:ILE:N	2:E:242:MET:HE1	2.34	0.41
2:E:359:GLN:O	2:E:360:LEU:HD12	2.20	0.41
2:B:161:ILE:N	2:B:162:PRO:CD	2.83	0.41
2:B:253:GLN:HE21	2:B:452:MET:HG3	1.85	0.41
3:C:280:TYR:CD1	3:C:280:TYR:C	2.97	0.41
3:C:391:ARG:HD2	3:C:391:ARG:HA	1.82	0.41
1:D:128:GLU:OE2	1:D:129:LYS:HE2	2.21	0.41
3:C:277:THR:HG23	3:F:303:PHE:HD2	1.84	0.41
3:C:297:ASP:O	3:C:298:ASP:CB	2.69	0.41
1:D:145:VAL:HG12	1:D:149:ARG:NH1	2.35	0.41
2:E:314:MET:HE1	2:E:437:TRP:CB	2.50	0.41
2:B:230:ASP:O	2:B:233:VAL:HG12	2.19	0.41
2:B:411:ASN:O	2:B:411:ASN:CG	2.62	0.41
3:C:264:MET:O	3:C:264:MET:HG2	2.19	0.41
3:C:346:GLY:HA3	3:C:366:GLY:CA	2.51	0.41
2:E:343:ASN:CG	2:E:344:LYS:HG2	2.45	0.41
2:E:379:ASP:OD1	2:E:379:ASP:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:157:ALA:HA	3:F:160:GLY:O	2.20	0.41
1:A:126:VAL:HG22	2:B:154:ASP:CB	2.50	0.41
2:B:199:VAL:O	3:C:141:ASP:OD2	2.38	0.41
2:B:326:TYR:CZ	2:B:353:LEU:HD12	2.55	0.41
2:E:336:ASN:O	2:E:338:TYR:N	2.53	0.41
2:E:352:ALA:O	2:E:370:HIS:HD2	2.03	0.41
3:F:140:LYS:HD3	3:F:141:ASP:N	2.35	0.41
3:F:166:LEU:H	3:F:166:LEU:CD1	2.28	0.41
3:F:204:PHE:O	3:F:332:SER:HA	2.20	0.41
3:F:253:TRP:NE1	3:F:379:MET:O	2.53	0.41
3:F:272:ASP:O	3:F:273:LYS:HB2	2.20	0.41
2:B:229:PRO:HG3	2:B:236:TYR:OH	2.21	0.41
2:B:406:ARG:HG2	2:B:406:ARG:O	2.21	0.41
2:B:413:ASN:N	2:B:435:VAL:HG22	2.34	0.41
3:C:304:PHE:HB3	3:C:338:LYS:HG3	2.01	0.41
2:E:172:LEU:HD21	3:F:114:TYR:HD2	1.86	0.41
2:E:177:SER:HA	2:E:180:GLN:HG2	2.02	0.41
2:E:412:PRO:HA	2:E:435:VAL:HG13	2.01	0.41
3:F:170:LYS:HE3	3:F:175:ASN:CA	2.49	0.41
2:B:301:GLN:HE21	2:B:301:GLN:HB3	1.53	0.41
2:B:337:LYS:O	2:B:338:TYR:C	2.62	0.41
2:E:162:PRO:O	2:E:165:LEU:HB2	2.21	0.41
2:E:309:GLU:HG2	2:E:455:ARG:O	2.21	0.41
2:E:438:MET:HA	2:E:442:GLY:CA	2.51	0.41
3:F:304:PHE:HB3	3:F:338:LYS:HB2	2.03	0.41
3:F:367:ILE:H	3:F:367:ILE:CD1	2.19	0.41
1:A:147:MET:O	1:A:150:LEU:HB2	2.21	0.41
3:C:227:TRP:O	3:C:228:LEU:C	2.62	0.41
3:C:344:LEU:HA	3:C:367:ILE:HG22	2.03	0.41
2:E:169:ARG:NH1	3:F:109:TYR:CD2	2.89	0.41
2:E:172:LEU:HD21	3:F:114:TYR:HB2	2.02	0.41
2:E:254:ASN:O	2:E:291:GLU:HA	2.21	0.41
2:E:449:LYS:HE3	2:E:449:LYS:HB2	1.88	0.41
3:F:196:LYS:O	3:F:225:GLU:HA	2.20	0.41
3:F:245:ALA:O	3:F:386:ILE:HA	2.21	0.41
3:C:100:ILE:O	3:C:103:HIS:CD2	2.73	0.41
3:C:205:LYS:HE2	3:C:331:GLY:CA	2.51	0.41
2:E:176:ARG:CG	3:F:120:LYS:NZ	2.82	0.41
3:F:186:GLY:O	3:F:188:GLY:N	2.54	0.41
3:F:194:PHE:HZ	3:F:384:MET:HE2	1.86	0.41
2:B:375:PHE:CE2	2:B:401:GLY:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:MET:SD	2:B:443:SER:HB3	2.61	0.40
2:B:445:TYR:HD1	2:B:447:MET:HE1	1.86	0.40
2:E:181:LYS:C	2:E:181:LYS:HD3	2.46	0.40
2:E:225:TYR:HD2	2:E:240:CYS:HB2	1.86	0.40
2:E:236:TYR:CD2	2:E:294:LEU:HD11	2.56	0.40
2:E:253:GLN:HG3	2:E:293:TRP:HE3	1.84	0.40
2:E:421:GLN:HE21	2:E:421:GLN:HB2	1.50	0.40
2:B:180:GLN:HG3	2:B:181:LYS:N	2.35	0.40
2:B:228:GLN:HB2	2:B:235:PRO:HG3	2.03	0.40
2:B:319:GLY:O	2:B:320:ASP:C	2.63	0.40
3:C:148:ILE:O	3:C:148:ILE:HG22	2.21	0.40
3:C:277:THR:CG2	3:F:303:PHE:HD2	2.34	0.40
2:E:168:LEU:O	2:E:172:LEU:HB2	2.22	0.40
3:F:185:ASP:C	3:F:187:SER:H	2.29	0.40
1:A:161:CYS:O	1:A:162:ARG:C	2.63	0.40
2:B:209:LYS:HD2	2:B:213:GLU:OE2	2.21	0.40
2:B:322:VAL:HB	2:B:349:ALA:HB2	2.03	0.40
2:B:325:HIS:HB3	2:B:346:ARG:HB2	2.02	0.40
3:C:175:ASN:O	3:C:176:GLN:O	2.39	0.40
3:C:272:ASP:O	3:C:273:LYS:HB2	2.19	0.40
3:C:305:THR:HB	3:C:341:ALA:CB	2.28	0.40
1:D:126:VAL:HG21	2:E:153:ILE:HG12	2.04	0.40
2:E:253:GLN:HE21	2:E:253:GLN:HB3	1.56	0.40
3:F:359:THR:HA	3:F:360:PRO:HD3	1.88	0.40
1:A:123:LYS:HE2	1:A:124:ARG:HH22	1.86	0.40
1:A:176:LYS:O	1:A:180:ASP:HB2	2.21	0.40
2:B:373:MET:HG3	2:B:405:ASN:CB	2.46	0.40
3:C:205:LYS:HG2	3:C:331:GLY:C	2.47	0.40
3:C:311:GLN:HB2	3:C:319:ASN:O	2.21	0.40
2:E:249:TRP:HH2	2:E:325:HIS:CE1	2.39	0.40
2:E:367:MET:O	2:E:367:MET:HG3	2.20	0.40
3:F:305:THR:CG2	3:F:338:LYS:HD2	2.51	0.40
3:F:334:TRP:CE2	3:F:343:HIS:HA	2.57	0.40
3:C:124:LEU:O	3:C:125:LYS:C	2.62	0.40
3:C:342:GLY:HA2	3:C:368:ILE:CD1	2.52	0.40
2:E:296:ASN:HD22	2:E:299:ILE:HD12	1.87	0.40
2:E:296:ASN:HA	2:E:299:ILE:HD12	2.03	0.40
3:F:198:LEU:O	3:F:200:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/197 (36%)	62 (86%)	6 (8%)	4 (6%)	1	14
1	D	72/197 (36%)	62 (86%)	7 (10%)	3 (4%)	2	19
2	B	306/458 (67%)	230 (75%)	57 (19%)	19 (6%)	1	12
2	E	306/458 (67%)	226 (74%)	63 (21%)	17 (6%)	1	14
3	C	299/317 (94%)	199 (67%)	67 (22%)	33 (11%)	0	5
3	F	294/317 (93%)	211 (72%)	54 (18%)	29 (10%)	0	6
4	M	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	N	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
All	All	1355/1954 (69%)	994 (73%)	256 (19%)	105 (8%)	1	9

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	153	ILE
2	B	238	VAL
2	B	289	PRO
2	B	349	ALA
3	C	98	ALA
3	C	101	LEU
3	C	161	ALA
3	C	199	ASP
3	C	336	MET
3	C	386	ILE
3	C	396	GLU
1	D	191	LYS
2	E	337	LYS
2	E	349	ALA
3	F	161	ALA
3	F	199	ASP
3	F	301	ASP

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Mol	Chain	Res	Type
3	F	371	THR
2	B	256	GLN
2	B	366	THR
2	B	405	ASN
2	B	416	TYR
3	C	202	VAL
3	C	235	LEU
3	C	266	LYS
3	C	295	PHE
3	C	300	SER
3	C	393	THR
2	E	153	ILE
2	E	245	GLU
2	E	256	GLN
2	E	289	PRO
2	E	347	GLY
2	E	399	GLY
2	E	433	ASP
3	F	177	GLN
3	F	202	VAL
3	F	315	TRP
3	F	324	GLY
3	F	325	ASN
3	F	336	MET
3	F	367	ILE
3	F	370	ALA
1	A	189	ILE
2	B	237	ARG
2	B	243	ASN
2	B	245	GLU
2	B	291	GLU
2	B	399	GLY
2	B	404	TYR
2	B	457	PHE
3	C	136	GLN
3	C	176	GLN
3	C	224	THR
3	C	228	LEU
3	C	330	ASP
3	C	342	GLY
3	C	353	THR
3	C	371	THR

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Mol	Chain	Res	Type
2	E	238	VAL
2	E	243	ASN
2	E	304	ARG
2	E	363	GLU
2	E	416	TYR
3	F	101	LEU
3	F	337	ASN
3	F	342	GLY
3	F	346	GLY
3	F	383	THR
1	A	164	SER
1	A	166	SER
3	C	203	ASP
3	C	367	ILE
3	C	390	ASN
2	E	291	GLU
3	F	203	ASP
3	F	224	THR
3	F	295	PHE
3	F	296	GLY
3	F	300	SER
3	F	331	GLY
3	F	353	THR
1	A	190	ALA
2	B	193	CYS
2	B	265	LYS
2	B	378	TYR
3	C	183	GLU
3	C	234	HIS
3	C	301	ASP
3	C	337	ASN
3	F	147	ASP
3	F	266	LYS
3	F	282	ALA
3	F	379	MET
3	F	228	LEU
3	C	283	GLY
3	C	292	GLY
3	C	296	GLY
3	C	331	GLY
3	C	395	GLY
2	B	196	PRO

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Mol	Chain	Res	Type
1	D	126	VAL
2	E	340	ILE
1	D	189	ILE
2	E	435	VAL

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	69/179 (38%)	59 (86%)	10 (14%)	3	18
1	D	69/179 (38%)	58 (84%)	11 (16%)	2	15
2	B	266/393 (68%)	236 (89%)	30 (11%)	5	26
2	E	266/393 (68%)	237 (89%)	29 (11%)	6	27
3	C	252/263 (96%)	221 (88%)	31 (12%)	4	23
3	F	249/263 (95%)	220 (88%)	29 (12%)	5	25
4	M	4/4 (100%)	4 (100%)	0	100	100
4	N	4/4 (100%)	4 (100%)	0	100	100
All	All	1179/1678 (70%)	1039 (88%)	140 (12%)	5	24

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LEU
1	A	123	LYS
1	A	131	GLN
1	A	139	ASN
1	A	162	ARG
1	A	164	SER
1	A	171	ARG
1	A	174	ASP
1	A	185	LEU
1	A	187	GLN
2	B	151	LEU

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Mol	Chain	Res	Type
2	B	152	TYR
2	B	153	ILE
2	B	159	SER
2	B	163	THR
2	B	172	LEU
2	B	176	ARG
2	B	193	CYS
2	B	197	CYS
2	B	203	ILE
2	B	206	VAL
2	B	237	ARG
2	B	246	ASN
2	B	250	THR
2	B	253	GLN
2	B	260	VAL
2	B	276	VAL
2	B	301	GLN
2	B	314	MET
2	B	322	VAL
2	B	323	LYS
2	B	330	THR
2	B	341	SER
2	B	342	VAL
2	B	355	ASP
2	B	377	THR
2	B	378	TYR
2	B	386	LEU
2	B	451	SER
2	B	453	LYS
3	C	100	ILE
3	C	103	HIS
3	C	110	LEU
3	C	114	TYR
3	C	115	ASN
3	C	145	ILE
3	C	166	LEU
3	C	175	ASN
3	C	177	GLN
3	C	179	LEU
3	C	180	VAL
3	C	192	THR
3	C	195	GLN

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Mol	Chain	Res	Type
3	C	217	HIS
3	C	250	LEU
3	C	308	ASN
3	C	315	TRP
3	C	317	ASN
3	C	343	HIS
3	C	344	LEU
3	C	361	ASN
3	C	364	ASP
3	C	365	ASN
3	C	367	ILE
3	C	371	THR
3	C	374	THR
3	C	383	THR
3	C	387	ILE
3	C	390	ASN
3	C	391	ARG
3	C	396	GLU
1	D	122	LEU
1	D	126	VAL
1	D	127	ILE
1	D	135	LEU
1	D	159	ARG
1	D	161	CYS
1	D	162	ARG
1	D	171	ARG
1	D	174	ASP
1	D	185	LEU
1	D	192	ASP
2	E	151	LEU
2	E	152	TYR
2	E	153	ILE
2	E	163	THR
2	E	184	SER
2	E	193	CYS
2	E	206	VAL
2	E	224	MET
2	E	237	ARG
2	E	246	ASN
2	E	253	GLN
2	E	255	ARG
2	E	276	VAL

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Mol	Chain	Res	Type
2	E	280	THR
2	E	301	GLN
2	E	308	THR
2	E	323	LYS
2	E	325	HIS
2	E	330	THR
2	E	331	VAL
2	E	342	VAL
2	E	377	THR
2	E	378	TYR
2	E	386	LEU
2	E	398	ASP
2	E	418	TRP
2	E	421	GLN
2	E	423	THR
2	E	453	LYS
3	F	100	ILE
3	F	103	HIS
3	F	108	ARG
3	F	166	LEU
3	F	169	ILE
3	F	175	ASN
3	F	177	GLN
3	F	192	THR
3	F	195	GLN
3	F	198	LEU
3	F	217	HIS
3	F	237	SER
3	F	250	LEU
3	F	276	LEU
3	F	295	PHE
3	F	305	THR
3	F	308	ASN
3	F	315	TRP
3	F	317	ASN
3	F	343	HIS
3	F	344	LEU
3	F	364	ASP
3	F	365	ASN
3	F	367	ILE
3	F	379	MET
3	F	383	THR

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Mol	Chain	Res	Type
3	F	387	ILE
3	F	390	ASN
3	F	391	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	139	ASN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	228	GLN
2	B	253	GLN
2	B	296	ASN
2	B	332	GLN
2	B	336	ASN
2	B	339	GLN
2	B	351	ASN
2	B	370	HIS
2	B	382	ASN
2	B	408	HIS
2	B	421	GLN
3	C	103	HIS
3	C	111	GLN
3	C	115	ASN
3	C	117	ASN
3	C	119	GLN
3	C	177	GLN
3	C	195	GLN
3	C	230	ASN
3	C	307	HIS
3	C	308	ASN
3	C	317	ASN
3	C	325	ASN
3	C	365	ASN
3	C	390	ASN
1	D	134	GLN

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Mol	Chain	Res	Type
1	D	139	ASN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	158	ASN
2	E	160	ASN
2	E	164	ASN
2	E	189	GLN
2	E	228	GLN
2	E	253	GLN
2	E	296	ASN
2	E	325	HIS
2	E	332	GLN
2	E	336	ASN
2	E	351	ASN
2	E	359	GLN
2	E	382	ASN
2	E	393	GLN
2	E	408	HIS
2	E	421	GLN
2	E	429	HIS
3	F	103	HIS
3	F	117	ASN
3	F	119	GLN
3	F	177	GLN
3	F	189	ASN
3	F	195	GLN
3	F	230	ASN
3	F	239	GLN
3	F	307	HIS
3	F	308	ASN
3	F	350	GLN
3	F	390	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 ⓘ

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	G	1	5,2	14,14,15	0.63	0	17,19,21	1.04	1 (5%)
5	NAG	G	2	5	14,14,15	1.05	1 (7%)	17,19,21	1.27	2 (11%)
5	MAN	G	3	5	11,11,12	0.96	0	15,15,17	1.35	2 (13%)
5	MAN	G	4	5	11,11,12	1.15	0	15,15,17	0.78	0
5	NAG	G	5	5	14,14,15	1.44	1 (7%)	17,19,21	1.75	3 (17%)
5	GAL	G	6	5	11,11,12	1.10	0	15,15,17	0.73	0
5	SIA	G	7	5	20,20,21	1.63	4 (20%)	21,28,31	1.16	2 (9%)
5	MAN	G	8	5	11,11,12	0.74	0	15,15,17	0.98	2 (13%)
5	NAG	H	1	5,2	14,14,15	0.67	0	17,19,21	1.05	1 (5%)
5	NAG	H	2	5	14,14,15	1.11	0	17,19,21	1.33	2 (11%)
5	MAN	H	3	5	11,11,12	1.23	0	15,15,17	0.73	0
5	MAN	H	4	5	11,11,12	1.66	1 (9%)	15,15,17	1.52	3 (20%)
5	NAG	H	5	5	14,14,15	1.67	2 (14%)	17,19,21	0.89	1 (5%)
5	GAL	H	6	5	11,11,12	1.04	1 (9%)	15,15,17	0.68	0
5	SIA	H	7	5	20,20,21	2.65	7 (35%)	21,28,31	1.77	3 (14%)
5	MAN	H	8	5	11,11,12	0.91	0	15,15,17	1.00	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	1/1/5/7	5/6/23/26	0/1/1/1
5	MAN	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	NAG	G	5	5	1/1/5/7	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	G	6	5	-	2/2/19/22	0/1/1/1
5	SIA	G	7	5	-	6/18/34/38	0/1/1/1
5	MAN	G	8	5	1/1/4/5	2/2/19/22	0/1/1/1
5	NAG	H	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	H	2	5	1/1/5/7	6/6/23/26	0/1/1/1
5	MAN	H	3	5	-	2/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	NAG	H	5	5	1/1/5/7	3/6/23/26	0/1/1/1
5	GAL	H	6	5	-	2/2/19/22	0/1/1/1
5	SIA	H	7	5	1/1/8/9	5/18/34/38	0/1/1/1
5	MAN	H	8	5	-	1/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	7	SIA	C7-C6	6.42	1.60	1.52
5	H	7	SIA	C6-C5	4.90	1.60	1.53
5	H	5	NAG	C1-C2	4.81	1.58	1.52
5	H	4	MAN	C2-C3	4.42	1.59	1.52
5	H	7	SIA	C4-C5	4.17	1.57	1.53
5	H	7	SIA	O6-C6	4.06	1.50	1.44
5	H	7	SIA	C2-C1	3.96	1.57	1.52
5	G	7	SIA	O6-C6	3.65	1.49	1.44
5	G	5	NAG	C1-C2	3.53	1.57	1.52
5	G	7	SIA	C2-C1	3.37	1.56	1.52
5	H	7	SIA	O6-C2	2.96	1.49	1.43
5	H	7	SIA	C8-C7	2.73	1.58	1.53
5	G	7	SIA	C7-C6	2.47	1.56	1.52
5	G	7	SIA	C4-C5	2.37	1.55	1.53
5	H	5	NAG	C3-C2	2.32	1.57	1.52
5	H	6	GAL	C1-C2	2.20	1.57	1.52
5	G	2	NAG	C4-C5	2.07	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	7	SIA	O6-C2-C3	6.55	119.36	110.56
5	G	5	NAG	C4-C3-C2	5.09	118.47	111.02
5	H	4	MAN	C2-C3-C4	3.96	117.82	110.86
5	G	1	NAG	C2-N2-C7	-3.45	118.28	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	MAN	C3-C4-C5	3.34	116.30	110.23
5	H	2	NAG	C4-C3-C2	3.28	115.82	111.02
5	G	2	NAG	C3-C4-C5	3.15	115.94	110.23
5	H	2	NAG	C3-C4-C5	2.94	115.57	110.23
5	H	8	MAN	C1-O5-C5	2.93	116.11	112.19
5	G	5	NAG	C3-C4-C5	2.69	115.10	110.23
5	G	8	MAN	C1-O5-C5	2.63	115.71	112.19
5	G	7	SIA	O1B-C1-C2	2.60	119.47	112.71
5	G	5	NAG	C1-C2-N2	2.56	114.46	110.43
5	G	3	MAN	C1-O5-C5	2.39	115.39	112.19
5	H	1	NAG	C4-C3-C2	2.30	114.39	111.02
5	G	7	SIA	O1A-C1-C2	-2.28	117.93	122.85
5	G	2	NAG	C2-N2-C7	-2.20	119.95	122.90
5	H	4	MAN	C3-C4-C5	2.13	114.10	110.23
5	G	8	MAN	C1-C2-C3	2.12	112.73	109.64
5	H	4	MAN	C1-C2-C3	2.09	112.68	109.64
5	H	5	NAG	C4-C3-C2	2.07	114.06	111.02
5	H	7	SIA	O10-C10-C11	-2.07	118.36	122.05
5	H	7	SIA	O1B-C1-C2	2.07	118.09	112.71

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	2	NAG	C1
5	G	5	NAG	C1
5	G	8	MAN	C1
5	H	2	NAG	C1
5	H	5	NAG	C1
5	H	7	SIA	C2

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	G	5	NAG	C3-C2-N2-C7
5	G	5	NAG	C8-C7-N2-C2
5	G	5	NAG	O7-C7-N2-C2
5	G	7	SIA	C11-C10-N5-C5
5	G	7	SIA	O10-C10-N5-C5

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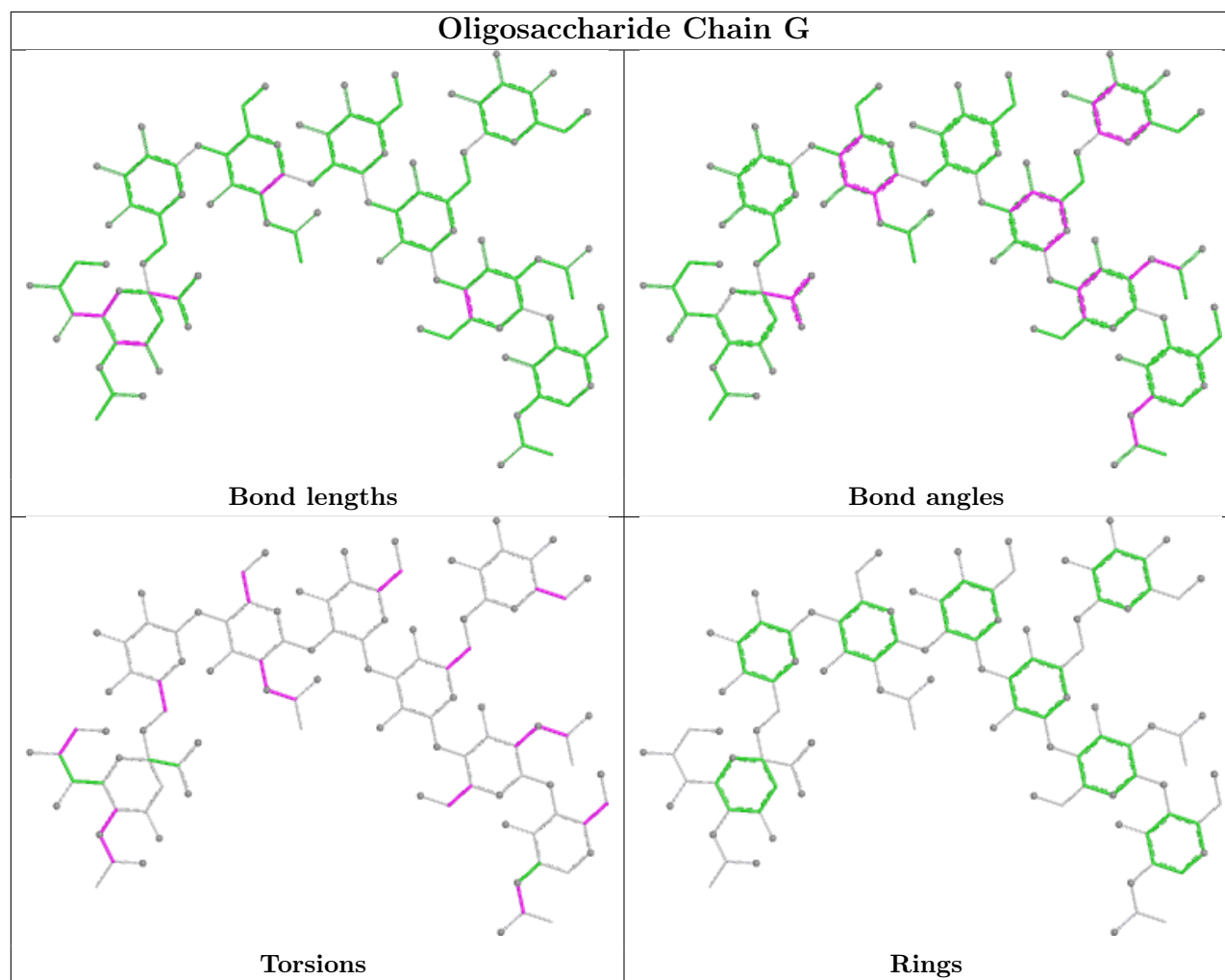
Mol	Chain	Res	Type	Atoms
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	H	7	SIA	C11-C10-N5-C5
5	H	7	SIA	O10-C10-N5-C5
5	H	3	MAN	C4-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
5	H	3	MAN	O5-C5-C6-O6
5	G	6	GAL	O5-C5-C6-O6
5	H	6	GAL	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	G	5	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	H	6	GAL	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	8	MAN	O5-C5-C6-O6
5	G	8	MAN	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	3	MAN	O5-C5-C6-O6
5	G	7	SIA	O8-C8-C9-O9
5	G	7	SIA	C7-C8-C9-O9
5	G	6	GAL	C4-C5-C6-O6
5	G	7	SIA	C4-C5-N5-C10
5	H	8	MAN	O5-C5-C6-O6
5	H	5	NAG	C8-C7-N2-C2
5	G	7	SIA	C6-C5-N5-C10
5	H	2	NAG	C1-C2-N2-C7
5	H	5	NAG	O7-C7-N2-C2
5	H	7	SIA	O8-C8-C9-O9
5	H	2	NAG	C3-C2-N2-C7
5	H	5	NAG	C3-C2-N2-C7
5	G	4	MAN	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C1-C2-N2-C7
5	G	3	MAN	C4-C5-C6-O6
5	H	7	SIA	O1A-C1-C2-O6
5	H	7	SIA	O7-C7-C8-C9

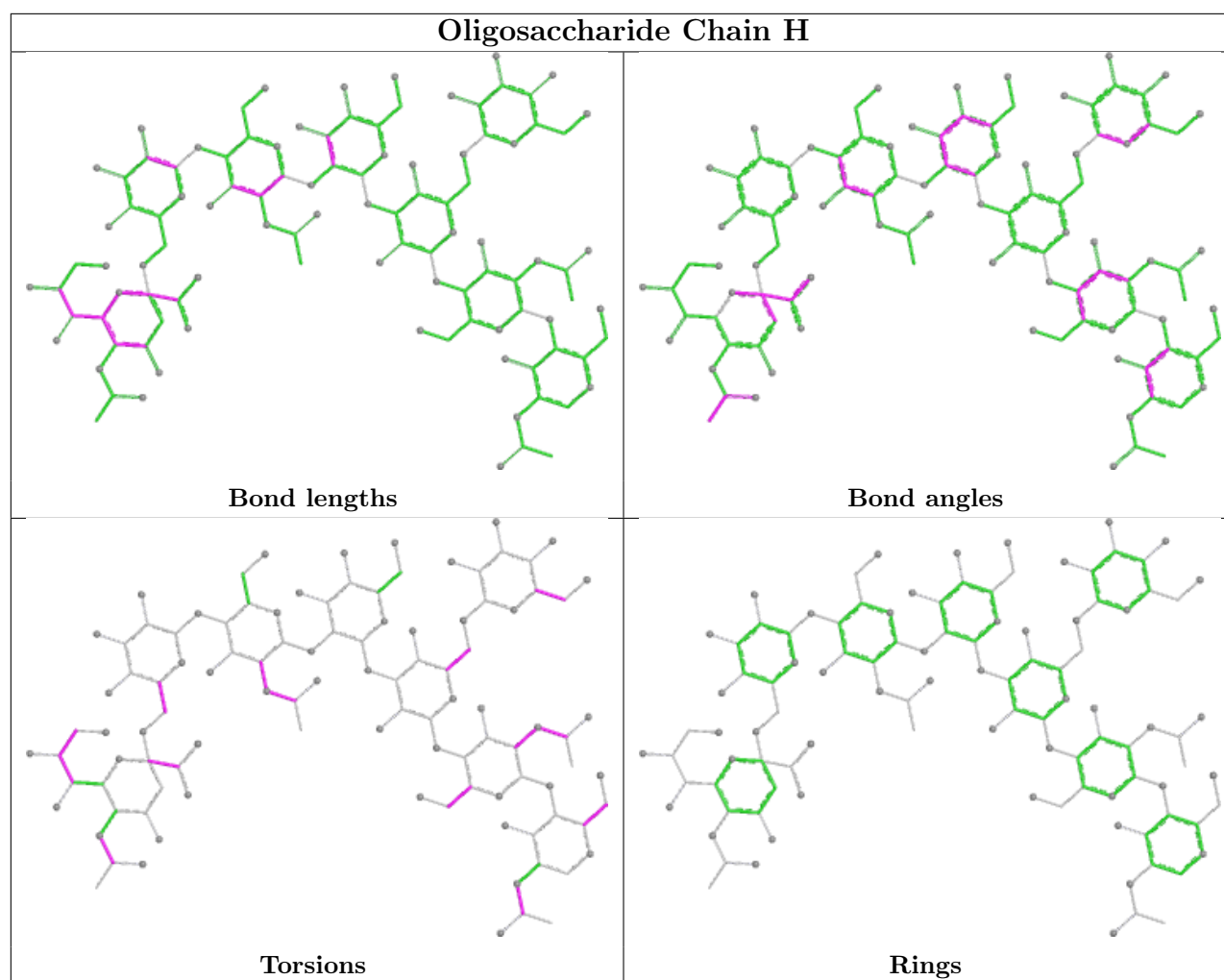
There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	6	GAL	2	0
5	H	3	MAN	2	0
5	G	7	SIA	4	0
5	H	7	SIA	2	0
5	H	8	MAN	2	0
5	G	6	GAL	2	0
5	G	4	MAN	1	0
5	G	3	MAN	1	0
5	H	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	74/197 (37%)	0.84	8 (10%) 11 9	77, 91, 103, 108	0
1	D	74/197 (37%)	0.37	3 (4%) 41 23	79, 93, 104, 108	0
2	B	308/458 (67%)	0.39	7 (2%) 61 35	65, 82, 98, 108	0
2	E	308/458 (67%)	0.38	7 (2%) 61 35	64, 83, 97, 106	0
3	C	301/317 (94%)	0.46	10 (3%) 49 28	67, 84, 98, 105	0
3	F	296/317 (93%)	0.45	13 (4%) 39 22	67, 85, 97, 105	0
4	M	5/5 (100%)	0.51	0 100 100	76, 80, 84, 85	0
4	N	5/5 (100%)	0.60	0 100 100	83, 87, 91, 93	0
All	All	1371/1954 (70%)	0.44	48 (3%) 47 27	64, 85, 100, 108	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	5.5
1	A	126	VAL	5.0
1	A	121	VAL	4.6
2	E	399	GLY	3.7
2	E	210	GLU	3.7
3	C	393	THR	3.7
3	C	363	TYR	3.6
1	D	126	VAL	3.5
3	C	394	ILE	3.4
3	F	163	GLN	3.4
3	F	135	CYS	3.2
3	C	321	LYS	3.0
3	F	360	PRO	3.0
3	F	103	HIS	2.8
2	B	220	GLU	2.8
2	B	399	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	341	SER	2.7
2	B	210	GLU	2.7
2	B	371	ASN	2.7
2	E	261	ASP	2.7
3	C	111	GLN	2.7
3	C	330	ASP	2.6
1	A	125	LYS	2.6
3	C	215	PHE	2.6
2	B	413	ASN	2.5
2	E	292	TYR	2.5
2	E	372	GLY	2.5
3	F	342	GLY	2.5
1	D	127	ILE	2.4
1	D	122	LEU	2.4
2	E	154	ASP	2.4
1	A	132	HIS	2.3
1	A	124	ARG	2.2
3	C	157	ALA	2.2
3	C	115	ASN	2.2
3	F	389	PHE	2.2
3	F	378	SER	2.1
3	F	330	ASP	2.1
3	F	367	ILE	2.1
3	F	102	THR	2.1
1	A	162	ARG	2.1
3	F	392	LEU	2.1
3	F	222	GLY	2.0
2	B	403	TRP	2.0
3	C	392	LEU	2.0
1	A	122	LEU	2.0
2	B	286	CYS	2.0
3	F	341	ALA	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,

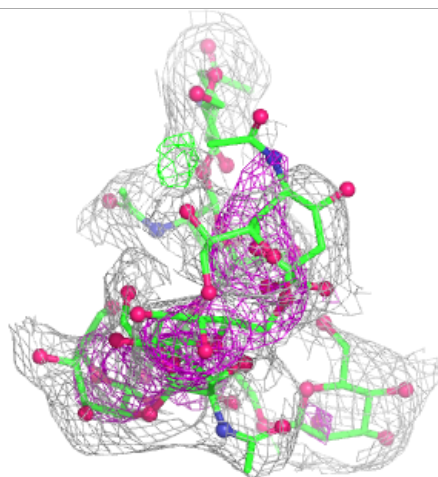
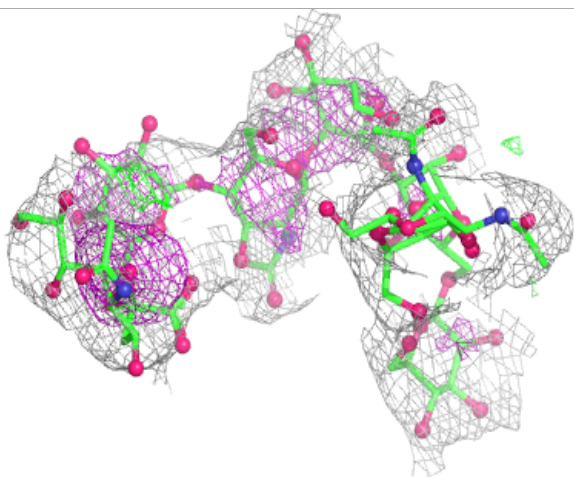
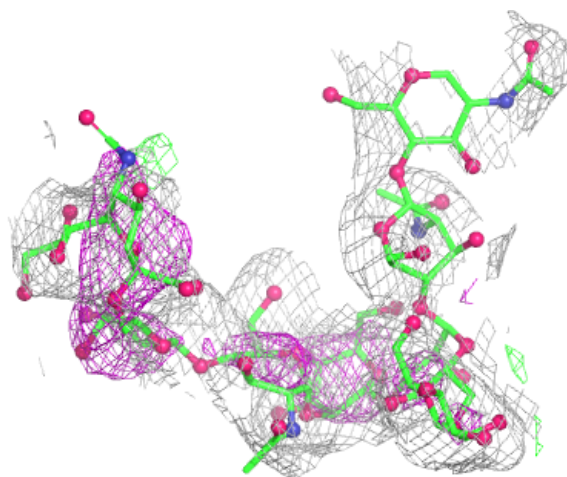
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

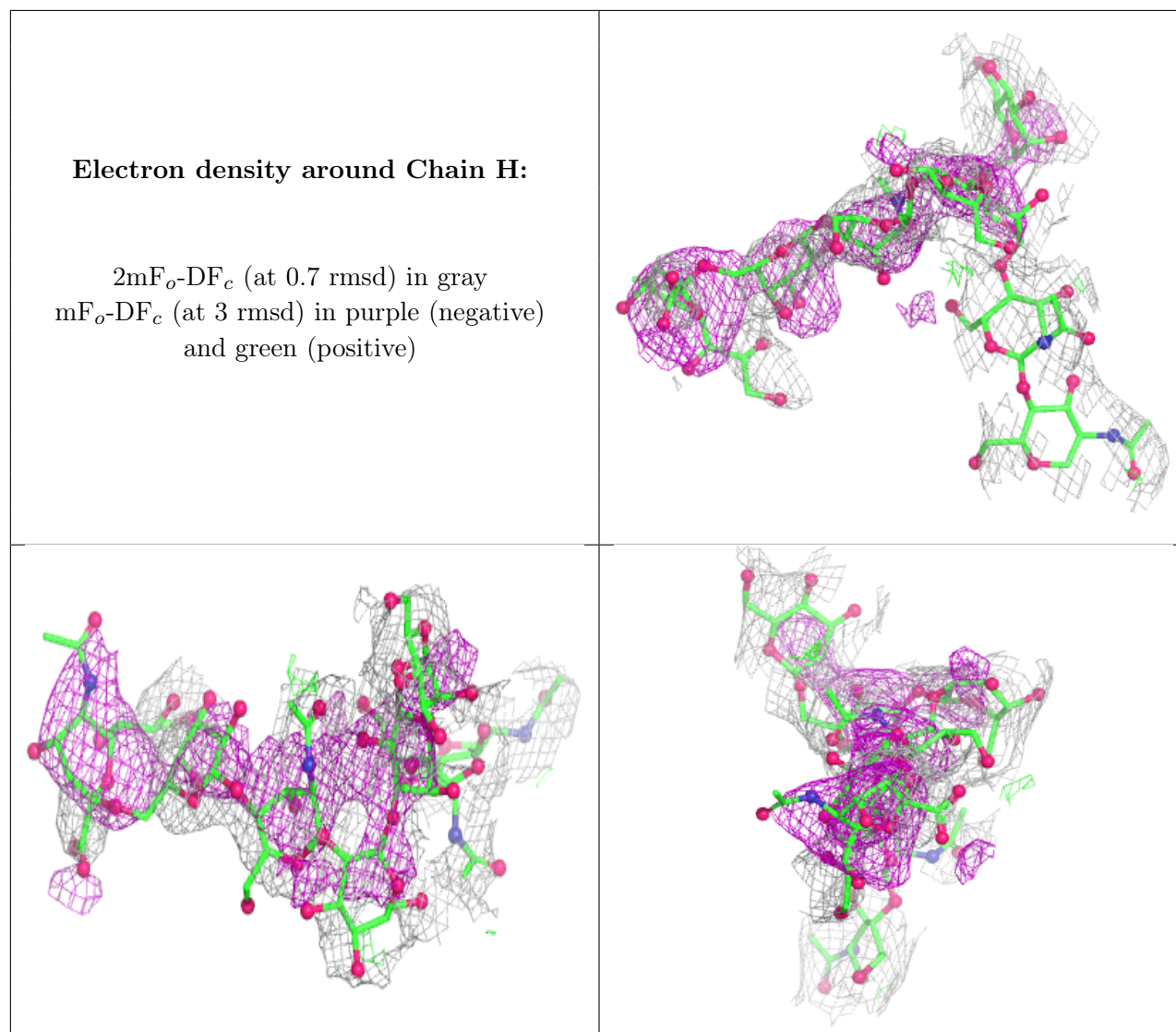
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	1	14/15	-	-	85,91,95,99	0
5	NAG	G	2	14/15	-	-	95,105,108,111	0
5	MAN	G	3	11/12	-	-	111,113,114,115	0
5	MAN	G	4	11/12	-	-	115,115,116,116	0
5	NAG	G	5	14/15	-	-	107,114,115,117	0
5	GAL	G	6	11/12	-	-	116,117,118,119	0
5	SIA	G	7	20/21	-	-	107,111,117,118	0
5	MAN	G	8	11/12	-	-	106,110,112,115	0
5	NAG	H	1	14/15	-	-	90,94,97,101	0
5	NAG	H	2	14/15	-	-	104,108,112,114	0
5	MAN	H	3	11/12	-	-	117,118,120,121	0
5	MAN	H	4	11/12	-	-	111,116,119,120	0
5	NAG	H	5	14/15	-	-	103,109,112,112	0
5	GAL	H	6	11/12	-	-	107,110,112,112	0
5	SIA	H	7	20/21	-	-	104,113,114,114	0
5	MAN	H	8	11/12	-	-	114,117,119,122	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)





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
6	CA	F	501	1/1	0.88	0.14	108,108,108,108	0
6	CA	B	502	1/1	0.97	0.04	40,40,40,40	0
6	CA	E	502	1/1	0.98	0.09	26,26,26,26	0
6	CA	C	501	1/1	0.99	0.03	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.