



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 2AJD / pdb_00002ajd
Title : Porcine dipeptidyl peptidase IV (CD26) in complex with L-Pro-boro-L-Pro (boroPro)
Authors : Engel, M.; Hoffmann, T.; Manhart, S.; Heiser, U.; Chambre, S.; Huber, R.; Demuth, H.U.; Bode, W.
Deposited on : 2005-08-01
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

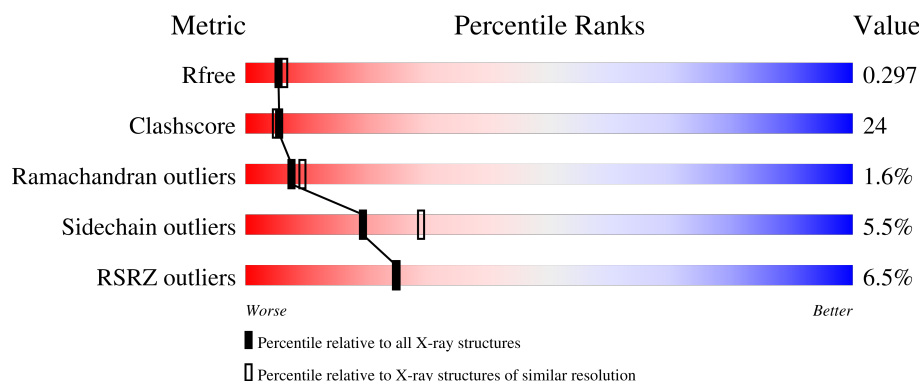
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

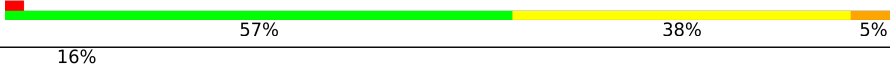
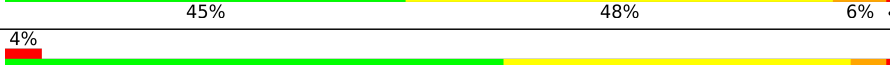
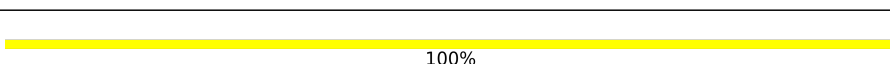
The reported resolution of this entry is 2.56 Å.

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.



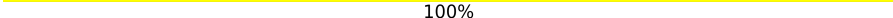
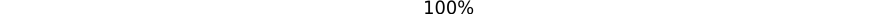
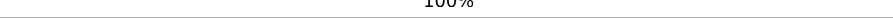
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	728	
1	B	728	
1	C	728	
1	D	728	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	H	2	 50%50%
2	I	2	 50%50%
2	K	2	 100%
2	L	2	 100%
2	M	2	 50%50%
3	G	3	 100%
3	J	3	 67%33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 25139 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	80	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	83	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

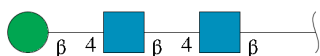
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

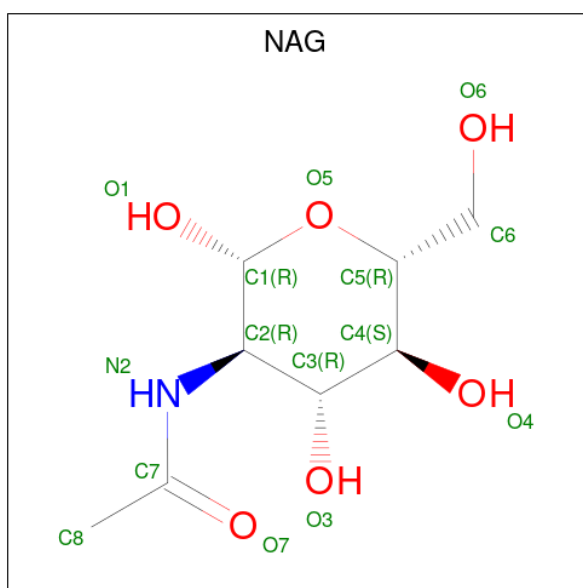
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

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



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	3	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



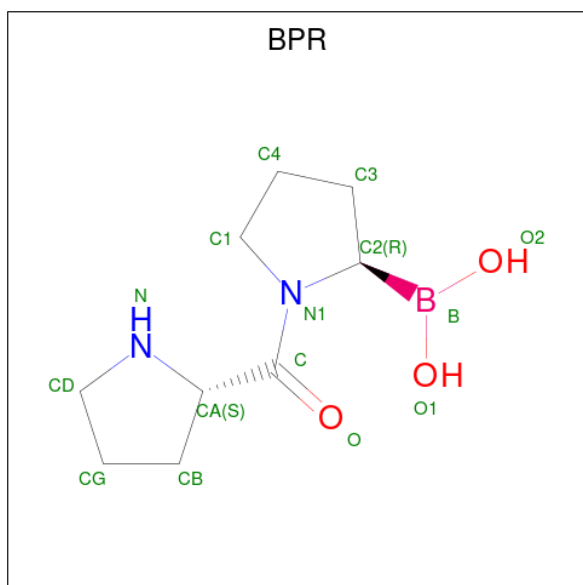
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (2R)-N-[(2R)-2-(DIHYDROXYBORYL)-1-L-PROLYLPYRROLIDIN-2-YL]-N-[(5R)-5-(DIHYDROXYBORYL)-1-L-PROLYLPYRROLIDIN-2-YL]-L-PROLINAMIDE (CCD ID: BPR) (formula: C₉H₁₇BN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	B	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	C	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
6	D	1	Total	B	C	N	O	0	0
			15	1	9	2	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	163	Total	O	0	0
			163	163		
7	B	224	Total	O	0	0
			224	224		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	138	Total 138	O 138	0	0
7	D	186	Total 186	O 186	0	0

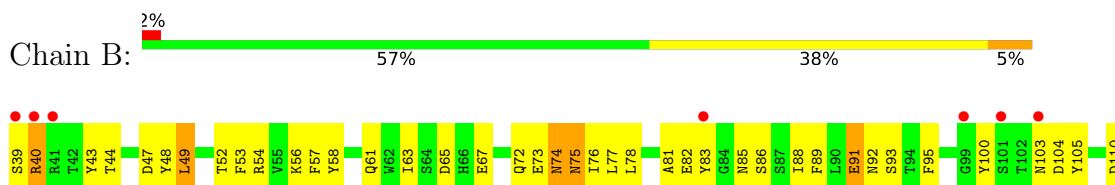
3 Residue-property plots

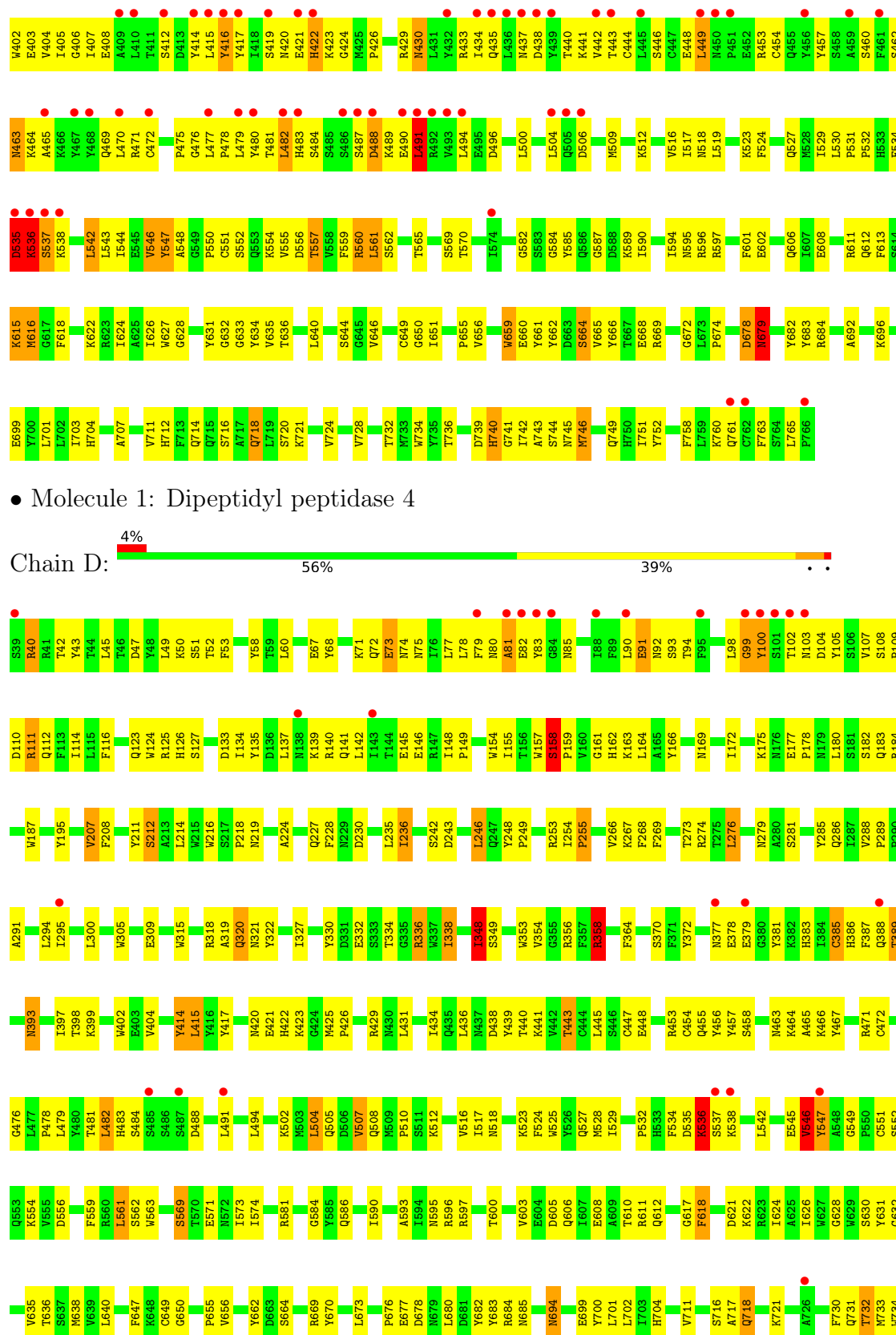
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4







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

Chain E:  100%



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

Chain F:  100%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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

Chain K:  100%



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

Chain L:  100%

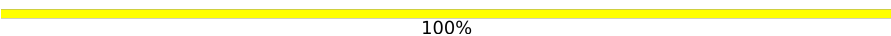


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2
BMA3

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

Chain J:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 122.07Å 134.03Å 111.41° 95.27° 94.52°	Depositor
Resolution (Å)	19.99 – 2.56 19.99 – 2.56	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.99-2.56) 96.8 (19.99-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.312 0.231 , 0.297	Depositor DCC
R_{free} test set	5808 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25139	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BPR, SO4, BMA

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	0.55	0/6141	1.04	31/8353 (0.4%)
1	B	0.59	0/6141	1.04	34/8353 (0.4%)
1	C	0.53	0/6141	1.03	31/8353 (0.4%)
1	D	0.57	0/6141	1.06	42/8353 (0.5%)
All	All	0.56	0/24564	1.04	138/33412 (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
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	GLU	N-CA-C	-11.96	98.69	113.28
1	D	378	GLU	N-CA-C	-11.27	99.57	113.20
1	B	656	VAL	N-CA-C	-10.60	94.92	109.55
1	D	656	VAL	N-CA-C	-9.38	99.83	110.05
1	D	744	SER	N-CA-C	-8.08	99.36	110.35
1	C	546	VAL	N-CA-C	8.02	120.03	108.48
1	A	212	SER	N-CA-C	7.81	120.97	110.35
1	C	150	ASN	N-CA-C	-7.64	99.73	110.50
1	B	150	ASN	N-CA-C	-7.62	100.45	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	ASN	N-CA-C	7.42	120.02	111.11
1	C	656	VAL	N-CA-C	-7.37	100.00	109.80
1	A	436	LEU	N-CA-C	7.33	121.14	111.75
1	C	633	GLY	N-CA-C	-7.31	102.89	113.86
1	A	207	VAL	N-CA-C	7.15	120.11	112.96
1	D	529	ILE	N-CA-C	-7.08	97.39	108.23
1	D	281	SER	N-CA-C	-7.03	101.76	110.41
1	D	664	SER	N-CA-C	7.02	118.93	111.28
1	B	201	TRP	N-CA-C	6.98	118.54	111.07
1	D	207	VAL	N-CA-C	6.98	117.13	111.62
1	B	562	SER	N-CA-C	6.92	117.63	108.07
1	B	454	CYS	N-CA-C	6.90	121.55	107.69
1	A	546	VAL	N-CA-C	6.86	118.68	108.46
1	B	321	ASN	N-CA-C	-6.84	103.00	112.30
1	B	664	SER	N-CA-C	6.84	118.81	111.36
1	D	536	LYS	N-CA-C	-6.82	101.53	110.33
1	A	656	VAL	N-CA-C	-6.79	99.97	109.21
1	B	546	VAL	N-CA-C	6.79	120.15	108.95
1	C	321	ASN	N-CA-C	-6.78	102.63	111.71
1	B	300	LEU	N-CA-C	-6.63	98.43	109.24
1	D	182	SER	N-CA-C	-6.62	100.99	110.59
1	B	448	GLU	N-CA-C	6.59	121.03	112.92
1	B	736	THR	N-CA-C	6.52	119.68	109.96
1	B	692	ALA	N-CA-C	6.51	120.09	111.75
1	D	743	ALA	N-CA-C	6.33	120.32	112.59
1	C	744	SER	N-CA-C	-6.31	101.61	110.50
1	A	683	TYR	N-CA-C	-6.29	103.73	111.40
1	C	615	LYS	N-CA-C	-6.22	104.40	112.23
1	C	529	ILE	N-CA-C	-6.19	98.95	107.99
1	C	664	SER	N-CA-C	6.16	117.79	111.14
1	D	45	LEU	N-CA-C	-6.15	104.66	111.36
1	D	158	SER	N-CA-C	-6.15	101.10	110.01
1	D	618	PHE	N-CA-C	6.14	119.72	112.72
1	C	448	GLU	N-CA-C	6.14	118.74	110.88
1	A	458	SER	N-CA-C	-6.13	99.98	109.24
1	A	601	PHE	N-CA-C	6.09	117.59	111.07
1	A	206	GLU	N-CA-C	6.09	121.76	113.97
1	D	274	ARG	N-CA-C	6.05	117.88	111.28
1	B	205	GLU	N-CA-C	6.05	117.95	111.36
1	C	740	HIS	N-CA-C	6.04	117.86	111.28
1	C	449	LEU	N-CA-C	-6.02	104.08	112.45
1	A	207	VAL	CB-CA-C	-5.96	105.81	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	GLU	N-CA-C	-5.95	105.97	113.23
1	A	450	ASN	CA-C-N	5.94	126.37	119.47
1	A	450	ASN	C-N-CA	5.94	126.37	119.47
1	C	537	SER	N-CA-C	-5.94	104.70	113.61
1	D	358	ARG	N-CA-C	-5.92	102.81	108.13
1	B	411	THR	N-CA-C	-5.91	101.45	110.14
1	D	338	ILE	N-CA-C	5.89	117.08	108.53
1	D	448	GLU	N-CA-C	5.86	119.74	112.59
1	D	319	ALA	N-CA-C	-5.85	98.16	108.23
1	D	606	GLN	N-CA-C	-5.83	104.52	111.69
1	A	677	GLU	N-CA-C	-5.82	105.94	113.16
1	D	320	GLN	N-CA-C	5.80	123.16	110.80
1	C	357	PHE	N-CA-C	-5.79	106.25	113.55
1	D	364	PHE	N-CA-C	5.76	119.00	110.48
1	D	547	TYR	N-CA-C	-5.76	98.54	110.80
1	A	547	TYR	N-CA-C	-5.74	102.79	111.34
1	A	281	SER	N-CA-C	-5.72	103.37	110.41
1	C	547	TYR	N-CA-C	-5.72	98.62	110.80
1	B	365	THR	N-CA-C	-5.71	103.00	110.53
1	B	357	PHE	N-CA-C	-5.71	105.05	113.61
1	C	692	ALA	N-CA-C	5.68	117.93	111.11
1	C	206	GLU	N-CA-C	5.67	120.31	113.17
1	C	236	ILE	N-CA-C	-5.67	100.16	109.12
1	C	683	TYR	N-CA-C	-5.65	104.51	111.40
1	D	300	LEU	N-CA-C	-5.65	99.53	108.73
1	D	348	ILE	N-CA-C	5.64	117.03	108.80
1	A	321	ASN	N-CA-C	-5.59	104.88	112.26
1	B	560	ARG	N-CA-C	5.59	117.51	108.34
1	A	617	GLY	N-CA-C	5.59	122.24	113.86
1	A	659	TRP	N-CA-C	5.58	119.60	112.34
1	C	679	ASN	N-CA-C	5.58	119.08	112.72
1	A	158	SER	N-CA-C	-5.56	101.95	110.07
1	C	392	SER	N-CA-C	5.54	119.75	113.15
1	D	546	VAL	N-CA-C	5.53	117.62	108.99
1	B	390	ASP	N-CA-C	5.53	119.72	112.92
1	D	563	TRP	N-CA-C	-5.53	105.34	111.36
1	C	684	ARG	N-CA-C	5.49	117.27	111.28
1	B	547	TYR	N-CA-C	-5.49	99.10	110.80
1	D	332	GLU	N-CA-C	5.49	118.02	111.71
1	D	463	ASN	N-CA-C	5.46	117.66	111.11
1	C	601	PHE	N-CA-C	5.45	116.90	111.07
1	B	209	SER	N-CA-C	-5.42	104.74	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	584	GLY	N-CA-C	5.42	119.11	111.42
1	A	397	ILE	N-CA-C	-5.41	107.85	113.10
1	B	753	THR	N-CA-C	-5.41	105.08	110.97
1	B	49	LEU	N-CA-C	5.40	117.24	111.36
1	D	255	PRO	N-CA-C	-5.39	101.37	112.47
1	A	545	GLU	N-CA-C	-5.38	99.96	108.73
1	B	75	ASN	N-CA-C	-5.37	102.10	110.42
1	A	163	LYS	N-CA-C	-5.34	103.56	110.19
1	B	484	SER	N-CA-C	-5.34	101.01	109.76
1	B	402	TRP	N-CA-C	-5.32	101.39	108.74
1	C	616	MET	N-CA-C	-5.32	102.40	110.28
1	A	92	ASN	N-CA-C	-5.31	99.48	110.80
1	C	430	ASN	N-CA-C	5.31	117.46	109.23
1	B	711	VAL	N-CA-C	-5.31	99.31	106.85
1	A	300	LEU	N-CA-C	-5.31	99.87	108.52
1	A	633	GLY	N-CA-C	-5.28	108.11	114.66
1	B	436	LEU	N-CA-C	5.28	118.98	112.54
1	D	630	SER	CB-CA-C	-5.28	110.50	116.63
1	C	659	TRP	N-CA-C	5.27	117.77	111.71
1	D	504	LEU	N-CA-C	5.23	117.89	111.82
1	B	388	GLN	N-CA-C	-5.22	100.66	108.96
1	C	89	PHE	N-CA-C	-5.20	107.07	113.41
1	B	561	LEU	N-CA-C	-5.19	100.62	108.67
1	A	410	LEU	N-CA-C	5.18	115.88	107.23
1	B	425	MET	CA-C-N	5.16	125.24	119.87
1	B	425	MET	C-N-CA	5.16	125.24	119.87
1	D	569	SER	N-CA-C	5.15	117.30	111.02
1	A	174	VAL	N-CA-C	5.15	115.26	107.75
1	D	617	GLY	N-CA-C	5.14	120.11	113.27
1	A	750	HIS	N-CA-C	5.14	116.57	111.07
1	D	236	ILE	N-CA-C	-5.14	101.06	108.87
1	D	683	TYR	N-CA-C	-5.13	104.62	111.24
1	D	212	SER	N-CA-C	5.13	117.73	110.50
1	D	562	SER	N-CA-C	5.12	118.06	109.96
1	D	447	CYS	N-CA-C	5.12	117.53	111.33
1	D	414	TYR	N-CA-C	5.12	117.45	109.52
1	B	338	ILE	N-CA-C	5.11	116.63	108.87
1	D	443	THR	N-CA-C	5.09	116.71	108.41
1	A	744	SER	N-CA-C	-5.08	103.77	110.43
1	C	199	THR	N-CA-C	5.08	118.40	110.32
1	C	215	TRP	N-CA-C	5.08	116.59	107.80
1	C	678	ASP	CB-CA-C	-5.08	109.13	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	492	ARG	N-CA-C	5.07	116.12	108.07
1	B	332	GLU	N-CA-C	5.04	118.53	112.38
1	C	560	ARG	N-CA-C	5.04	116.58	108.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	256	TYR	Sidechain
1	C	285	TYR	Sidechain
1	D	700	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	5966	0	5662	253	0
1	B	5966	0	5662	231	0
1	C	5966	0	5661	374	0
1	D	5966	0	5661	266	0
2	E	28	0	25	0	0
2	F	28	0	25	4	0
2	H	28	0	25	4	0
2	I	28	0	25	2	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	4	0
3	G	39	0	34	1	0
3	J	39	0	34	1	0
4	A	56	0	52	1	0
4	B	56	0	52	2	0
4	C	70	0	65	6	0
4	D	28	0	26	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	15	0	17	2	0
6	B	15	0	17	3	0
6	C	15	0	17	4	0
6	D	15	0	17	1	0
7	A	163	0	0	14	0
7	B	224	0	0	14	0
7	C	138	0	0	22	0
7	D	186	0	0	13	0
All	All	25139	0	23152	1115	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 24.

All (1115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HG2	1:C:537:SER:H	1.09	1.18
1:D:600:THR:HG22	2:M:1:NAG:H83	1.42	1.02
1:A:500:LEU:HA	1:A:503:MET:HE3	1.43	1.00
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.65	0.95
1:D:393:ASN:H	1:D:393:ASN:HD22	1.11	0.92
1:A:453:ARG:HH21	1:A:479:LEU:HB2	1.36	0.91
1:C:536:LYS:HG2	1:C:537:SER:N	1.86	0.91
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.72	0.89
1:D:581:ARG:HB2	1:D:605:ASP:OD2	1.74	0.88
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.75	0.87
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.40	0.86
1:A:67:GLU:HB3	1:A:78:LEU:HD11	1.56	0.86
1:A:377:ASN:HB2	1:A:381:TYR:H	1.40	0.86
1:C:382:LYS:H	1:C:403:GLU:HG2	1.39	0.85
1:C:536:LYS:CG	1:C:537:SER:H	1.88	0.85
1:C:696:LYS:HG2	1:C:728:VAL:HG22	1.57	0.84
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.13	0.84
1:C:516:VAL:HG11	1:C:523:LYS:HB2	1.60	0.84
1:C:516:VAL:HG12	1:C:517:ILE:H	1.41	0.84
1:C:184:ARG:HD3	1:C:186:THR:O	1.77	0.84
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.43	0.83
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.59	0.82
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.61	0.81
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.46	0.81
1:C:612:GLN:O	1:C:615:LYS:HG2	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HD3	1:B:186:THR:O	1.81	0.81
1:C:343:ARG:HG3	1:C:343:ARG:HH11	1.46	0.81
1:A:377:ASN:HB3	1:A:379:GLU:H	1.46	0.80
1:B:500:LEU:HA	1:B:503:MET:HE3	1.63	0.80
1:B:175:LYS:NZ	1:B:178:PRO:HA	1.97	0.80
1:D:718:GLN:HE22	1:D:721:LYS:NZ	1.81	0.79
1:C:438:ASP:OD2	1:C:441:LYS:HG3	1.82	0.79
1:D:327:ILE:HD13	1:D:389:THR:HG23	1.66	0.78
1:B:113:PHE:HE2	1:B:162:HIS:ND1	1.82	0.77
1:A:460:SER:HB2	1:A:471:ARG:HH21	1.48	0.76
1:C:221:THR:HB	1:C:222:PHE:CD2	2.20	0.76
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.01	0.76
1:D:40:ARG:HH11	1:D:40:ARG:HB2	1.50	0.75
1:A:92:ASN:O	1:A:94:THR:N	2.19	0.75
1:A:438:ASP:OD1	1:A:440:THR:HB	1.87	0.74
1:C:516:VAL:HG12	1:C:517:ILE:N	2.00	0.74
1:C:109:PRO:HG2	1:C:161:GLY:O	1.87	0.74
1:C:137:LEU:HA	7:C:1579:HOH:O	1.86	0.74
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.52	0.74
1:B:73:GLU:O	1:B:74:ASN:HB2	1.87	0.74
1:A:159:PRO:HG2	1:A:217:SER:O	1.88	0.74
1:C:666:TYR:CE2	6:C:801:BPR:HB1	2.23	0.74
1:A:414:TYR:CD2	1:A:433:ARG:HD2	2.22	0.73
1:B:393:ASN:HD22	1:B:393:ASN:H	1.35	0.73
1:C:330:TYR:CE1	1:C:335:GLY:HA2	2.24	0.73
1:D:377:ASN:HD21	1:D:383:HIS:CD2	2.06	0.73
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.03	0.73
1:B:356:ARG:HD3	1:B:551:CYS:SG	2.29	0.72
1:B:428:GLY:O	1:B:429:ARG:HD3	1.89	0.72
1:C:746:MET:HE2	1:C:746:MET:H	1.53	0.72
1:A:413:ASP:O	1:A:436:LEU:HB2	1.90	0.72
1:C:67:GLU:HB3	1:C:78:LEU:HD11	1.72	0.72
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.25	0.72
1:B:175:LYS:HZ3	1:B:178:PRO:HA	1.55	0.71
1:C:104:ASP:HA	7:C:1617:HOH:O	1.88	0.71
1:C:435:GLN:NE2	1:C:441:LYS:HD2	2.05	0.71
1:A:438:ASP:OD1	1:A:441:LYS:HG3	1.91	0.70
1:C:134:ILE:HD13	1:C:178:PRO:HB3	1.71	0.70
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.91	0.70
1:C:662:TYR:CE2	6:C:801:BPR:H12	2.26	0.70
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD11	1:A:544:ILE:HD11	1.72	0.70
1:D:377:ASN:ND2	1:D:383:HIS:HD2	1.89	0.70
1:C:416:TYR:CD1	1:C:416:TYR:N	2.58	0.70
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.73	0.70
1:B:378:GLU:CD	1:B:378:GLU:H	1.99	0.70
1:C:470:LEU:HD12	1:C:483:HIS:CE1	2.26	0.70
1:A:438:ASP:HB3	1:A:441:LYS:HD2	1.73	0.69
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.92	0.69
1:C:664:SER:O	1:C:668:GLU:HG3	1.92	0.69
1:D:425:MET:HE1	1:D:455:GLN:OE1	1.92	0.69
1:C:590:ILE:HG13	7:C:1555:HOH:O	1.92	0.69
1:B:457:TYR:CD2	1:B:470:LEU:HD13	2.27	0.69
1:D:377:ASN:HD21	1:D:383:HIS:HD2	1.40	0.69
1:C:471:ARG:HG2	1:C:480:TYR:HD2	1.55	0.69
1:B:133:ASP:HB3	1:B:142:LEU:HD21	1.75	0.69
1:D:676:PRO:HG2	1:D:677:GLU:OE1	1.93	0.69
1:A:718:GLN:HE21	1:A:718:GLN:HA	1.58	0.68
1:B:218:PRO:HB2	7:B:1586:HOH:O	1.92	0.68
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.59	0.68
1:B:143:ILE:HD12	1:B:143:ILE:H	1.58	0.68
1:C:87:SER:OG	4:C:767(A):NAG:H81	1.93	0.68
1:B:65:ASP:HB2	1:B:466:LYS:HD2	1.75	0.68
1:B:125:ARG:HH11	1:B:125:ARG:HG3	1.59	0.68
1:B:457:TYR:CE2	1:B:470:LEU:HD13	2.29	0.68
1:C:63:ILE:HD11	1:C:111:ARG:NH1	2.08	0.68
1:C:701:LEU:HD11	1:C:703:ILE:HD11	1.75	0.68
1:D:75:ASN:HD21	1:D:92:ASN:ND2	1.91	0.68
1:D:536:LYS:NZ	1:D:536:LYS:HB3	2.09	0.68
1:C:289:PRO:HG2	1:C:294:LEU:CD2	2.24	0.68
1:C:535:ASP:C	1:C:536:LYS:HD3	2.18	0.68
1:A:71:LYS:HD2	1:A:105:TYR:HE2	1.59	0.68
1:D:600:THR:HG22	2:M:1:NAG:C8	2.22	0.68
1:A:201:TRP:CH2	1:A:205:GLU:HG2	2.29	0.67
1:A:309:GLU:HG2	1:A:330:TYR:HB3	1.76	0.67
1:C:159:PRO:HB2	1:C:218:PRO:O	1.94	0.67
1:A:490:GLU:O	1:A:492:ARG:N	2.27	0.67
1:C:222:PHE:CD2	1:C:222:PHE:N	2.63	0.67
1:C:225:TYR:CE1	1:C:269:PHE:HB2	2.30	0.67
1:C:292:SER:HA	1:C:295:ILE:HD11	1.74	0.67
1:A:526:TYR:HE1	1:A:528:MET:HE2	1.60	0.67
1:C:517:ILE:HB	1:C:612:GLN:HE22	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:N	1:B:308:GLU:OE2	2.19	0.67
1:B:751:ILE:O	1:B:755:MET:HG3	1.94	0.67
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.24	0.67
1:B:39:SER:O	1:B:40:ARG:HB2	1.93	0.67
1:B:516:VAL:HG11	1:B:523:LYS:HB2	1.76	0.67
1:C:374:ILE:HD11	1:C:406:GLY:HA2	1.76	0.66
1:D:704:HIS:HD2	1:D:716:SER:OG	1.78	0.66
1:A:246:LEU:HD22	1:A:248:TYR:H	1.60	0.66
1:A:378:GLU:CD	1:A:378:GLU:H	2.03	0.66
1:C:743:ALA:HB1	7:C:1589:HOH:O	1.95	0.66
1:A:496:ASP:OD2	1:A:498:SER:HB3	1.96	0.66
1:B:83:TYR:CE2	4:B:767(A):NAG:H62	2.30	0.66
1:B:660:GLU:HG3	1:B:683:TYR:HD1	1.60	0.66
1:A:675:THR:HB	1:A:677:GLU:OE1	1.96	0.66
1:B:487:SER:OG	1:B:489:LYS:HB3	1.96	0.66
1:A:403:GLU:OE1	1:A:585:TYR:HA	1.97	0.65
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.31	0.65
2:F:1:NAG:H61	2:F:2:NAG:H82	1.78	0.65
1:C:307:THR:C	1:C:309:GLU:H	2.04	0.65
1:B:54:ARG:O	1:B:500:LEU:HD13	1.96	0.65
1:B:334:THR:OG1	1:B:336:ARG:HG2	1.96	0.65
1:B:403:GLU:OE1	1:B:585:TYR:HA	1.95	0.65
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.78	0.65
1:D:100:TYR:HE1	1:D:102:THR:HG1	1.45	0.65
1:D:169:ASN:N	1:D:169:ASN:HD22	1.94	0.65
1:C:516:VAL:HG13	1:C:524:PHE:O	1.96	0.65
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.31	0.65
1:C:487:SER:C	1:C:489:LYS:H	2.05	0.65
1:C:704:HIS:HD2	1:C:716:SER:OG	1.81	0.64
1:D:414:TYR:HA	1:D:436:LEU:HD13	1.79	0.64
1:B:327:ILE:CD1	1:B:389:THR:HG23	2.28	0.64
1:C:422:HIS:HA	7:C:1628:HOH:O	1.96	0.64
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.96	0.64
1:C:718:GLN:HE21	1:C:718:GLN:CA	2.10	0.64
1:D:242:SER:HB3	1:D:246:LEU:HD12	1.80	0.64
1:D:718:GLN:HE22	1:D:721:LYS:HZ1	1.46	0.64
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.78	0.64
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.78	0.64
1:C:416:TYR:HD1	1:C:416:TYR:H	1.43	0.64
1:C:138:ASN:C	1:C:140:ARG:H	2.06	0.64
1:C:221:THR:HB	1:C:222:PHE:CE2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.27	0.64
1:D:731:GLN:OE1	7:D:1507:HOH:O	2.14	0.64
1:C:291:ALA:O	1:C:295:ILE:HG13	1.97	0.64
1:C:746:MET:H	1:C:746:MET:CE	2.11	0.64
1:B:660:GLU:HG3	1:B:683:TYR:CD1	2.32	0.64
1:A:214:LEU:HD22	1:A:223:LEU:HD11	1.80	0.64
1:C:134:ILE:HG21	1:C:178:PRO:HB3	1.80	0.64
1:C:491:LEU:H	1:C:491:LEU:CD2	2.11	0.63
1:D:40:ARG:HB2	1:D:40:ARG:NH1	2.13	0.63
1:D:484:SER:O	1:D:488:ASP:HA	1.99	0.63
1:B:143:ILE:HD12	1:B:143:ILE:N	2.13	0.63
1:C:316:ILE:HG22	1:C:323:SER:HB2	1.79	0.63
1:A:704:HIS:HE1	1:A:711:VAL:O	1.81	0.63
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.33	0.63
1:A:327:ILE:CD1	1:A:389:THR:HG23	2.29	0.63
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.79	0.63
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.80	0.63
7:C:1562:HOH:O	1:D:243:ASP:HA	1.98	0.63
1:C:535:ASP:O	1:C:536:LYS:HB3	1.98	0.63
1:C:718:GLN:HA	1:C:718:GLN:NE2	2.12	0.63
1:C:343:ARG:HG3	1:C:343:ARG:NH1	2.12	0.62
1:C:453:ARG:O	1:C:453:ARG:HG2	1.99	0.62
1:D:393:ASN:H	1:D:393:ASN:ND2	1.89	0.62
1:B:516:VAL:CG1	1:B:523:LYS:HB2	2.28	0.62
1:C:484:SER:HB2	1:C:491:LEU:HD21	1.81	0.62
1:C:631:TYR:O	1:C:634:TYR:HB3	1.99	0.62
1:B:113:PHE:CE2	1:B:162:HIS:ND1	2.67	0.62
1:C:435:GLN:HG2	1:C:437:ASN:OD1	1.99	0.62
1:C:678:ASP:OD1	1:C:679:ASN:N	2.32	0.62
1:B:614:SER:HA	1:B:619:VAL:HG11	1.80	0.62
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.34	0.62
1:D:266:VAL:HG22	1:D:267:LYS:N	2.14	0.62
1:D:516:VAL:HG13	1:D:524:PHE:O	1.99	0.62
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.34	0.62
1:A:422:HIS:NE2	1:A:423:LYS:HD3	2.14	0.62
1:D:291:ALA:O	1:D:295:ILE:HG13	1.99	0.62
1:C:429:ARG:HB2	1:C:457:TYR:H	1.65	0.62
1:D:457:TYR:HA	1:D:471:ARG:O	2.00	0.62
1:A:65:ASP:HA	1:A:463:ASN:HB2	1.82	0.61
1:A:107:VAL:HG22	1:A:114:ILE:HG13	1.82	0.61
1:B:500:LEU:CA	1:B:503:MET:HE3	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:TYR:N	1:C:416:TYR:HD1	1.95	0.61
1:C:438:ASP:OD2	1:C:440:THR:HB	2.00	0.61
1:D:60:LEU:HD12	1:D:60:LEU:C	2.25	0.61
1:D:377:ASN:HB3	1:D:379:GLU:H	1.64	0.61
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.36	0.61
1:C:272:ASP:OD2	1:C:274:ARG:HB2	2.00	0.61
1:C:718:GLN:HE22	1:C:721:LYS:NZ	1.99	0.61
1:A:704:HIS:HD2	1:A:716:SER:OG	1.84	0.61
1:A:336:ARG:NH2	1:A:338:ILE:HD11	2.15	0.61
1:C:536:LYS:HD3	1:C:536:LYS:N	2.15	0.61
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.83	0.61
1:C:90:LEU:HD13	1:C:90:LEU:O	2.01	0.60
1:D:81:ALA:O	1:D:82:GLU:HB3	2.00	0.60
1:B:91:GLU:C	1:B:93:SER:H	2.09	0.60
3:G:2:NAG:O6	3:G:3:BMA:H2	2.00	0.60
1:A:271:VAL:HG22	1:A:284:SER:HB3	1.82	0.60
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.12	0.60
1:C:317:ARG:NH1	1:C:322:TYR:CD2	2.70	0.60
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.84	0.60
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.83	0.60
1:D:762:CYS:HA	7:D:1584:HOH:O	2.00	0.60
1:C:463:ASN:N	1:C:463:ASN:HD22	2.00	0.60
1:A:249:PRO:HD2	7:B:1521:HOH:O	2.00	0.60
1:A:378:GLU:CD	1:A:378:GLU:N	2.60	0.60
1:D:502:LYS:O	1:D:505:GLN:HG2	2.01	0.60
1:B:410:LEU:HD13	1:B:415:LEU:HD22	1.83	0.60
1:C:415:LEU:HD23	1:C:415:LEU:C	2.26	0.60
1:C:512:LYS:HE3	1:C:527:GLN:NE2	2.17	0.60
1:C:547:TYR:HD2	1:C:552:SER:HB2	1.67	0.60
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.84	0.60
1:C:87:SER:CB	4:C:767(A):NAG:H81	2.31	0.60
1:C:374:ILE:CD1	1:C:406:GLY:HA2	2.30	0.60
1:D:372:TYR:CE2	1:D:386:HIS:HD2	2.20	0.60
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.83	0.59
1:C:430:ASN:HB2	7:C:1527:HOH:O	2.02	0.59
1:A:435:GLN:HB3	1:A:441:LYS:HB2	1.84	0.59
1:D:98:LEU:HD22	1:D:142:LEU:HD12	1.84	0.59
1:D:100:TYR:HE1	1:D:102:THR:OG1	1.85	0.59
1:A:295:ILE:HG23	1:A:296:GLY:N	2.16	0.59
1:C:402:TRP:HA	7:C:1560:HOH:O	2.01	0.59
1:D:662:TYR:CE2	6:D:801:BPR:H12	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.83	0.59
1:C:491:LEU:H	1:C:491:LEU:HD22	1.66	0.59
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.02	0.59
1:D:40:ARG:HB3	1:D:508:GLN:HG3	1.83	0.59
1:C:236:ILE:HD13	1:C:712:HIS:ND1	2.18	0.59
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.02	0.59
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.17	0.59
1:A:543:LEU:HD21	1:A:627:TRP:HD1	1.67	0.59
1:D:94:THR:O	1:D:98:LEU:HG	2.01	0.59
1:D:155:ILE:HG13	1:D:166:TYR:HB3	1.85	0.59
1:C:153:GLN:OE1	1:C:167:VAL:HG12	2.02	0.59
1:C:589:LYS:HB3	7:C:1555:HOH:O	2.02	0.59
1:A:78:LEU:HD12	1:A:79:PHE:N	2.17	0.59
1:A:91:GLU:C	1:A:92:ASN:O	2.39	0.59
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.01	0.59
1:B:429:ARG:HH11	1:B:429:ARG:HG3	1.68	0.59
1:B:696:LYS:HG2	1:B:728:VAL:HG22	1.85	0.59
1:D:385:CYS:HB3	1:D:387:PHE:CE1	2.37	0.58
1:B:718:GLN:HA	1:B:718:GLN:HE21	1.68	0.58
1:D:484:SER:HB2	1:D:491:LEU:HD21	1.85	0.58
1:B:327:ILE:HD13	1:B:389:THR:HG23	1.84	0.58
1:A:685:ASN:O	2:F:1:NAG:H82	2.04	0.58
1:C:651:ILE:HG23	1:C:701:LEU:HD12	1.86	0.58
1:D:472:CYS:O	1:D:478:PRO:HA	2.04	0.58
1:A:295:ILE:CG2	1:A:296:GLY:N	2.67	0.58
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.86	0.58
1:A:534:PHE:CE1	1:A:540:TYR:CE1	2.92	0.58
1:C:307:THR:O	1:C:309:GLU:N	2.37	0.58
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.39	0.58
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.33	0.58
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.39	0.58
1:C:487:SER:O	1:C:489:LYS:N	2.37	0.57
1:A:477:LEU:HD22	1:A:500:LEU:HD23	1.85	0.57
1:C:732:THR:CG2	1:D:733:MET:HA	2.35	0.57
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.34	0.57
1:B:327:ILE:HB	1:B:343:ARG:HB3	1.86	0.57
1:D:536:LYS:HB3	1:D:536:LYS:HZ3	1.68	0.57
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.86	0.57
1:B:143:ILE:H	1:B:143:ILE:CD1	2.18	0.57
1:C:565:THR:O	1:C:569:SER:HB3	2.03	0.57
1:C:718:GLN:HE22	1:C:721:LYS:HZ1	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.85	0.57
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.84	0.57
1:A:340:SER:O	1:A:344:GLN:HG3	2.05	0.57
1:B:75:ASN:ND2	1:B:92:ASN:H	2.02	0.57
1:A:534:PHE:CD2	1:A:536:LYS:HD2	2.39	0.57
1:B:214:LEU:HD12	1:B:214:LEU:O	2.05	0.57
1:D:532:PRO:HD3	1:D:569:SER:HA	1.86	0.57
1:A:631:TYR:O	1:A:634:TYR:HB3	2.05	0.57
1:B:77:LEU:HD23	1:B:88:ILE:HA	1.86	0.57
1:B:370:SER:HB2	1:B:387:PHE:O	2.05	0.57
1:C:372:TYR:CE2	1:C:386:HIS:CG	2.93	0.57
1:C:372:TYR:HE2	1:C:386:HIS:CG	2.22	0.57
1:C:546:VAL:HG21	1:C:635:VAL:HG11	1.87	0.57
1:B:232:GLU:CB	1:B:262:GLU:HG2	2.35	0.56
1:C:197:GLY:C	1:C:213:ALA:HB3	2.30	0.56
1:C:301:CYS:SG	1:C:316:ILE:HG12	2.45	0.56
1:D:169:ASN:HB2	7:D:1515:HOH:O	2.04	0.56
1:C:602:GLU:O	1:C:606:GLN:HG2	2.05	0.56
1:D:536:LYS:O	1:D:537:SER:CB	2.51	0.56
1:A:526:TYR:CE1	1:A:528:MET:HE2	2.38	0.56
1:B:393:ASN:H	1:B:393:ASN:ND2	2.01	0.56
1:C:60:LEU:C	1:C:60:LEU:HD12	2.30	0.56
1:D:438:ASP:OD2	1:D:441:LYS:HG2	2.05	0.56
1:B:159:PRO:HG2	1:B:217:SER:O	2.04	0.56
1:C:43:TYR:OH	1:C:561:LEU:HB3	2.05	0.56
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.41	0.56
1:C:460:SER:HB3	1:C:469:GLN:HB3	1.86	0.56
1:D:536:LYS:O	1:D:537:SER:HB2	2.05	0.56
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.87	0.56
1:C:316:ILE:CG2	1:C:323:SER:HB2	2.36	0.56
1:D:289:PRO:HB3	1:D:315:TRP:CE2	2.41	0.56
1:B:546:VAL:HG23	7:B:1516:HOH:O	2.04	0.56
1:A:464:LYS:O	1:A:465:ALA:HB3	2.05	0.56
1:C:269:PHE:CE2	1:C:286:GLN:HG3	2.40	0.56
1:C:483:HIS:CE1	1:C:490:GLU:HG3	2.41	0.56
1:C:417:TYR:HE1	1:C:419:SER:HB3	1.71	0.56
1:D:139:LYS:HG3	1:D:141:GLN:HG3	1.88	0.56
1:D:454:CYS:HB3	1:D:457:TYR:CZ	2.41	0.56
1:C:160:VAL:HG13	1:C:218:PRO:O	2.05	0.55
1:C:194:ILE:HD12	4:C:769(A):NAG:H82	1.87	0.55
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ASN:H	1:C:308:GLU:CD	2.12	0.55
1:D:600:THR:CG2	2:M:1:NAG:H83	2.27	0.55
1:C:90:LEU:C	1:C:90:LEU:HD22	2.32	0.55
1:A:415:LEU:C	1:A:415:LEU:HD13	2.30	0.55
1:A:519:LEU:HD22	1:A:608:GLU:HG2	1.89	0.55
1:A:675:THR:C	1:A:680:LEU:HB2	2.32	0.55
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.21	0.55
1:B:44:THR:O	1:B:47:ASP:HB2	2.07	0.55
1:C:400:GLY:C	7:C:1546:HOH:O	2.50	0.55
1:D:482:LEU:HD13	1:D:491:LEU:HD12	1.88	0.55
1:C:63:ILE:HG21	1:C:69:LEU:HG	1.89	0.55
1:D:75:ASN:ND2	1:D:92:ASN:H	2.04	0.55
1:D:183:GLN:HB2	7:D:1574:HOH:O	2.07	0.55
1:B:125:ARG:HG3	1:B:125:ARG:NH1	2.20	0.55
1:B:379:GLU:OE2	1:B:399:LYS:NZ	2.39	0.55
1:C:177:GLU:CB	1:C:180:LEU:HD23	2.37	0.55
1:C:443:THR:HG22	1:C:444:CYS:N	2.22	0.55
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.89	0.55
1:C:479:LEU:HD12	1:C:496:ASP:HA	1.88	0.55
1:C:741:GLY:O	1:C:742:ILE:C	2.50	0.55
1:D:164:LEU:HB2	1:D:175:LYS:HB2	1.88	0.55
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.06	0.55
1:C:666:TYR:HE2	6:C:801:BPR:HB1	1.70	0.55
1:B:67:GLU:HB3	1:B:78:LEU:HD11	1.89	0.54
1:C:194:ILE:CD1	4:C:769(A):NAG:H82	2.37	0.54
1:C:358:ARG:HG2	1:C:358:ARG:HH11	1.72	0.54
1:A:741:GLY:O	1:A:742:ILE:C	2.50	0.54
1:C:108:SER:HB3	1:C:157:TRP:CE3	2.42	0.54
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.42	0.54
1:D:718:GLN:NE2	1:D:721:LYS:NZ	2.53	0.54
1:C:136:ASP:HB2	1:C:143:ILE:HD11	1.88	0.54
1:C:307:THR:C	1:C:309:GLU:N	2.66	0.54
1:C:536:LYS:HE3	1:C:538:LYS:HB2	1.89	0.54
1:D:718:GLN:HE22	1:D:721:LYS:HZ2	1.56	0.54
1:A:295:ILE:CG2	1:A:296:GLY:H	2.21	0.54
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.89	0.54
1:B:377:ASN:HA	1:B:396:PHE:CZ	2.42	0.54
1:B:513:LYS:HE2	1:B:530:LEU:HD11	1.90	0.54
1:C:472:CYS:O	1:C:478:PRO:HA	2.06	0.54
1:D:415:LEU:C	1:D:415:LEU:HD23	2.31	0.54
1:B:410:LEU:HD13	1:B:415:LEU:CD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:MET:HE3	1:B:754:HIS:CE1	2.43	0.54
1:C:288:VAL:HG12	1:C:294:LEU:HD11	1.88	0.54
1:D:49:LEU:HD22	1:D:749:GLN:HA	1.88	0.54
1:A:91:GLU:O	1:A:92:ASN:O	2.26	0.54
1:A:306:VAL:HB	1:A:310:ARG:HG2	1.90	0.54
1:A:336:ARG:HG3	1:A:336:ARG:NH1	2.21	0.54
1:A:479:LEU:HD12	1:A:496:ASP:HA	1.90	0.54
1:C:143:ILE:HG21	1:C:178:PRO:O	2.08	0.54
1:C:582:GLY:HA3	1:C:594:ILE:HD13	1.90	0.54
1:C:760:LYS:HB3	1:C:765:LEU:O	2.06	0.54
1:D:47:ASP:HA	1:D:52:THR:HG23	1.89	0.54
1:A:400:GLY:HA3	1:A:402:TRP:NE1	2.22	0.54
1:D:334:THR:OG1	1:D:336:ARG:HG3	2.08	0.54
1:A:571:GLU:CD	1:A:760:LYS:HD3	2.33	0.54
1:B:420:ASN:ND2	1:B:426:PRO:HA	2.23	0.54
1:B:515:ASP:HB3	1:B:526:TYR:CE2	2.42	0.54
1:C:145:GLU:O	1:C:146:GLU:HB2	2.08	0.54
1:C:325:ILE:O	1:C:344:GLN:HA	2.08	0.54
1:B:134:ILE:O	1:B:142:LEU:HD23	2.07	0.53
1:C:292:SER:O	1:C:295:ILE:HD12	2.08	0.53
1:D:372:TYR:CE2	1:D:386:HIS:CD2	2.96	0.53
1:A:439:TYR:HE1	7:A:1568:HOH:O	1.90	0.53
1:B:704:HIS:HE1	1:B:711:VAL:O	1.90	0.53
1:C:156:THR:HG21	1:C:214:LEU:HD11	1.90	0.53
1:A:270:VAL:HG11	1:A:337:TRP:CE2	2.43	0.53
1:A:310:ARG:NE	1:A:329:ASP:OD1	2.27	0.53
1:B:420:ASN:HD22	1:B:426:PRO:HA	1.73	0.53
1:C:41:ARG:HA	7:C:1515:HOH:O	2.08	0.53
1:C:127:SER:HB3	1:C:204:GLU:OE1	2.08	0.53
1:C:435:GLN:HB3	1:C:438:ASP:O	2.08	0.53
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.38	0.53
1:D:377:ASN:HD22	1:D:381:TYR:HB2	1.74	0.53
1:A:143:ILE:N	1:A:143:ILE:HD12	2.24	0.53
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.89	0.53
1:D:82:GLU:HA	1:D:491:LEU:HD13	1.89	0.53
1:D:334:THR:CB	1:D:336:ARG:HG3	2.39	0.53
1:A:319:ALA:O	1:A:320:GLN:HB2	2.09	0.53
1:A:528:MET:HG2	1:A:576:ALA:HB2	1.89	0.53
1:C:386:HIS:C	1:C:386:HIS:CD2	2.87	0.53
1:C:484:SER:O	1:C:488:ASP:HA	2.09	0.53
7:C:1506:HOH:O	1:D:249:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.44	0.53
1:B:600:THR:HG22	2:H:1:NAG:HN2	1.73	0.53
1:C:536:LYS:CE	1:C:538:LYS:HB2	2.38	0.53
1:B:105:TYR:HA	1:B:115:LEU:O	2.09	0.53
1:C:111:ARG:O	1:C:137:LEU:HD12	2.09	0.53
1:C:302:GLY:HA2	7:C:1537:HOH:O	2.08	0.53
1:C:454:CYS:HB3	1:C:457:TYR:CE1	2.43	0.53
1:D:694:ASN:N	1:D:694:ASN:HD22	2.06	0.53
1:B:103:ASN:O	1:B:104:ASP:HB2	2.09	0.53
1:B:429:ARG:HG3	1:B:429:ARG:NH1	2.24	0.53
1:D:443:THR:HG22	1:D:445:LEU:HD23	1.91	0.53
1:A:718:GLN:HE22	1:A:721:LYS:HZ1	1.55	0.53
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.90	0.53
1:C:415:LEU:O	1:C:434:ILE:HG22	2.08	0.53
1:A:415:LEU:C	1:A:415:LEU:CD1	2.82	0.52
1:A:718:GLN:HE21	1:A:718:GLN:CA	2.18	0.52
1:C:109:PRO:HG3	1:C:158:SER:O	2.08	0.52
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.44	0.52
1:C:516:VAL:CG1	1:C:517:ILE:H	2.16	0.52
1:D:98:LEU:HD13	1:D:100:TYR:OH	2.09	0.52
1:D:372:TYR:CZ	1:D:386:HIS:HD2	2.26	0.52
1:D:404:VAL:HG13	1:D:417:TYR:CD1	2.44	0.52
1:C:167:VAL:HA	1:C:171:ASP:O	2.09	0.52
1:D:90:LEU:HD11	1:D:94:THR:HG21	1.92	0.52
1:A:93:SER:C	1:A:95:PHE:N	2.67	0.52
1:A:458:SER:OG	1:A:471:ARG:HD2	2.08	0.52
1:A:751:ILE:O	1:A:755:MET:HG3	2.08	0.52
1:C:65:ASP:HB2	1:C:463:ASN:O	2.09	0.52
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.89	0.52
1:A:686:SER:HA	2:F:1:NAG:H82	1.91	0.52
1:C:519:LEU:HD22	1:C:608:GLU:CD	2.31	0.52
1:C:662:TYR:CZ	6:C:801:BPR:H12	2.45	0.52
1:D:158:SER:OG	1:D:163:LYS:HB2	2.08	0.52
1:A:246:LEU:CD2	1:A:248:TYR:H	2.23	0.52
1:B:232:GLU:HB3	1:B:262:GLU:HG2	1.90	0.52
1:B:687:THR:HG22	7:B:1575:HOH:O	2.09	0.52
1:D:718:GLN:NE2	1:D:721:LYS:HZ2	2.07	0.52
1:A:454:CYS:HB3	1:A:457:TYR:CZ	2.45	0.52
1:C:109:PRO:O	1:C:111:ARG:HG3	2.10	0.52
1:C:353:TRP:HZ3	1:C:595:ASN:HD22	1.54	0.52
1:C:414:TYR:CG	1:C:433:ARG:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:ARG:HD2	7:C:1524:HOH:O	2.10	0.52
1:C:720:SER:O	1:C:724:VAL:HG23	2.10	0.52
1:D:73:GLU:O	1:D:74:ASN:HB2	2.10	0.52
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.90	0.52
1:D:535:ASP:C	1:D:536:LYS:O	2.51	0.52
1:D:748:HIS:HD2	7:D:1558:HOH:O	1.91	0.52
1:C:155:ILE:HG13	1:C:166:TYR:HB3	1.92	0.52
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.92	0.52
1:C:616:MET:HB3	1:C:618:PHE:CE2	2.45	0.52
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.91	0.52
1:D:358:ARG:HA	7:D:1683:HOH:O	2.10	0.52
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.75	0.52
1:B:258:LYS:NZ	1:B:714:GLN:OE1	2.43	0.52
1:C:463:ASN:C	1:C:465:ALA:H	2.18	0.52
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.74	0.52
1:D:517:ILE:HB	1:D:612:GLN:HE22	1.75	0.52
1:D:523:LYS:O	1:D:523:LYS:HG3	2.10	0.52
1:A:410:LEU:HD11	1:A:436:LEU:HD21	1.92	0.52
1:B:206:GLU:OE1	6:B:801:BPR:HD2	2.10	0.52
1:C:289:PRO:HG2	1:C:294:LEU:HD21	1.92	0.52
1:A:158:SER:HA	1:A:216:TRP:CD1	2.45	0.51
1:A:738:GLU:OE2	1:A:744:SER:HB3	2.10	0.51
1:D:571:GLU:HA	1:D:571:GLU:OE1	2.10	0.51
1:A:438:ASP:C	1:A:440:THR:H	2.18	0.51
1:B:500:LEU:HG	1:B:504:LEU:CD1	2.40	0.51
1:D:83:TYR:HB2	1:D:85:ASN:OD1	2.10	0.51
1:D:266:VAL:CG2	1:D:267:LYS:N	2.74	0.51
1:C:627:TRP:HB2	1:C:651:ILE:HB	1.92	0.51
1:A:724:VAL:HG22	1:B:750:HIS:CG	2.45	0.51
1:B:546:VAL:HG22	1:B:547:TYR:N	2.24	0.51
1:A:377:ASN:HB2	1:A:381:TYR:N	2.18	0.51
1:C:58:TYR:CE1	1:C:494:LEU:HD13	2.45	0.51
1:C:363:HIS:O	1:C:371:PHE:HB2	2.10	0.51
1:D:377:ASN:ND2	1:D:383:HIS:CD2	2.71	0.51
1:B:761:GLN:HG2	1:B:762:CYS:N	2.26	0.51
1:C:365:THR:O	1:C:368:GLY:N	2.43	0.51
1:C:636:THR:HG21	1:C:651:ILE:O	2.11	0.51
1:D:273:THR:HA	1:D:276:LEU:HD22	1.93	0.51
1:D:516:VAL:CG1	1:D:523:LYS:HB2	2.38	0.51
1:A:489:LYS:HG3	1:A:491:LEU:H	1.74	0.51
1:B:402:TRP:HA	7:B:1508:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:C	1:C:142:LEU:HD23	2.36	0.51
1:C:222:PHE:N	1:C:222:PHE:HD2	2.09	0.51
1:D:472:CYS:HB3	1:D:479:LEU:HB3	1.92	0.51
1:A:61:GLN:HA	7:A:1550:HOH:O	2.11	0.51
1:A:246:LEU:HD22	1:A:248:TYR:N	2.24	0.51
1:A:589:LYS:HB2	7:A:1642:HOH:O	2.10	0.51
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.46	0.51
1:B:516:VAL:HG12	1:B:517:ILE:N	2.25	0.51
1:C:518:ASN:HB3	7:C:1614:HOH:O	2.10	0.51
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.92	0.50
1:B:658:LYS:HB3	1:B:661:TYR:CD2	2.46	0.50
1:C:704:HIS:CE1	1:C:711:VAL:O	2.63	0.50
1:D:334:THR:HB	1:D:336:ARG:HG3	1.92	0.50
1:B:516:VAL:CG1	1:B:517:ILE:N	2.75	0.50
1:D:107:VAL:HG12	1:D:114:ILE:HB	1.93	0.50
1:D:458:SER:OG	1:D:471:ARG:HB2	2.12	0.50
1:D:718:GLN:HE21	1:D:718:GLN:CA	2.14	0.50
1:B:91:GLU:C	1:B:93:SER:N	2.70	0.50
1:B:214:LEU:HD12	1:B:214:LEU:C	2.37	0.50
1:C:214:LEU:HD12	1:C:214:LEU:O	2.11	0.50
1:C:701:LEU:CD1	1:C:703:ILE:HD11	2.40	0.50
1:D:516:VAL:HG12	1:D:517:ILE:N	2.27	0.50
2:H:1:NAG:H61	2:H:2:NAG:H82	1.94	0.50
1:A:199:THR:HA	1:A:228:PHE:CE2	2.47	0.50
1:A:504:LEU:C	1:A:506:ASP:H	2.20	0.50
1:D:123:GLN:HG2	1:D:124:TRP:N	2.27	0.50
1:D:273:THR:O	1:D:276:LEU:HB2	2.11	0.50
1:A:547:TYR:HE2	7:A:1607:HOH:O	1.93	0.50
1:C:120:TYR:HA	1:C:130:ALA:HB2	1.92	0.50
1:C:150:ASN:O	1:C:151:ASN:HB2	2.10	0.50
1:A:551:CYS:O	1:A:551:CYS:SG	2.70	0.50
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.41	0.50
7:B:1604:HOH:O	2:H:1:NAG:H82	2.11	0.50
1:C:547:TYR:HD2	1:C:552:SER:CB	2.24	0.50
1:D:99:GLY:O	1:D:100:TYR:HB3	2.12	0.50
1:A:327:ILE:HD12	1:A:389:THR:HG23	1.94	0.50
1:D:175:LYS:HE3	1:D:177:GLU:O	2.12	0.50
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.94	0.49
1:B:519:LEU:HD21	1:B:608:GLU:HB3	1.94	0.49
1:B:693:GLU:OE1	1:B:696:LYS:HE3	2.11	0.49
1:C:375:ILE:HG12	1:C:385:CYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:ALA:HB2	7:C:1520:HOH:O	2.11	0.49
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.19	0.49
1:B:73:GLU:O	1:B:74:ASN:CB	2.59	0.49
1:B:208:PHE:O	1:B:209:SER:C	2.55	0.49
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.43	0.49
1:C:559:PHE:C	1:C:560:ARG:HG3	2.37	0.49
1:C:628:GLY:HA3	1:C:632:GLY:O	2.12	0.49
1:B:658:LYS:HD3	1:B:661:TYR:CZ	2.47	0.49
1:C:475:PRO:HA	1:C:557:THR:O	2.12	0.49
1:C:517:ILE:HB	1:C:612:GLN:NE2	2.27	0.49
1:C:651:ILE:HD11	1:C:758:PHE:HD2	1.77	0.49
1:D:434:ILE:HD11	1:D:439:TYR:HB3	1.93	0.49
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.12	0.49
1:C:536:LYS:HE3	1:C:538:LYS:N	2.27	0.49
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.95	0.49
1:B:280:ALA:HB2	1:D:285:TYR:HD1	1.77	0.49
1:C:148:ILE:HD13	1:C:155:ILE:CD1	2.42	0.49
1:D:547:TYR:HD2	1:D:552:SER:HB2	1.76	0.49
1:A:438:ASP:CG	1:A:441:LYS:HG3	2.37	0.49
1:B:65:ASP:HB2	1:B:466:LYS:CD	2.41	0.49
1:D:682:TYR:OH	2:M:2:NAG:H83	2.13	0.49
1:B:289:PRO:HG2	1:B:294:LEU:HG	1.94	0.49
1:D:512:LYS:HA	1:D:528:MET:O	2.12	0.49
1:D:549:GLY:HA2	1:D:631:TYR:CE1	2.48	0.49
1:B:734:TRP:CD1	1:B:734:TRP:C	2.91	0.49
1:C:322:TYR:CD1	1:C:322:TYR:C	2.91	0.49
1:C:613:PHE:HA	1:C:616:MET:HE3	1.94	0.49
1:A:429:ARG:HB2	1:A:457:TYR:H	1.78	0.49
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.48	0.49
1:C:388:GLN:O	1:C:390:ASP:N	2.46	0.49
1:C:421:GLU:O	1:C:422:HIS:C	2.56	0.49
1:C:516:VAL:O	1:C:517:ILE:HG23	2.13	0.49
1:A:65:ASP:CA	1:A:463:ASN:HB2	2.42	0.48
1:B:76:ILE:O	1:B:89:PHE:HB3	2.13	0.48
1:B:405:ILE:HG13	1:B:429:ARG:HD2	1.95	0.48
1:C:289:PRO:HD2	1:C:294:LEU:HD21	1.95	0.48
1:C:487:SER:C	1:C:489:LYS:N	2.70	0.48
1:D:294:LEU:O	1:D:294:LEU:HD23	2.13	0.48
1:D:438:ASP:OD2	1:D:440:THR:HB	2.13	0.48
1:A:270:VAL:HG11	1:A:337:TRP:CZ2	2.48	0.48
1:C:125:ARG:NH2	1:C:205:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:HIS:ND1	1:C:345:HIS:N	2.60	0.48
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.94	0.48
1:C:438:ASP:CG	1:C:440:THR:HB	2.38	0.48
1:D:43:TYR:HE1	1:D:53:PHE:HD2	1.60	0.48
1:D:105:TYR:CD1	1:D:105:TYR:C	2.91	0.48
1:A:96:ASP:HA	7:A:1510:HOH:O	2.13	0.48
1:A:515:ASP:HB3	1:A:526:TYR:CE2	2.48	0.48
1:B:61:GLN:O	1:B:63:ILE:HG23	2.13	0.48
1:B:219:ASN:ND2	7:B:1534:HOH:O	2.44	0.48
1:B:596:ARG:NH2	1:B:679:ASN:HB2	2.28	0.48
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.28	0.48
1:D:512:LYS:HE3	1:D:527:GLN:CD	2.37	0.48
1:A:689:MET:HE3	1:B:244:GLU:HG3	1.95	0.48
1:A:734:TRP:C	1:A:734:TRP:CD1	2.91	0.48
1:B:438:ASP:OD2	1:B:441:LYS:HE3	2.13	0.48
1:C:177:GLU:HB3	1:C:180:LEU:HD23	1.96	0.48
1:C:197:GLY:O	1:C:213:ALA:N	2.42	0.48
1:C:562:SER:O	1:C:565:THR:HB	2.13	0.48
1:D:453:ARG:HG3	1:D:476:GLY:HA3	1.95	0.48
1:A:347:GLU:OE2	1:A:354:VAL:HG13	2.13	0.48
1:B:603:VAL:HG22	1:B:635:VAL:HG13	1.95	0.48
1:D:289:PRO:HA	7:D:1603:HOH:O	2.13	0.48
4:A:768(A):NAG:N2	7:A:1651:HOH:O	2.31	0.48
1:D:77:LEU:HB2	1:D:79:PHE:CE2	2.48	0.48
1:D:236:ILE:HD12	7:D:1557:HOH:O	2.13	0.48
1:D:628:GLY:HA3	1:D:632:GLY:O	2.13	0.48
1:A:258:LYS:O	1:A:259:ALA:C	2.55	0.48
1:D:377:ASN:C	1:D:379:GLU:H	2.16	0.48
1:A:453:ARG:NH2	1:A:479:LEU:HD13	2.29	0.48
1:B:197:GLY:C	1:B:213:ALA:HB3	2.39	0.48
1:C:712:HIS:C	1:C:714:GLN:N	2.69	0.48
1:D:67:GLU:HB3	1:D:78:LEU:HD11	1.95	0.48
1:D:110:ASP:O	1:D:111:ARG:HB2	2.13	0.48
1:B:208:PHE:C	1:B:210:ALA:N	2.68	0.48
1:C:542:LEU:HB3	1:C:624:ILE:HG23	1.96	0.48
1:D:321:ASN:HA	1:D:354:VAL:HG23	1.95	0.48
1:D:546:VAL:HG21	1:D:635:VAL:HG11	1.96	0.48
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.32	0.48
1:A:246:LEU:HD22	1:A:248:TYR:O	2.14	0.48
1:C:114:ILE:HG23	1:C:114:ILE:O	2.14	0.48
1:C:704:HIS:HE1	1:C:711:VAL:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.49	0.48
1:C:90:LEU:O	1:C:90:LEU:HD22	2.13	0.47
1:B:155:ILE:HG13	1:B:166:TYR:HB3	1.96	0.47
1:C:356:ARG:NH1	1:C:382:LYS:HG2	2.29	0.47
1:D:127:SER:HB3	1:D:211:TYR:CD1	2.48	0.47
1:D:734:TRP:CD1	1:D:734:TRP:C	2.92	0.47
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.49	0.47
1:B:230:ASP:OD2	1:B:255:PRO:HB2	2.14	0.47
1:C:75:ASN:HD21	1:C:92:ASN:HB2	1.74	0.47
1:C:108:SER:HB3	1:C:157:TRP:CZ3	2.50	0.47
1:C:429:ARG:HG2	1:C:429:ARG:HH11	1.79	0.47
1:D:523:LYS:NZ	1:D:525:TRP:HE1	2.13	0.47
1:D:556:ASP:C	1:D:556:ASP:OD1	2.56	0.47
1:A:614:SER:HA	1:A:619:VAL:HG11	1.97	0.47
1:B:263:ASN:ND2	1:B:318:ARG:CZ	2.76	0.47
1:C:108:SER:HB3	1:C:157:TRP:CD2	2.49	0.47
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.44	0.47
1:D:183:GLN:HG2	1:D:276:LEU:HG	1.96	0.47
1:A:103:ASN:HD21	1:A:117:GLU:CD	2.20	0.47
1:D:162:HIS:HD2	1:D:178:PRO:HD3	1.80	0.47
1:C:317:ARG:HB3	7:C:1624:HOH:O	2.13	0.47
1:D:322:TYR:CD1	1:D:322:TYR:C	2.93	0.47
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.49	0.47
1:A:90:LEU:HD23	1:A:91:GLU:O	2.15	0.47
1:A:289:PRO:HG2	1:A:294:LEU:HG	1.96	0.47
1:A:322:TYR:CD1	1:A:322:TYR:C	2.93	0.47
1:A:455:GLN:HA	7:A:1575:HOH:O	2.14	0.47
1:A:724:VAL:HG22	1:B:750:HIS:CD2	2.49	0.47
1:C:288:VAL:CG1	1:C:289:PRO:HD2	2.44	0.47
1:C:476:GLY:O	1:C:477:LEU:C	2.58	0.47
1:D:103:ASN:O	1:D:104:ASP:HB2	2.13	0.47
1:D:235:LEU:HA	1:D:254:ILE:O	2.15	0.47
1:B:127:SER:HB3	1:B:211:TYR:CG	2.49	0.47
1:C:80:ASN:OD1	1:C:82:GLU:HB3	2.15	0.47
1:A:625:ALA:HB2	1:A:649:CYS:SG	2.55	0.47
1:C:644:SER:C	1:C:646:VAL:H	2.22	0.47
1:D:739:ASP:HB2	7:D:1550:HOH:O	2.14	0.47
1:A:591:MET:CE	7:A:1522:HOH:O	2.62	0.47
1:B:177:GLU:HB2	1:B:180:LEU:HB2	1.96	0.47
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.79	0.47
1:D:218:PRO:HD3	1:D:305:TRP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.45	0.46
1:A:547:TYR:HD2	1:A:552:SER:CB	2.28	0.46
1:C:516:VAL:CG1	1:C:517:ILE:N	2.71	0.46
1:D:72:GLN:HE21	1:D:77:LEU:HD12	1.79	0.46
1:A:175:LYS:HG2	1:A:182:SER:HB3	1.97	0.46
1:A:658:LYS:HB3	1:A:661:TYR:CD2	2.50	0.46
1:B:100:TYR:HE2	1:B:133:ASP:OD2	1.98	0.46
1:B:199:THR:HA	1:B:228:PHE:CE2	2.51	0.46
1:C:108:SER:O	1:C:109:PRO:C	2.56	0.46
1:A:658:LYS:HB3	1:A:661:TYR:CE2	2.50	0.46
1:A:681:ASP:HA	7:A:1544:HOH:O	2.15	0.46
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.16	0.46
1:C:356:ARG:CZ	1:C:382:LYS:HG2	2.45	0.46
1:D:348:ILE:HG13	1:D:349:SER:N	2.28	0.46
1:A:549:GLY:O	1:A:550:PRO:C	2.59	0.46
1:C:68:TYR:CD1	1:C:68:TYR:C	2.93	0.46
1:C:301:CYS:HB3	1:C:316:ILE:HD11	1.97	0.46
1:C:490:GLU:O	1:C:491:LEU:C	2.58	0.46
1:C:547:TYR:HB2	1:C:554:LYS:HD3	1.98	0.46
1:D:423:LYS:HB3	1:D:425:MET:HG3	1.98	0.46
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.97	0.46
1:A:542:LEU:HD22	1:A:543:LEU:N	2.30	0.46
1:C:72:GLN:O	1:C:74:ASN:N	2.48	0.46
1:C:126:HIS:O	1:C:128:TYR:HD2	1.98	0.46
1:C:345:HIS:CD2	1:C:371:PHE:HZ	2.32	0.46
4:C:768(A):NAG:O3	4:C:768(A):NAG:H83	2.16	0.46
1:D:110:ASP:OD2	1:D:162:HIS:ND1	2.49	0.46
1:D:184:ARG:HD2	1:D:187:TRP:CZ3	2.51	0.46
1:C:183:GLN:HE21	1:C:183:GLN:HB2	1.54	0.46
1:C:226:ALA:HA	1:C:267:LYS:O	2.16	0.46
1:C:550:PRO:HD2	1:C:631:TYR:CE2	2.50	0.46
1:D:68:TYR:CD1	1:D:68:TYR:C	2.93	0.46
1:D:169:ASN:N	1:D:169:ASN:ND2	2.61	0.46
1:D:216:TRP:HZ3	1:D:273:THR:HG21	1.81	0.46
1:D:288:VAL:HG12	1:D:289:PRO:HD2	1.98	0.46
1:D:47:ASP:HA	1:D:52:THR:CG2	2.46	0.46
1:A:60:LEU:HD12	1:A:60:LEU:C	2.41	0.46
1:A:630:SER:HA	1:A:654:ALA:O	2.16	0.46
1:B:256:TYR:CE2	1:B:712:HIS:NE2	2.84	0.46
1:B:403:GLU:OE1	1:B:585:TYR:CA	2.64	0.46
1:C:407:ILE:HG22	1:C:408:GLU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:HB2	1:D:112:GLN:HE21	1.81	0.46
1:A:310:ARG:HD2	7:A:1659:HOH:O	2.15	0.46
1:C:114:ILE:HG12	1:C:116:PHE:CE2	2.51	0.46
1:C:230:ASP:OD1	1:C:264:PRO:HB3	2.16	0.46
1:C:664:SER:HB2	1:C:668:GLU:CD	2.40	0.46
1:D:109:PRO:HG2	1:D:161:GLY:O	2.16	0.46
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.80	0.46
1:A:714:GLN:HG2	1:A:715:GLN:N	2.29	0.46
1:A:759:LEU:HA	1:A:759:LEU:HD23	1.66	0.46
1:C:136:ASP:HB2	1:C:143:ILE:CD1	2.46	0.46
1:D:635:VAL:O	1:D:636:THR:C	2.58	0.46
1:A:704:HIS:CE1	1:A:711:VAL:O	2.65	0.45
1:B:571:GLU:HA	1:B:571:GLU:OE1	2.15	0.45
1:C:43:TYR:O	1:C:570:THR:OG1	2.34	0.45
1:C:271:VAL:HG22	1:C:284:SER:OG	2.15	0.45
1:C:627:TRP:HA	1:C:651:ILE:O	2.17	0.45
1:D:547:TYR:HD2	1:D:552:SER:CB	2.30	0.45
1:A:134:ILE:O	1:A:143:ILE:HD13	2.16	0.45
1:B:232:GLU:HB2	1:B:262:GLU:HG2	1.97	0.45
1:B:686:SER:HA	2:H:1:NAG:H81	1.98	0.45
1:C:62:TRP:CG	1:C:462:SER:HA	2.51	0.45
1:D:50:LYS:O	1:D:51:SER:C	2.58	0.45
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.51	0.45
1:A:597:ARG:HH21	1:A:600:THR:HB	1.81	0.45
1:B:95:PHE:HE1	1:B:116:PHE:CE2	2.34	0.45
1:B:692:ALA:O	1:B:728:VAL:HG21	2.17	0.45
1:C:356:ARG:HB3	1:C:551:CYS:SG	2.57	0.45
1:C:382:LYS:N	1:C:403:GLU:HG2	2.20	0.45
1:C:463:ASN:O	1:C:464:LYS:HB2	2.16	0.45
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.98	0.45
1:D:546:VAL:CG2	1:D:547:TYR:N	2.78	0.45
1:A:499:ALA:O	1:A:502:LYS:HB3	2.17	0.45
1:A:660:GLU:HG3	7:A:1564:HOH:O	2.17	0.45
1:B:420:ASN:HB2	1:B:426:PRO:HA	1.98	0.45
1:B:443:THR:HG22	1:B:444:CYS:N	2.32	0.45
1:C:148:ILE:HD13	1:C:155:ILE:HD11	1.97	0.45
1:C:375:ILE:HD11	1:C:385:CYS:SG	2.56	0.45
1:D:680:LEU:HD11	1:D:684:ARG:HE	1.81	0.45
1:D:704:HIS:CD2	1:D:716:SER:OG	2.65	0.45
1:A:142:LEU:HD23	1:A:143:ILE:O	2.16	0.45
1:B:56:LYS:HG3	7:B:1681:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:GLN:HG3	7:B:1676:HOH:O	2.17	0.45
1:C:76:ILE:HB	1:C:90:LEU:HD13	1.98	0.45
1:C:193:VAL:HG12	1:C:194:ILE:HG12	1.98	0.45
1:C:536:LYS:CG	1:C:537:SER:N	2.58	0.45
1:D:573:ILE:HD13	1:D:763:PHE:CD2	2.52	0.45
1:B:308:GLU:HG2	7:B:1586:HOH:O	2.16	0.45
1:B:513:LYS:HE2	1:B:513:LYS:HB3	1.81	0.45
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.17	0.45
1:C:340:SER:O	1:C:344:GLN:HG3	2.17	0.45
1:C:454:CYS:HB3	1:C:457:TYR:CZ	2.52	0.45
1:D:80:ASN:O	1:D:81:ALA:O	2.35	0.45
1:D:135:TYR:CD2	1:D:137:LEU:HD23	2.52	0.45
1:D:148:ILE:HG23	1:D:149:PRO:HD2	1.99	0.45
1:A:195:TYR:CD1	1:A:195:TYR:N	2.84	0.45
1:A:364:PHE:HB2	7:A:1654:HOH:O	2.16	0.45
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.99	0.45
1:C:66:HIS:CD2	1:C:67:GLU:HG3	2.52	0.45
1:C:227:GLN:O	1:C:266:VAL:HA	2.17	0.45
1:C:266:VAL:HG22	1:C:267:LYS:N	2.31	0.45
1:C:306:VAL:CG2	1:C:310:ARG:HG2	2.46	0.45
1:C:597:ARG:NH1	2:I:2:NAG:O7	2.49	0.45
1:D:40:ARG:O	1:D:508:GLN:NE2	2.50	0.45
1:A:534:PHE:HZ	1:A:618:PHE:CG	2.35	0.45
1:B:301:CYS:SG	1:B:314:GLN:HG2	2.57	0.45
1:B:415:LEU:CD1	1:B:415:LEU:C	2.90	0.45
1:C:43:TYR:HE1	1:C:53:PHE:HD2	1.63	0.45
1:C:288:VAL:CG1	1:C:294:LEU:HD11	2.45	0.45
1:C:326:ASP:OD1	1:C:339:SER:OG	2.35	0.45
1:C:380:GLY:O	1:C:587:GLY:HA2	2.16	0.45
1:D:269:PHE:CE2	1:D:286:GLN:HG3	2.52	0.45
1:A:438:ASP:CG	1:A:441:LYS:HE3	2.42	0.45
1:A:504:LEU:O	1:A:507:VAL:HG12	2.17	0.45
1:B:184:ARG:O	1:B:185:ILE:HD13	2.17	0.45
1:B:487:SER:O	1:B:488:ASP:C	2.59	0.45
1:C:107:VAL:HG12	1:C:108:SER:O	2.16	0.45
1:C:164:LEU:HB2	1:C:175:LYS:HB2	1.99	0.45
1:C:668:GLU:HA	1:C:672:GLY:O	2.17	0.45
1:D:414:TYR:CA	1:D:436:LEU:HD13	2.45	0.45
1:A:420:ASN:HB2	1:A:426:PRO:HA	1.99	0.45
1:B:584:GLY:HA2	7:B:1503:HOH:O	2.16	0.45
1:C:661:TYR:OH	1:C:718:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:THR:HB	1:D:569:SER:OG	2.17	0.45
1:A:273:THR:HA	1:A:276:LEU:HG	1.98	0.44
1:A:336:ARG:NH1	1:A:336:ARG:CG	2.76	0.44
1:C:110:ASP:C	1:C:111:ARG:HG3	2.42	0.44
1:C:167:VAL:HG21	1:C:198:VAL:HG13	1.98	0.44
1:C:219:ASN:N	1:C:308:GLU:OE2	2.40	0.44
1:C:482:LEU:HD23	1:C:483:HIS:H	1.80	0.44
1:D:464:LYS:O	1:D:465:ALA:HB3	2.17	0.44
1:A:651:ILE:HG23	1:A:701:LEU:HB3	1.99	0.44
1:B:113:PHE:HE2	1:B:162:HIS:CE1	2.34	0.44
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.60	0.44
1:C:527:GLN:HB3	1:C:555:VAL:HG13	1.99	0.44
1:D:318:ARG:O	1:D:320:GLN:HG3	2.18	0.44
1:D:377:ASN:C	1:D:379:GLU:N	2.68	0.44
1:D:429:ARG:HB2	1:D:456:TYR:HA	1.99	0.44
1:D:635:VAL:O	1:D:638:MET:N	2.51	0.44
1:D:680:LEU:HD11	1:D:684:ARG:NE	2.32	0.44
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.99	0.44
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.00	0.44
1:A:653:VAL:O	1:A:654:ALA:C	2.60	0.44
1:B:47:ASP:HA	1:B:52:THR:HG23	2.00	0.44
1:B:662:TYR:CE2	6:B:801:BPR:H12	2.51	0.44
1:A:306:VAL:HG12	1:A:307:THR:HG23	2.00	0.44
1:B:146:GLU:OE1	1:B:181:SER:HA	2.17	0.44
1:C:358:ARG:HG2	1:C:358:ARG:NH1	2.32	0.44
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.47	0.44
1:B:666:TYR:CE2	6:B:801:BPR:HB1	2.53	0.44
1:B:704:HIS:CE1	1:B:711:VAL:O	2.71	0.44
1:D:75:ASN:ND2	1:D:92:ASN:ND2	2.64	0.44
1:D:422:HIS:NE2	1:D:423:LYS:HD3	2.32	0.44
1:B:566:TYR:CE2	1:B:567:LEU:HD23	2.52	0.44
1:C:92:ASN:O	1:C:94:THR:N	2.49	0.44
1:C:482:LEU:HB2	1:C:494:LEU:HD21	1.99	0.44
1:A:72:GLN:O	1:A:73:GLU:C	2.59	0.44
1:A:76:ILE:O	1:A:77:LEU:HD23	2.18	0.44
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.51	0.44
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.53	0.44
1:B:434:ILE:HD11	1:B:439:TYR:HB3	1.99	0.44
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.53	0.44
1:C:712:HIS:C	1:C:714:GLN:H	2.26	0.44
1:A:620:ASP:O	1:A:622:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.16	0.44
1:C:43:TYR:CE1	1:C:53:PHE:HD2	2.36	0.44
1:D:422:HIS:O	1:D:423:LYS:HB2	2.17	0.44
1:B:322:TYR:CD1	1:B:322:TYR:C	2.95	0.43
1:B:704:HIS:HD2	1:B:716:SER:OG	2.01	0.43
1:C:104:ASP:O	1:C:105:TYR:O	2.36	0.43
1:C:329:ASP:OD2	1:C:343:ARG:NH2	2.51	0.43
1:C:365:THR:HG21	1:C:370:SER:OG	2.18	0.43
1:C:736:THR:HB	1:D:721:LYS:HB2	2.00	0.43
1:D:751:ILE:O	1:D:755:MET:HG3	2.18	0.43
1:B:386:HIS:CD2	1:B:386:HIS:C	2.96	0.43
1:B:689:MET:HG2	1:B:722:ALA:HB2	2.00	0.43
1:C:138:ASN:C	1:C:140:ARG:N	2.73	0.43
1:C:306:VAL:HG21	1:C:310:ARG:HG2	1.99	0.43
1:C:548:ALA:HA	7:C:1608:HOH:O	2.17	0.43
1:C:734:TRP:H	1:D:732:THR:HG21	1.82	0.43
1:A:70:TYR:HB3	1:A:79:PHE:CE2	2.53	0.43
1:A:246:LEU:CD2	1:A:248:TYR:O	2.66	0.43
1:B:95:PHE:HE1	1:B:116:PHE:HE2	1.65	0.43
1:B:118:TYR:CE2	1:B:119:ASN:ND2	2.86	0.43
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.83	0.43
1:C:53:PHE:HB3	1:C:500:LEU:CD1	2.48	0.43
1:C:118:TYR:O	1:C:119:ASN:HB3	2.18	0.43
1:D:73:GLU:OE2	3:J:1:NAG:H4	2.19	0.43
1:D:107:VAL:HG12	1:D:114:ILE:CB	2.48	0.43
1:D:127:SER:HB3	1:D:211:TYR:CG	2.53	0.43
1:D:536:LYS:C	1:D:538:LYS:H	2.26	0.43
1:B:694:ASN:HA	1:B:697:GLN:NE2	2.32	0.43
1:C:44:THR:O	1:C:47:ASP:HB2	2.18	0.43
1:C:397:ILE:HD12	1:C:434:ILE:HD13	1.99	0.43
1:D:49:LEU:HB3	1:D:749:GLN:HG2	1.99	0.43
1:D:704:HIS:CE1	1:D:711:VAL:O	2.71	0.43
1:A:110:ASP:OD1	1:A:110:ASP:C	2.61	0.43
1:A:143:ILE:N	1:A:143:ILE:CD1	2.81	0.43
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.54	0.43
1:A:329:ASP:OD2	1:A:343:ARG:NH1	2.52	0.43
1:A:385:CYS:HA	1:A:396:PHE:HA	1.99	0.43
1:A:429:ARG:HG3	1:A:456:TYR:CE1	2.54	0.43
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.44	0.43
1:B:288:VAL:HG22	7:B:1598:HOH:O	2.18	0.43
1:B:422:HIS:C	1:B:424:GLY:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:TYR:HA	1:B:555:VAL:HG21	2.00	0.43
1:C:158:SER:OG	1:C:163:LYS:HB2	2.18	0.43
1:D:58:TYR:CE1	1:D:494:LEU:HD13	2.53	0.43
1:D:309:GLU:HB3	1:D:330:TYR:HB3	2.01	0.43
1:D:417:TYR:O	1:D:431:LEU:HD12	2.18	0.43
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.49	0.43
1:D:542:LEU:HD12	1:D:574:ILE:O	2.18	0.43
1:A:124:TRP:HA	1:A:124:TRP:HE3	1.84	0.43
1:A:453:ARG:HG2	1:A:454:CYS:SG	2.59	0.43
1:C:118:TYR:O	1:C:119:ASN:CB	2.66	0.43
1:C:422:HIS:O	1:C:424:GLY:N	2.52	0.43
1:D:673:LEU:O	1:D:678:ASP:HB3	2.18	0.43
1:A:136:ASP:HB2	1:A:143:ILE:HD11	2.01	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.54	0.43
1:A:633:GLY:C	1:A:655:PRO:HB3	2.43	0.43
1:A:702:LEU:O	1:A:732:THR:HA	2.19	0.43
1:B:158:SER:OG	1:B:163:LYS:HB2	2.18	0.43
1:B:200:ASP:OD1	1:B:203:TYR:HB2	2.18	0.43
1:C:367:ASP:OD2	1:C:369:ASN:HB2	2.18	0.43
1:D:92:ASN:O	1:D:93:SER:C	2.62	0.43
1:D:397:ILE:HG13	1:D:398:THR:HG23	2.00	0.43
1:D:610:THR:O	1:D:611:ARG:C	2.60	0.43
1:A:72:GLN:C	1:A:74:ASN:N	2.75	0.43
1:D:72:GLN:NE2	1:D:77:LEU:HD12	2.32	0.43
1:D:72:GLN:O	1:D:73:GLU:HB2	2.18	0.43
1:D:75:ASN:HD22	1:D:91:GLU:HA	1.83	0.43
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.33	0.43
1:D:279:ASN:OD1	4:D:773(A):NAG:N2	2.52	0.43
1:D:481:THR:OG1	1:D:483:HIS:HE1	2.02	0.43
1:D:581:ARG:HG3	1:D:593:ALA:CB	2.48	0.43
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.99	0.43
1:D:733:MET:HE2	1:D:754:HIS:CE1	2.54	0.43
1:A:334:THR:OG1	1:A:336:ARG:NH1	2.51	0.43
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.54	0.43
1:A:497:ASN:HA	7:A:1609:HOH:O	2.18	0.43
1:B:320:GLN:NE2	1:B:669:ARG:HB2	2.34	0.43
1:C:214:LEU:HD12	1:C:214:LEU:C	2.43	0.43
1:C:340:SER:CB	1:C:343:ARG:NH1	2.82	0.43
1:C:402:TRP:CD1	7:C:1546:HOH:O	2.71	0.43
1:C:751:ILE:HG23	1:C:752:TYR:N	2.33	0.43
1:D:454:CYS:HB2	1:D:457:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:PHE:C	1:A:697:GLN:N	2.77	0.42
1:B:266:VAL:HG22	1:B:267:LYS:N	2.33	0.42
1:C:165:ALA:HA	1:C:173:TYR:O	2.19	0.42
1:C:538:LYS:HE3	7:C:1635:HOH:O	2.19	0.42
1:D:100:TYR:CD1	1:D:100:TYR:C	2.97	0.42
1:D:207:VAL:HG12	1:D:208:PHE:HD1	1.84	0.42
1:D:586:GLN:HB2	7:D:1679:HOH:O	2.18	0.42
1:A:158:SER:CB	1:A:163:LYS:HB2	2.49	0.42
1:A:318:ARG:O	1:A:320:GLN:HG3	2.18	0.42
1:A:330:TYR:CE2	1:A:332:GLU:HA	2.54	0.42
1:A:438:ASP:C	1:A:440:THR:N	2.75	0.42
1:A:631:TYR:CD1	1:A:635:VAL:HG23	2.54	0.42
1:B:91:GLU:CD	1:B:91:GLU:H	2.27	0.42
1:B:258:LYS:O	1:B:259:ALA:C	2.61	0.42
1:B:402:TRP:CE3	1:B:421:GLU:HB2	2.54	0.42
1:C:330:TYR:HE1	1:C:335:GLY:HA2	1.80	0.42
1:C:504:LEU:HD22	1:C:509:MET:HE2	2.01	0.42
1:C:544:ILE:O	1:C:626:ILE:HA	2.19	0.42
1:C:556:ASP:OD1	1:C:556:ASP:C	2.62	0.42
1:C:763:PHE:CB	1:C:765:LEU:HG	2.49	0.42
1:D:370:SER:HB3	1:D:388:GLN:NE2	2.33	0.42
1:D:429:ARG:HG3	1:D:456:TYR:CZ	2.53	0.42
1:D:626:ILE:HB	1:D:647:PHE:CE2	2.54	0.42
1:A:128:TYR:C	1:A:128:TYR:CD1	2.96	0.42
1:A:150:ASN:O	1:A:151:ASN:HB2	2.19	0.42
1:B:155:ILE:HD11	1:B:164:LEU:HD22	2.02	0.42
1:B:438:ASP:OD2	1:B:441:LYS:CE	2.67	0.42
1:C:437:ASN:OD1	1:C:438:ASP:N	2.51	0.42
1:D:183:GLN:O	1:D:183:GLN:HG3	2.19	0.42
1:A:64:SER:C	1:A:463:ASN:OD1	2.63	0.42
1:A:200:ASP:HB2	7:A:1539:HOH:O	2.19	0.42
1:B:297:ASP:HA	7:B:1662:HOH:O	2.19	0.42
1:B:454:CYS:HB3	1:B:457:TYR:CZ	2.54	0.42
1:B:602:GLU:HG2	1:B:603:VAL:N	2.33	0.42
1:C:317:ARG:HD2	1:C:322:TYR:HB3	2.02	0.42
1:A:207:VAL:O	1:A:207:VAL:HG12	2.20	0.42
1:A:256:TYR:CD1	1:A:256:TYR:C	2.97	0.42
1:A:423:LYS:HD2	1:A:423:LYS:N	2.34	0.42
1:B:184:ARG:C	1:B:185:ILE:HD13	2.44	0.42
1:B:365:THR:HG23	1:B:370:SER:O	2.20	0.42
1:C:141:GLN:HE21	1:C:141:GLN:HB3	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:PHE:CD2	1:C:394:CYS:HB3	2.54	0.42
1:D:145:GLU:O	1:D:146:GLU:HB2	2.19	0.42
1:A:410:LEU:HD12	1:A:414:TYR:O	2.20	0.42
1:A:662:TYR:OH	6:A:801:BPR:C	2.68	0.42
1:A:735:TYR:OH	1:A:751:ILE:HA	2.20	0.42
1:B:177:GLU:HA	1:B:178:PRO:HD3	1.90	0.42
1:B:334:THR:OG1	1:B:336:ARG:CG	2.65	0.42
1:B:510:PRO:HB2	1:B:530:LEU:O	2.19	0.42
1:B:631:TYR:O	1:B:634:TYR:HB3	2.19	0.42
1:B:664:SER:O	1:B:668:GLU:HB2	2.20	0.42
1:D:420:ASN:ND2	1:D:426:PRO:HA	2.35	0.42
1:A:93:SER:C	1:A:95:PHE:H	2.27	0.42
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.88	0.42
1:A:666:TYR:CE2	6:A:801:BPR:HB1	2.55	0.42
1:A:742:ILE:O	1:A:742:ILE:HG22	2.19	0.42
1:B:500:LEU:HG	1:B:504:LEU:HD11	2.01	0.42
1:C:330:TYR:CZ	1:C:335:GLY:HA2	2.53	0.42
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.01	0.42
1:D:730:PHE:CD1	1:D:730:PHE:N	2.88	0.42
1:A:446:SER:HB2	1:A:457:TYR:CE1	2.54	0.42
1:A:516:VAL:HA	1:A:524:PHE:O	2.20	0.42
1:A:703:ILE:HG23	1:A:733:MET:O	2.20	0.42
1:B:491:LEU:O	1:B:492:ARG:HB3	2.18	0.42
1:D:532:PRO:CD	1:D:569:SER:HA	2.50	0.42
1:A:423:LYS:O	1:A:425:MET:N	2.53	0.42
1:B:53:PHE:HE1	1:B:503:MET:HB3	1.85	0.42
1:B:136:ASP:HB2	1:B:143:ILE:HD11	2.01	0.42
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.55	0.42
1:B:658:LYS:HB3	1:B:661:TYR:CE2	2.55	0.42
1:C:53:PHE:HB3	1:C:500:LEU:HD11	2.02	0.42
1:C:168:TRP:O	1:C:169:ASN:HB2	2.20	0.42
1:C:236:ILE:HG13	1:C:237:GLU:N	2.35	0.42
1:C:682:TYR:CE2	2:I:1:NAG:H5	2.55	0.42
1:A:72:GLN:HG2	1:A:73:GLU:HG3	2.02	0.42
1:A:75:ASN:HB3	1:A:92:ASN:N	2.35	0.42
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.49	0.42
1:A:169:ASN:N	1:A:169:ASN:HD22	2.17	0.42
1:A:415:LEU:HD13	1:A:416:TYR:N	2.35	0.42
1:A:434:ILE:HD11	1:A:439:TYR:HA	2.01	0.42
1:A:633:GLY:HA3	1:A:655:PRO:HB3	2.01	0.42
1:B:81:ALA:O	1:B:492:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ASP:HB3	1:B:526:TYR:CZ	2.55	0.42
1:C:310:ARG:NE	1:C:329:ASP:OD1	2.51	0.42
1:C:318:ARG:N	7:C:1624:HOH:O	2.53	0.42
1:C:370:SER:HA	1:C:389:THR:H	1.84	0.42
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.55	0.41
1:B:626:ILE:HG23	1:B:636:THR:HG23	2.02	0.41
1:C:242:SER:OG	1:C:243:ASP:N	2.52	0.41
1:D:195:TYR:O	1:D:227:GLN:HA	2.19	0.41
1:D:372:TYR:CZ	1:D:386:HIS:CD2	3.08	0.41
1:A:453:ARG:HH21	1:A:479:LEU:CB	2.21	0.41
1:B:86:SER:C	4:B:767(A):NAG:H81	2.45	0.41
1:B:405:ILE:N	1:B:418:ILE:O	2.49	0.41
1:C:217:SER:HB3	1:C:305:TRP:CZ2	2.55	0.41
1:C:446:SER:HA	1:C:449:LEU:CD1	2.50	0.41
1:C:506:ASP:OD1	1:C:506:ASP:O	2.38	0.41
1:C:763:PHE:HB3	1:C:765:LEU:HG	2.02	0.41
1:D:276:LEU:HD12	7:D:1664:HOH:O	2.19	0.41
1:D:327:ILE:CD1	1:D:389:THR:HG23	2.43	0.41
1:D:436:LEU:O	1:D:439:TYR:CE1	2.73	0.41
1:D:516:VAL:HG13	1:D:524:PHE:C	2.45	0.41
1:D:596:ARG:N	1:D:670:TYR:O	2.49	0.41
1:A:664:SER:HB2	1:A:668:GLU:CD	2.45	0.41
1:A:714:GLN:HA	1:B:241:TYR:CE2	2.56	0.41
1:B:374:ILE:CD1	1:B:406:GLY:HA2	2.50	0.41
1:B:547:TYR:HD2	1:B:549:GLY:H	1.66	0.41
1:C:328:CYS:HA	1:C:338:ILE:O	2.20	0.41
1:C:546:VAL:HG22	1:C:547:TYR:N	2.35	0.41
1:D:534:PHE:HZ	1:D:618:PHE:CG	2.38	0.41
1:D:621:ASP:C	1:D:621:ASP:OD1	2.64	0.41
1:A:663:ASP:OD1	1:A:663:ASP:C	2.63	0.41
1:B:118:TYR:CD2	1:B:119:ASN:ND2	2.88	0.41
1:C:110:ASP:O	1:C:111:ARG:HB2	2.21	0.41
1:C:234:PRO:HB2	1:D:248:TYR:OH	2.20	0.41
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.98	0.41
1:C:542:LEU:HD22	1:C:543:LEU:N	2.35	0.41
1:C:736:THR:HG23	1:D:717:ALA:HB1	2.02	0.41
1:D:466:LYS:HG2	1:D:467:TYR:CE2	2.55	0.41
1:A:246:LEU:CD2	1:A:246:LEU:C	2.94	0.41
1:C:122:LYS:HG2	1:C:123:GLN:N	2.36	0.41
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.90	0.41
1:C:341:VAL:O	1:C:341:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:SER:O	1:C:665:VAL:C	2.62	0.41
1:D:246:LEU:HD22	1:D:248:TYR:O	2.20	0.41
1:A:42:THR:HB	1:A:569:SER:OG	2.21	0.41
1:A:75:ASN:HD22	1:A:92:ASN:ND2	2.19	0.41
1:A:422:HIS:CE1	1:A:423:LYS:HD3	2.56	0.41
1:A:682:TYR:OH	2:F:2:NAG:H81	2.21	0.41
1:B:43:TYR:HE2	1:B:48:TYR:HB2	1.86	0.41
1:B:153:GLN:HE22	1:B:170:ASN:ND2	2.18	0.41
1:B:410:LEU:HD11	1:B:436:LEU:HD21	2.03	0.41
1:B:411:THR:CG2	1:B:465:ALA:HB3	2.51	0.41
1:B:524:PHE:CB	1:B:578:PHE:CE1	3.03	0.41
1:B:612:GLN:HE21	1:B:612:GLN:HB3	1.69	0.41
1:C:732:THR:HG22	1:D:733:MET:HA	2.01	0.41
1:D:230:ASP:OD2	1:D:255:PRO:HB2	2.21	0.41
1:D:542:LEU:HB3	1:D:624:ILE:HG12	2.02	0.41
1:A:57:PHE:HA	1:A:480:TYR:CE1	2.55	0.41
1:A:154:TRP:HD1	1:A:214:LEU:HD12	1.85	0.41
1:B:357:PHE:O	1:B:358:ARG:HB3	2.21	0.41
1:B:524:PHE:HB2	1:B:578:PHE:CE1	2.55	0.41
1:C:114:ILE:CG2	1:C:137:LEU:HD21	2.51	0.41
1:C:659:TRP:C	1:C:661:TYR:N	2.78	0.41
1:D:60:LEU:HD22	1:D:68:TYR:CD2	2.56	0.41
1:D:133:ASP:HB3	1:D:142:LEU:HD21	2.02	0.41
1:D:545:GLU:HG2	1:D:554:LYS:NZ	2.35	0.41
1:D:559:PHE:CZ	1:D:561:LEU:HD13	2.55	0.41
1:D:624:ILE:HB	7:D:1593:HOH:O	2.19	0.41
1:A:74:ASN:O	1:A:92:ASN:HB3	2.21	0.41
1:B:515:ASP:CG	1:B:516:VAL:H	2.29	0.41
1:B:748:HIS:O	1:B:751:ILE:HG22	2.21	0.41
1:C:113:PHE:HE2	1:C:162:HIS:CD2	2.38	0.41
1:C:343:ARG:NH1	1:C:343:ARG:CG	2.82	0.41
1:C:388:GLN:C	1:C:390:ASP:N	2.78	0.41
1:C:711:VAL:HG23	1:C:740:HIS:CE1	2.56	0.41
1:D:125:ARG:HD2	1:D:126:HIS:NE2	2.36	0.41
1:D:429:ARG:HG3	1:D:456:TYR:CE1	2.55	0.41
1:D:611:ARG:O	1:D:612:GLN:C	2.64	0.41
1:A:68:TYR:CD1	1:A:68:TYR:C	2.99	0.41
1:A:90:LEU:HD23	1:A:90:LEU:C	2.45	0.41
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.18	0.41
1:A:157:TRP:HE3	1:A:163:LYS:O	2.04	0.41
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:TYR:CG	1:A:433:ARG:HD2	2.54	0.41
1:B:168:TRP:HZ2	7:B:1627:HOH:O	2.04	0.41
1:B:285:TYR:CE1	1:B:336:ARG:HB3	2.55	0.41
1:C:97:GLU:OE1	1:C:97:GLU:N	2.46	0.41
1:C:149:PRO:HB2	1:C:168:TRP:CD1	2.56	0.41
1:C:417:TYR:CD1	1:C:417:TYR:C	2.99	0.41
1:C:471:ARG:HG2	1:C:480:TYR:CE2	2.55	0.41
1:C:595:ASN:O	1:C:596:ARG:HB2	2.20	0.41
1:C:734:TRP:CE3	1:D:732:THR:HG23	2.56	0.41
1:D:60:LEU:C	1:D:60:LEU:CD1	2.94	0.41
1:D:135:TYR:CE2	1:D:137:LEU:HD23	2.56	0.41
1:D:338:ILE:HA	7:D:1518:HOH:O	2.20	0.41
1:D:353:TRP:CE3	1:D:595:ASN:ND2	2.88	0.41
1:D:381:TYR:N	1:D:381:TYR:CD1	2.89	0.41
1:D:510:PRO:HD3	1:D:569:SER:HB2	2.02	0.41
1:B:377:ASN:OD1	1:B:377:ASN:C	2.64	0.41
1:C:415:LEU:C	1:C:415:LEU:CD2	2.93	0.41
1:C:435:GLN:HE22	1:C:441:LYS:HD2	1.81	0.41
1:C:613:PHE:HD1	1:C:616:MET:HE1	1.86	0.41
1:D:58:TYR:CD1	1:D:494:LEU:HD13	2.56	0.41
1:D:102:THR:HG21	1:D:116:PHE:CD2	2.56	0.41
1:D:195:TYR:HB2	1:D:228:PHE:HB2	2.02	0.41
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.55	0.40
1:A:236:ILE:HG22	1:A:254:ILE:O	2.21	0.40
1:A:546:VAL:O	1:A:632:GLY:HA3	2.20	0.40
1:B:118:TYR:O	1:B:119:ASN:HB2	2.20	0.40
1:B:148:ILE:HD13	1:B:155:ILE:CD1	2.51	0.40
1:B:148:ILE:HD13	1:B:155:ILE:HD12	2.03	0.40
1:B:256:TYR:C	1:B:256:TYR:CD1	2.99	0.40
1:C:87:SER:HB3	4:C:767(A):NAG:H81	2.01	0.40
1:D:216:TRP:CZ3	1:D:273:THR:HG21	2.56	0.40
1:D:356:ARG:HG2	1:D:551:CYS:SG	2.60	0.40
1:A:317:ARG:HD2	1:A:322:TYR:HB3	2.02	0.40
1:B:325:ILE:HD11	1:B:373:LYS:HE2	2.03	0.40
1:C:206:GLU:HB2	1:C:665:VAL:HG11	2.03	0.40
1:C:532:PRO:HD3	1:C:569:SER:HA	2.03	0.40
1:C:739:ASP:OD1	1:C:739:ASP:C	2.64	0.40
1:D:597:ARG:HG3	1:D:597:ARG:O	2.21	0.40
1:A:103:ASN:ND2	1:A:117:GLU:OE2	2.36	0.40
1:A:704:HIS:CD2	1:A:716:SER:OG	2.71	0.40
1:C:42:THR:N	7:C:1515:HOH:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PHE:HE1	1:C:137:LEU:HD13	1.86	0.40
1:C:170:ASN:N	1:C:170:ASN:HD22	2.19	0.40
1:C:442:VAL:O	1:C:442:VAL:HG13	2.21	0.40
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.34	0.40
1:A:377:ASN:HD22	1:A:381:TYR:HB2	1.86	0.40
1:B:519:LEU:C	1:B:521:GLY:N	2.79	0.40
1:C:72:GLN:HG2	1:C:73:GLU:HG3	2.02	0.40
1:C:91:GLU:HB3	1:C:92:ASN:H	1.69	0.40
1:C:344:GLN:C	1:C:345:HIS:ND1	2.80	0.40
1:C:415:LEU:HD23	1:C:415:LEU:O	2.21	0.40
1:C:584:GLY:O	1:C:585:TYR:HB2	2.21	0.40
1:D:466:LYS:C	1:D:467:TYR:CD2	3.00	0.40
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.03	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.97	0.40
1:B:95:PHE:CE1	1:B:116:PHE:HE2	2.39	0.40
1:B:110:ASP:C	1:B:110:ASP:OD1	2.65	0.40
1:B:140:ARG:HH11	1:B:140:ARG:CG	2.34	0.40
1:B:142:LEU:O	1:B:144:THR:HG23	2.22	0.40
1:C:123:GLN:HG2	1:C:124:TRP:CD2	2.56	0.40
1:C:307:THR:OG1	1:C:310:ARG:HB3	2.21	0.40
1:C:345:HIS:CD2	1:C:371:PHE:CZ	3.10	0.40
1:C:626:ILE:HG23	1:C:636:THR:HG23	2.04	0.40
1:D:108:SER:HB3	1:D:157:TRP:CZ3	2.56	0.40
1:D:154:TRP:CD2	1:D:212:SER:HB3	2.56	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	726/728 (100%)	655 (90%)	60 (8%)	11 (2%)	8 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/728 (100%)	658 (91%)	60 (8%)	8 (1%)	11	15
1	C	726/728 (100%)	610 (84%)	93 (13%)	23 (3%)	3	2
1	D	726/728 (100%)	664 (92%)	58 (8%)	4 (1%)	21	28
All	All	2904/2912 (100%)	2587 (89%)	271 (9%)	46 (2%)	7	9

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	GLU
1	A	491	LEU
1	B	140	ARG
1	C	91	GLU
1	C	103	ASN
1	C	104	ASP
1	C	105	TYR
1	C	423	LYS
1	C	488	ASP
1	C	536	LYS
1	D	81	ALA
1	A	92	ASN
1	A	424	GLY
1	B	438	ASP
1	B	538	LYS
1	C	97	GLU
1	C	308	GLU
1	C	389	THR
1	C	535	ASP
1	D	99	GLY
1	A	244	GLU
1	A	621	ASP
1	B	678	ASP
1	C	73	GLU
1	C	93	SER
1	C	139	LYS
1	C	355	GLY
1	C	491	LEU
1	C	534	PHE
1	D	100	TYR
1	D	389	THR
1	A	93	SER
1	B	520	HIS

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Mol	Chain	Res	Type
1	C	94	THR
1	C	422	HIS
1	B	40	ARG
1	B	138	ASN
1	C	138	ASN
1	C	332	GLU
1	A	66	HIS
1	A	520	HIS
1	A	534	PHE
1	B	465	ALA
1	C	99	GLY
1	C	674	PRO
1	A	178	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	652/652 (100%)	623 (96%)	29 (4%)	25	37
1	B	652/652 (100%)	608 (93%)	44 (7%)	15	21
1	C	652/652 (100%)	616 (94%)	36 (6%)	19	29
1	D	652/652 (100%)	618 (95%)	34 (5%)	21	31
All	All	2608/2608 (100%)	2465 (94%)	143 (6%)	19	29

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	115	LEU
1	A	144	THR
1	A	212	SER
1	A	219	ASN
1	A	231	THR
1	A	246	LEU
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	343	ARG
1	A	358	ARG
1	A	399	LYS
1	A	415	LEU
1	A	436	LEU
1	A	443	THR
1	A	492	ARG
1	A	514	LEU
1	A	520	HIS
1	A	536	LYS
1	A	542	LEU
1	A	543	LEU
1	A	561	LEU
1	A	630	SER
1	A	679	ASN
1	A	687	THR
1	A	701	LEU
1	A	714	GLN
1	A	718	GLN
1	A	745	ASN
1	A	761	GLN
1	B	74	ASN
1	B	91	GLU
1	B	142	LEU
1	B	143	ILE
1	B	152	THR
1	B	158	SER
1	B	212	SER
1	B	230	ASP
1	B	246	LEU
1	B	256	TYR
1	B	284	SER
1	B	293	VAL
1	B	323	SER
1	B	336	ARG
1	B	340	SER
1	B	393	ASN
1	B	415	LEU
1	B	418	ILE
1	B	421	GLU
1	B	435	GLN
1	B	436	LEU

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Mol	Chain	Res	Type
1	B	450	ASN
1	B	470	LEU
1	B	472	CYS
1	B	514	LEU
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	561	LEU
1	B	621	ASP
1	B	622	LYS
1	B	627	TRP
1	B	630	SER
1	B	685	ASN
1	B	699	GLU
1	B	701	LEU
1	B	702	LEU
1	B	714	GLN
1	B	718	GLN
1	B	732	THR
1	B	759	LEU
1	B	761	GLN
1	C	75	ASN
1	C	90	LEU
1	C	147	ARG
1	C	156	THR
1	C	158	SER
1	C	183	GLN
1	C	188	THR
1	C	202	VAL
1	C	222	PHE
1	C	236	ILE
1	C	246	LEU
1	C	250	LYS
1	C	284	SER
1	C	313	LEU
1	C	316	ILE
1	C	345	HIS
1	C	399	LYS
1	C	412	SER
1	C	416	TYR

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Mol	Chain	Res	Type
1	C	463	ASN
1	C	482	LEU
1	C	491	LEU
1	C	535	ASP
1	C	536	LYS
1	C	542	LEU
1	C	557	THR
1	C	561	LEU
1	C	611	ARG
1	C	622	LYS
1	C	655	PRO
1	C	660	GLU
1	C	679	ASN
1	C	718	GLN
1	C	745	ASN
1	C	746	MET
1	C	761	GLN
1	D	40	ARG
1	D	71	LYS
1	D	91	GLU
1	D	111	ARG
1	D	158	SER
1	D	180	LEU
1	D	219	ASN
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	336	ARG
1	D	348	ILE
1	D	358	ARG
1	D	385	CYS
1	D	393	ASN
1	D	399	LYS
1	D	415	LEU
1	D	482	LEU
1	D	507	VAL
1	D	518	ASN
1	D	536	LYS
1	D	546	VAL
1	D	561	LEU
1	D	590	ILE
1	D	603	VAL

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Mol	Chain	Res	Type
1	D	608	GLU
1	D	622	LYS
1	D	655	PRO
1	D	685	ASN
1	D	694	ASN
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	732	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	192	ASN
1	A	227	GLN
1	A	247	GLN
1	A	298	HIS
1	A	314	GLN
1	A	377	ASN
1	A	386	HIS
1	A	393	ASN
1	A	435	GLN
1	A	483	HIS
1	A	505	GLN
1	A	508	GLN
1	A	572	ASN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	A	761	GLN
1	B	61	GLN
1	B	74	ASN
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	179	ASN
1	B	183	GLN
1	B	192	ASN
1	B	227	GLN
1	B	247	GLN
1	B	314	GLN
1	B	369	ASN
1	B	386	HIS
1	B	393	ASN
1	B	430	ASN
1	B	450	ASN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	520	HIS
1	B	527	GLN
1	B	572	ASN
1	B	586	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	748	HIS
1	B	761	GLN
1	C	72	GLN
1	C	112	GLN
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	192	ASN
1	C	247	GLN
1	C	286	GLN
1	C	430	ASN
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN

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Mol	Chain	Res	Type
1	C	572	ASN
1	C	595	ASN
1	C	606	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	697	GLN
1	C	704	HIS
1	C	718	GLN
1	C	761	GLN
1	D	72	GLN
1	D	75	ASN
1	D	80	ASN
1	D	103	ASN
1	D	112	GLN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	247	GLN
1	D	314	GLN
1	D	369	ASN
1	D	377	ASN
1	D	383	HIS
1	D	386	HIS
1	D	388	GLN
1	D	393	ASN
1	D	430	ASN
1	D	463	ASN
1	D	483	HIS
1	D	505	GLN
1	D	508	GLN
1	D	533	HIS
1	D	586	GLN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS

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Mol	Chain	Res	Type
1	D	718	GLN
1	D	731	GLN
1	D	745	ASN
1	D	748	HIS
1	D	757	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

20 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.60	0	17,19,21	0.78	0
2	NAG	F	2	2	14,14,15	0.63	0	17,19,21	0.74	0
3	NAG	G	1	3,1	14,14,15	0.67	0	17,19,21	0.72	1 (5%)
3	NAG	G	2	3	14,14,15	0.73	0	17,19,21	0.80	0
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	0.29	0
2	NAG	H	1	2,1	14,14,15	0.59	0	17,19,21	0.68	0
2	NAG	H	2	2	14,14,15	0.83	1 (7%)	17,19,21	0.68	0
2	NAG	I	1	2,1	14,14,15	0.85	1 (7%)	17,19,21	0.76	0
2	NAG	I	2	2	14,14,15	0.69	0	17,19,21	0.68	0
3	NAG	J	1	3,1	14,14,15	0.53	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	2	3	14,14,15	0.54	0	17,19,21	0.66	0
3	BMA	J	3	3	11,11,12	0.61	0	15,15,17	0.22	0
2	NAG	K	1	2,1	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
2	NAG	K	2	2	14,14,15	0.60	0	17,19,21	0.92	1 (5%)
2	NAG	L	1	2,1	14,14,15	0.52	0	17,19,21	0.98	1 (5%)
2	NAG	L	2	2	14,14,15	0.65	0	17,19,21	0.82	1 (5%)
2	NAG	M	1	2,1	14,14,15	0.64	0	17,19,21	0.80	0
2	NAG	M	2	2	14,14,15	0.66	0	17,19,21	1.18	3 (17%)

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
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	6/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	C1-C2	2.40	1.55	1.52
2	I	1	NAG	C1-C2	2.34	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	-2.69	119.30	122.90
2	K	2	NAG	C2-N2-C7	-2.65	119.35	122.90
2	L	1	NAG	C2-N2-C7	-2.47	119.59	122.90
2	L	2	NAG	C2-N2-C7	-2.26	119.87	122.90
2	E	1	NAG	C2-N2-C7	-2.22	119.92	122.90
2	M	2	NAG	C1-C2-N2	2.18	113.87	110.43
2	M	2	NAG	O5-C1-C2	-2.16	107.94	111.29
2	M	2	NAG	C4-C3-C2	-2.03	108.04	111.02
3	G	1	NAG	C2-N2-C7	-2.02	120.19	122.90
2	K	1	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7
2	H	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
2	M	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O7-C7-N2-C2
2	K	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	M	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C8-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	M	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	H	2	NAG	C1-C2-N2-C7
2	L	1	NAG	C4-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O7-C7-N2-C2
3	J	3	BMA	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C1-C2-N2-C7
2	H	1	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 16 short contacts:

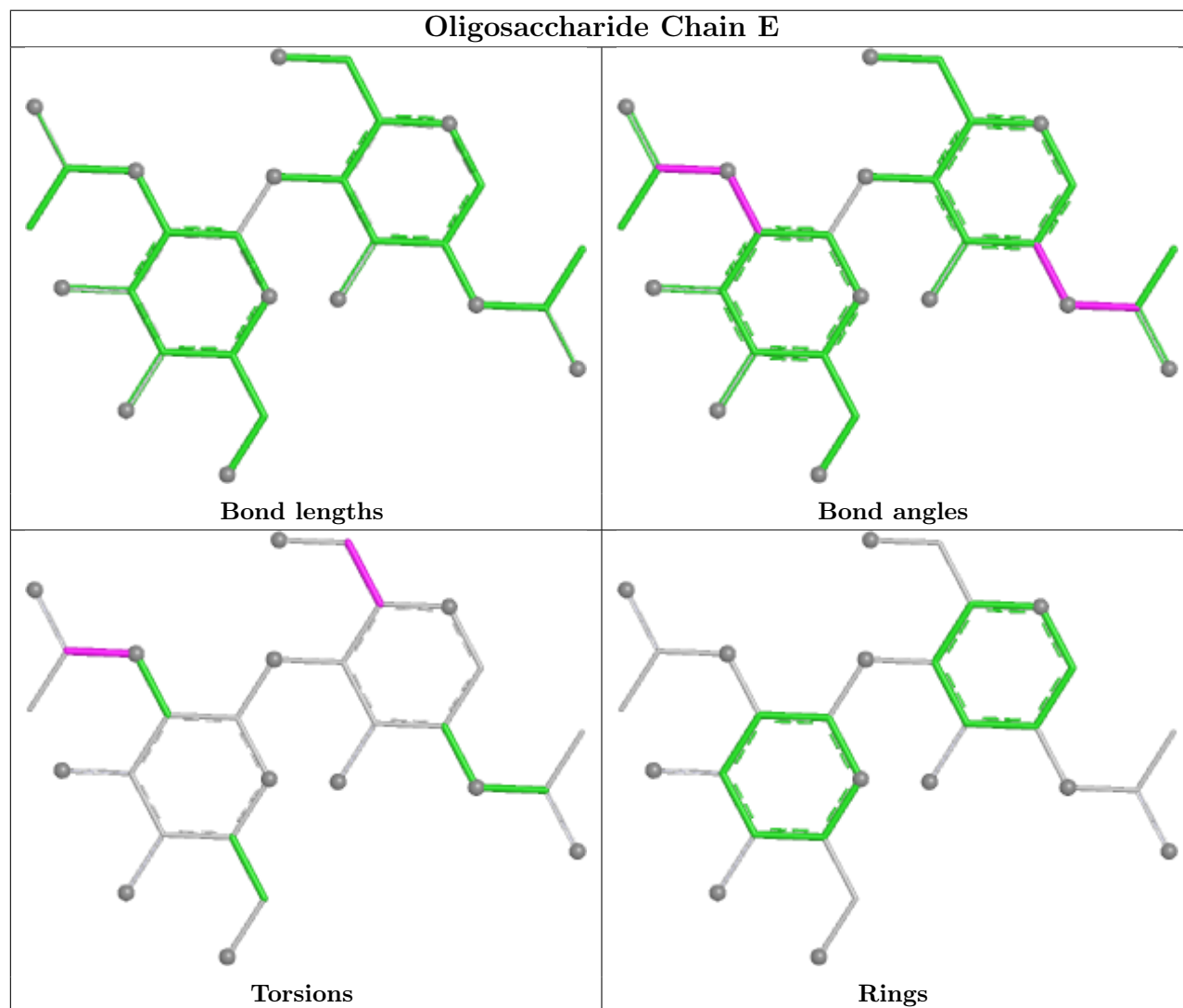
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	2	NAG	1	0
2	I	2	NAG	1	0
2	H	2	NAG	1	0
2	F	2	NAG	2	0
2	I	1	NAG	1	0
3	J	1	NAG	1	0
2	H	1	NAG	4	0

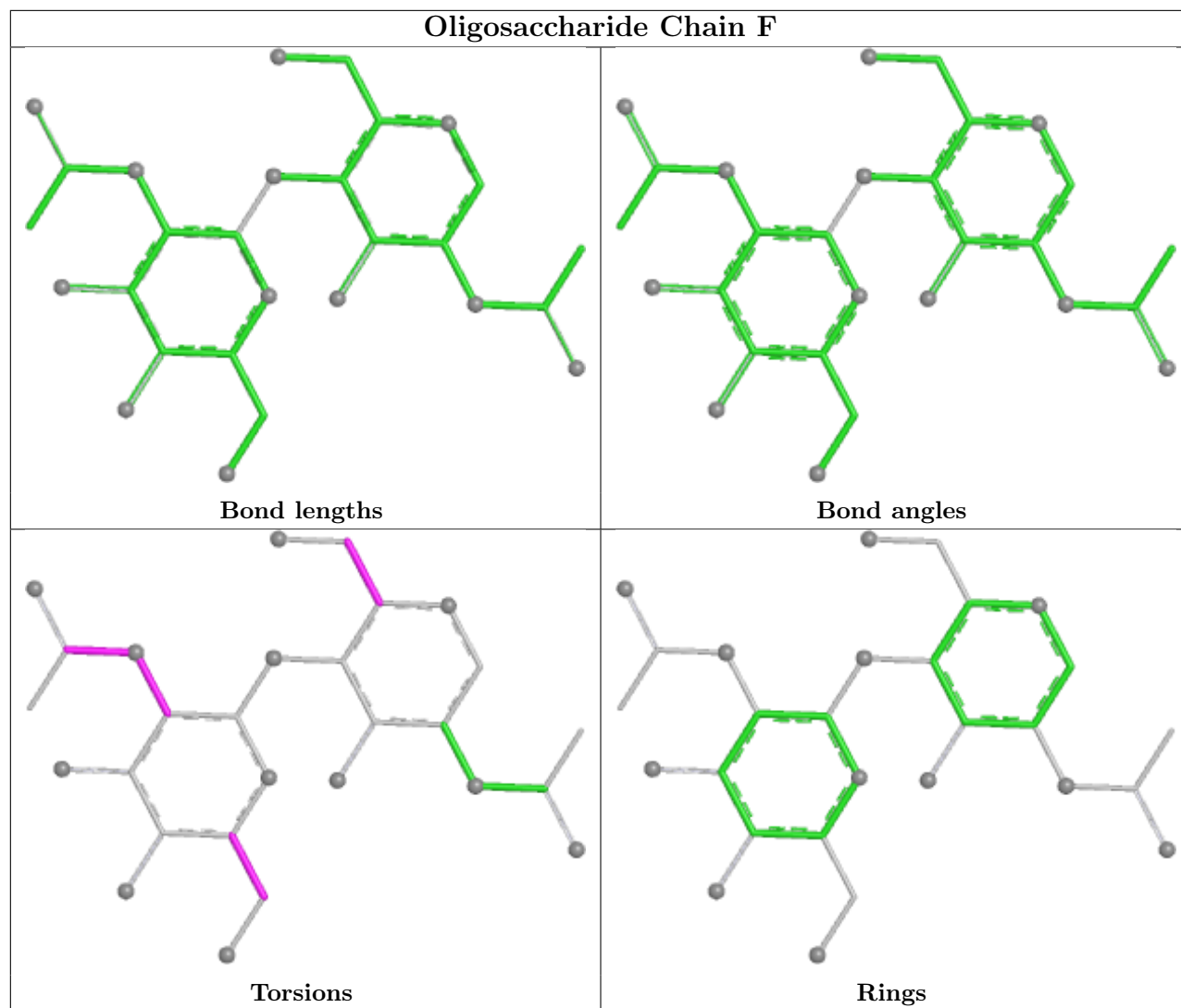
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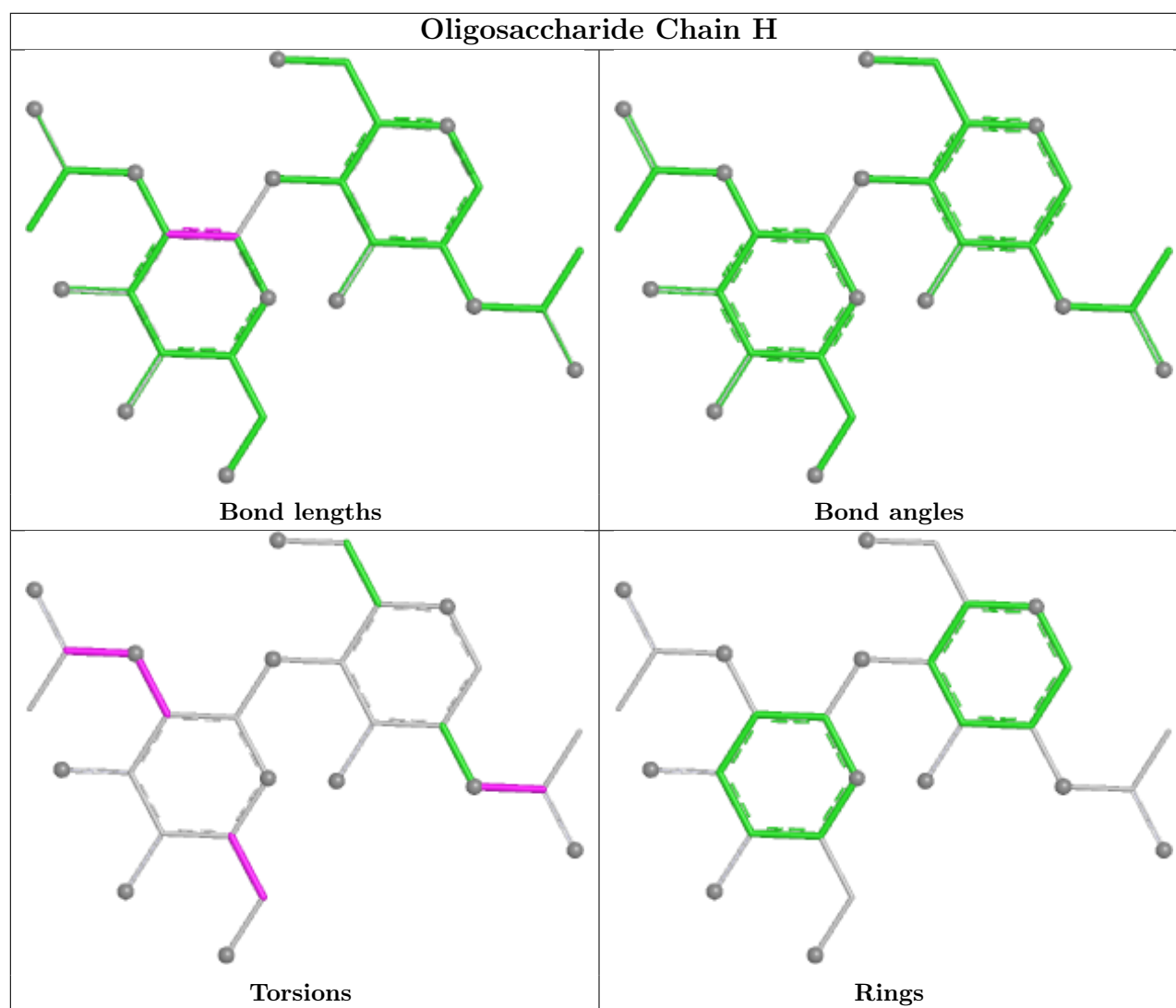
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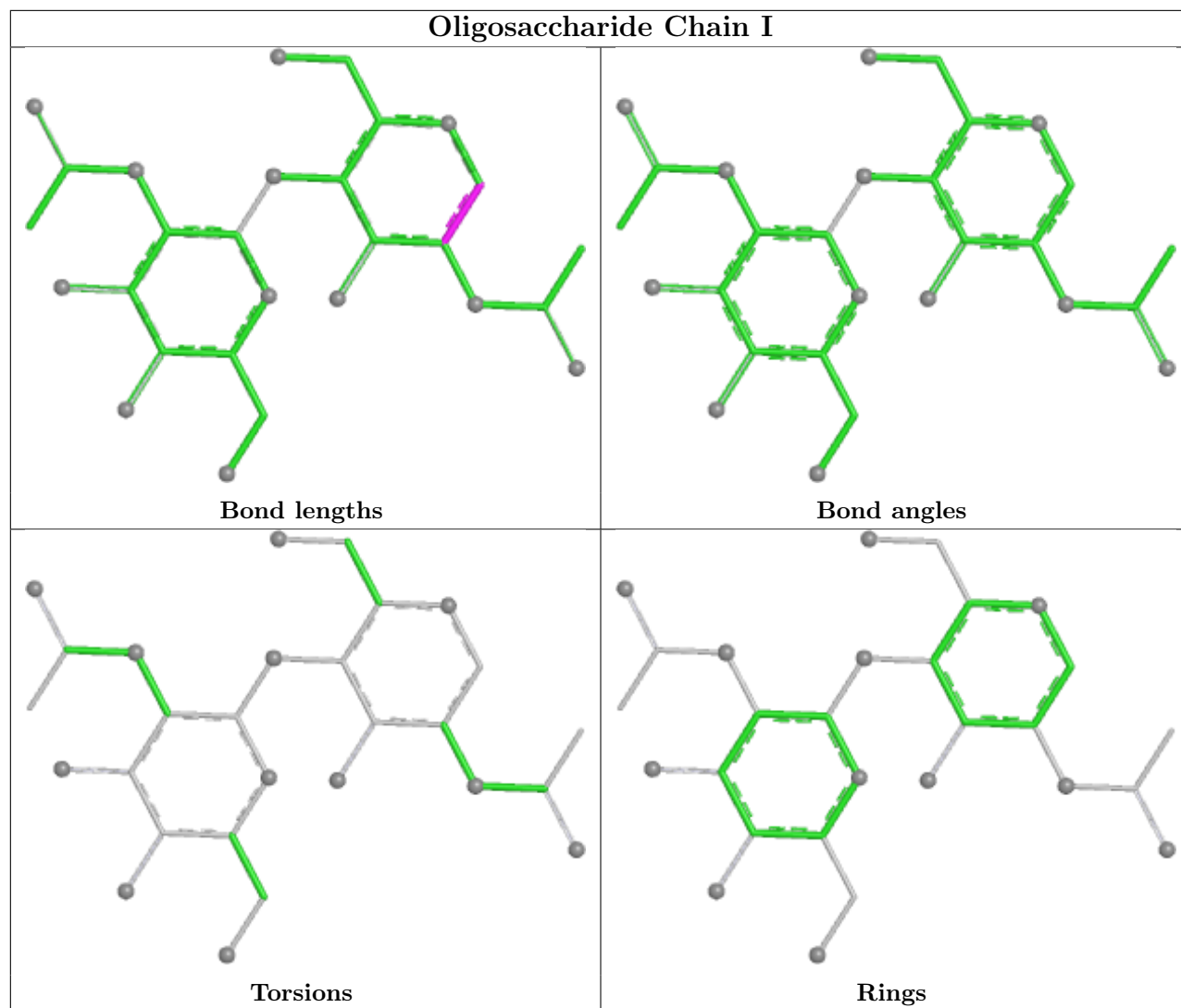
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	3	BMA	1	0
3	G	2	NAG	1	0
2	F	1	NAG	3	0
2	M	1	NAG	3	0

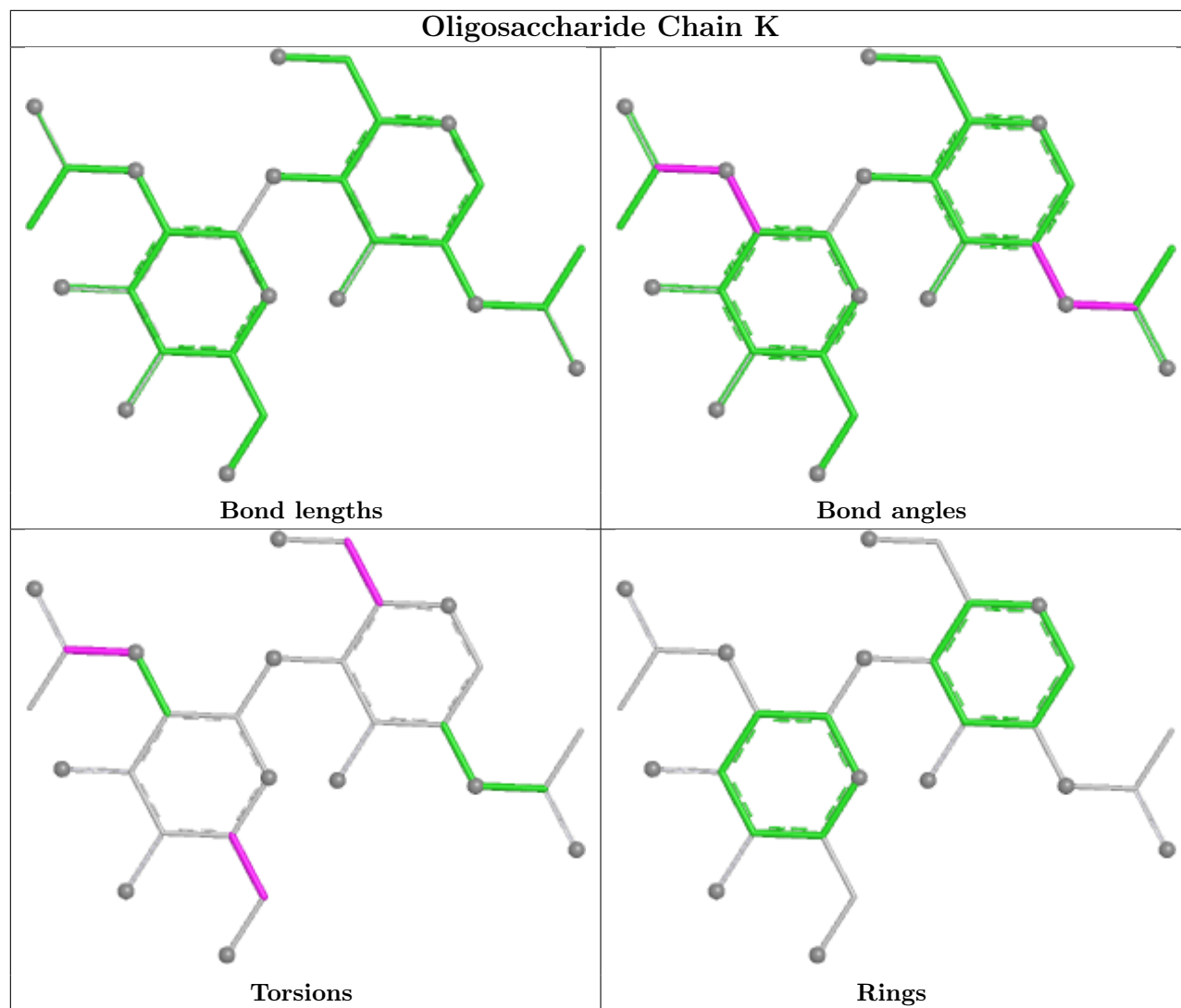
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

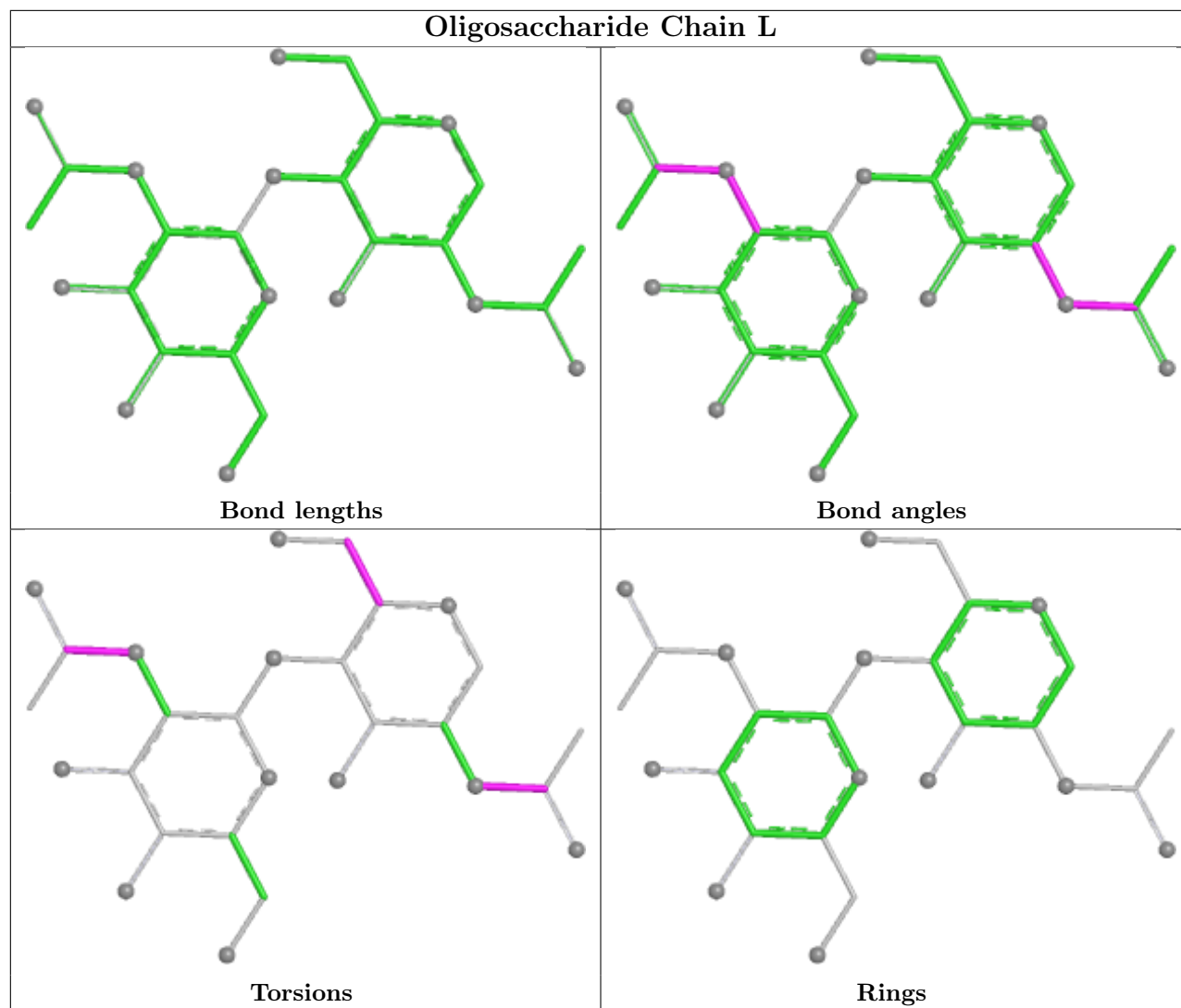


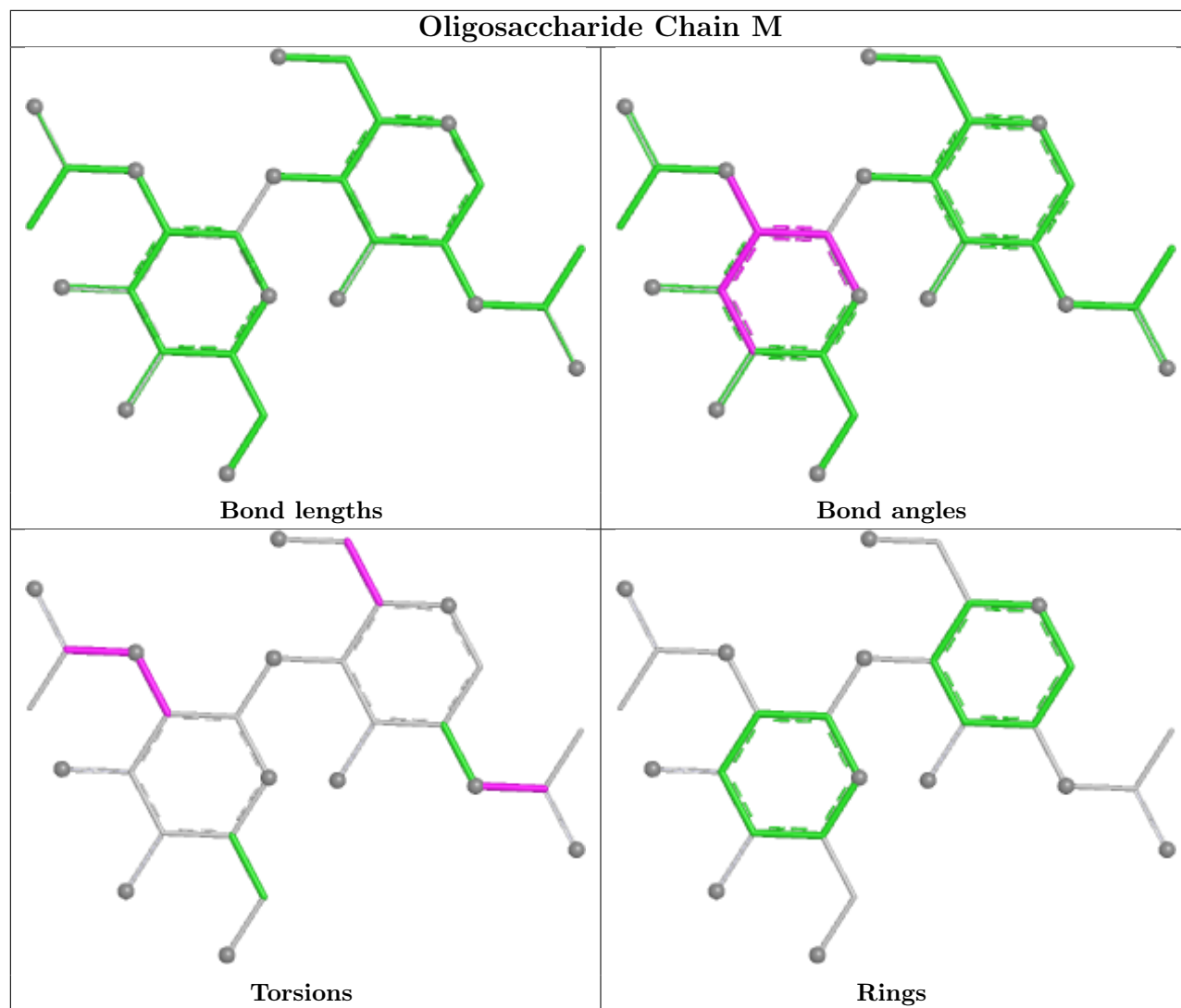


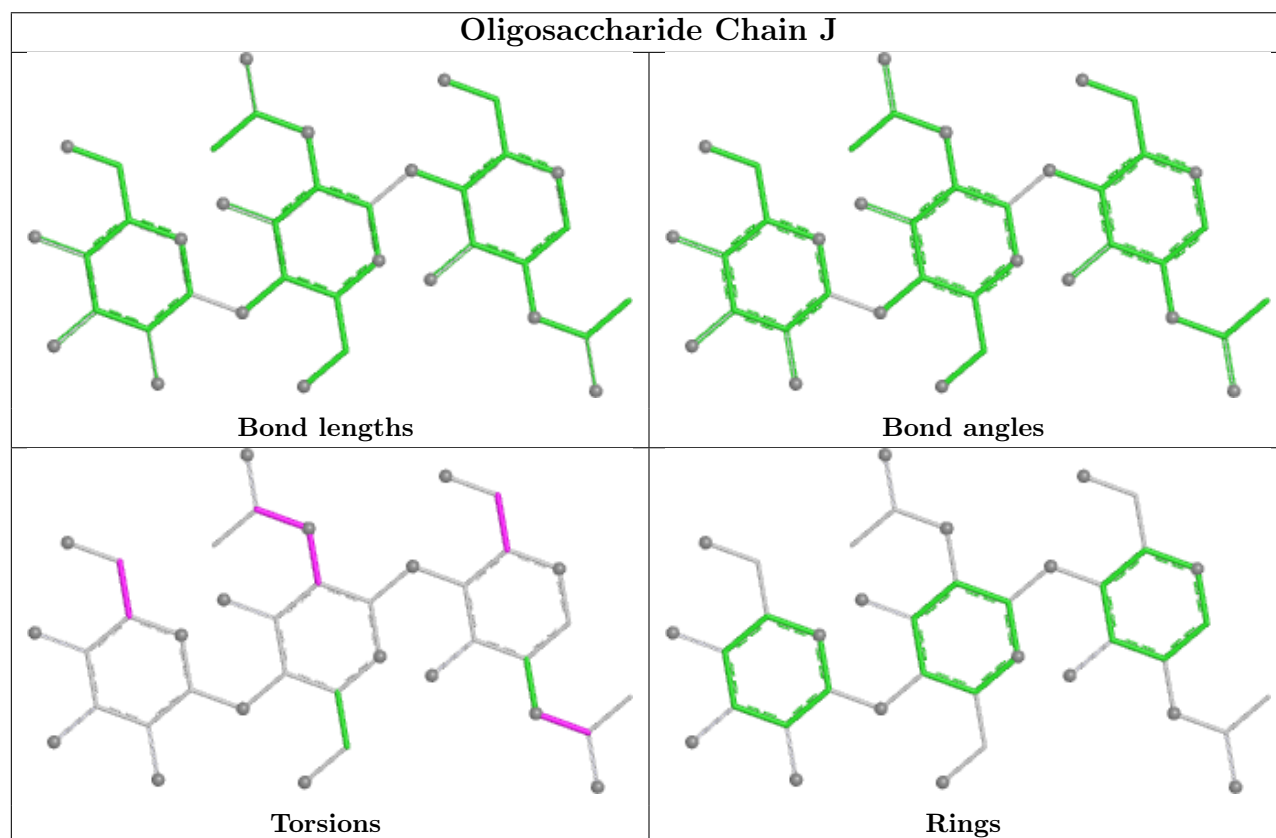
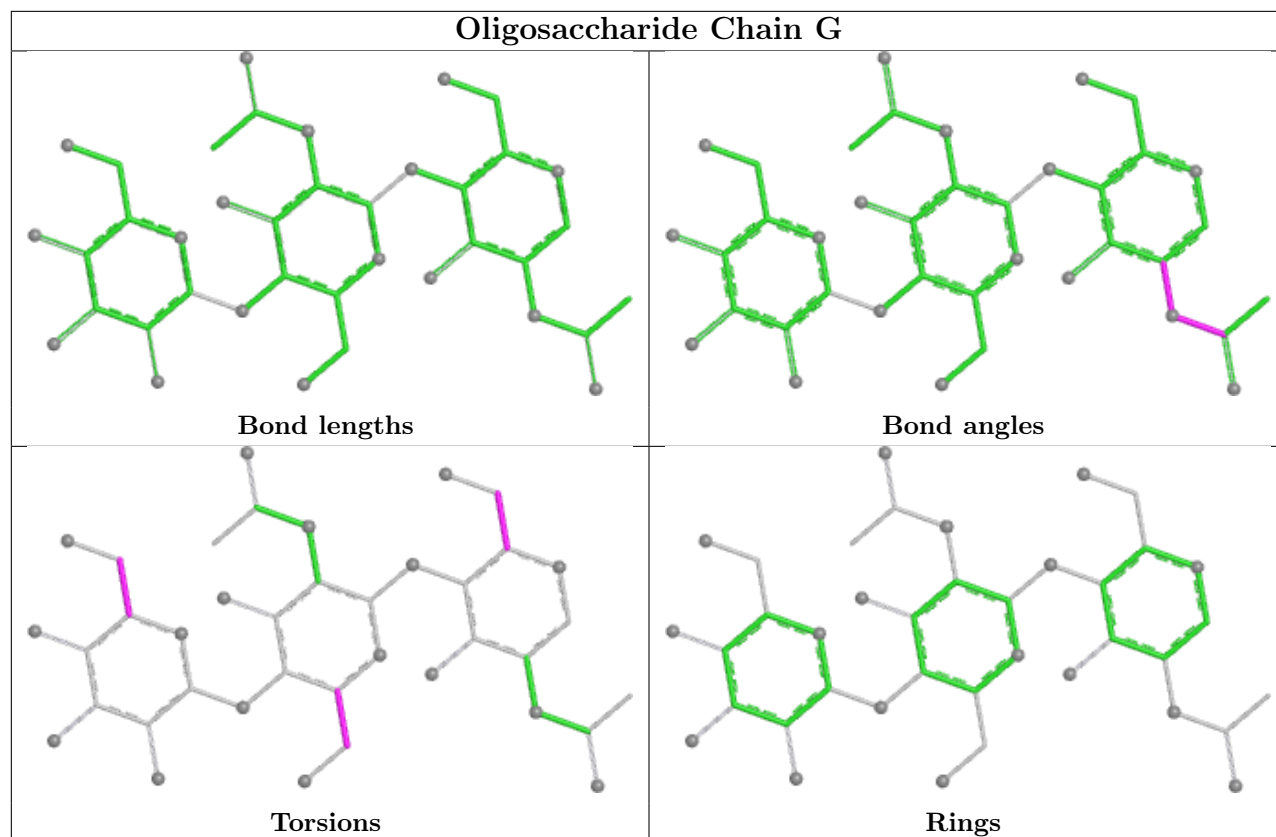












5.6 Ligand geometry

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	1502	-	4,4,4	0.56	0	6,6,6	0.75	0
4	NAG	B	772(A)	1	14,14,15	0.70	0	17,19,21	0.60	0
4	NAG	C	767(A)	1	14,14,15	0.61	0	17,19,21	0.63	0
5	SO4	A	1500	-	4,4,4	0.41	0	6,6,6	0.63	0
4	NAG	C	768(A)	1	14,14,15	0.58	0	17,19,21	0.65	0
4	NAG	A	768(A)	1	14,14,15	0.60	0	17,19,21	0.99	2 (11%)
4	NAG	C	771(A)	1	14,14,15	0.66	0	17,19,21	0.93	0
4	NAG	C	770(A)	1	14,14,15	0.70	0	17,19,21	0.62	0
6	BPR	D	801	1	12,16,16	0.48	0	15,22,22	0.57	0
4	NAG	A	767(A)	1	14,14,15	0.53	0	17,19,21	0.73	0
6	BPR	A	801	1	12,16,16	0.56	0	15,22,22	0.74	0
5	SO4	B	1501	-	4,4,4	0.50	0	6,6,6	0.61	0
6	BPR	B	801	1	12,16,16	0.68	0	15,22,22	0.77	0
4	NAG	A	771(A)	1	14,14,15	0.67	0	17,19,21	0.64	0
4	NAG	D	767(A)	1	14,14,15	0.66	0	17,19,21	0.66	0
4	NAG	D	773(A)	1	14,14,15	0.65	0	17,19,21	0.68	0
4	NAG	B	771(A)	1	14,14,15	0.68	0	17,19,21	0.78	0
5	SO4	D	1503	-	4,4,4	0.59	0	6,6,6	0.63	0
4	NAG	C	769(A)	1	14,14,15	0.56	0	17,19,21	0.79	0
4	NAG	B	773(A)	1	14,14,15	0.51	0	17,19,21	1.06	1 (5%)
6	BPR	C	801	1	12,16,16	0.73	0	15,22,22	0.96	1 (6%)
4	NAG	B	767(A)	1	14,14,15	0.81	1 (7%)	17,19,21	0.62	0
4	NAG	A	772(A)	1	14,14,15	0.54	0	17,19,21	0.97	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	772(A)	1	-	3/6/23/26	0/1/1/1
4	NAG	C	767(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	768(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	768(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	771(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	C	770(A)	1	-	4/6/23/26	0/1/1/1
6	BPR	D	801	1	-	1/8/29/29	0/2/2/2
4	NAG	A	767(A)	1	-	2/6/23/26	0/1/1/1
6	BPR	A	801	1	-	0/8/29/29	0/2/2/2
6	BPR	B	801	1	-	0/8/29/29	0/2/2/2
4	NAG	A	771(A)	1	-	3/6/23/26	0/1/1/1
4	NAG	D	767(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	D	773(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	C	769(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	773(A)	1	-	4/6/23/26	0/1/1/1
6	BPR	C	801	1	-	0/8/29/29	0/2/2/2
4	NAG	B	767(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	772(A)	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	767(A)	NAG	C1-C2	2.11	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	801	BPR	C-CA-N	2.85	116.67	110.98
4	B	773(A)	NAG	C2-N2-C7	-2.74	119.23	122.90
4	A	772(A)	NAG	C2-N2-C7	-2.67	119.33	122.90
4	A	768(A)	NAG	C2-N2-C7	-2.41	119.67	122.90
4	A	768(A)	NAG	C4-C3-C2	-2.03	108.05	111.02

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	767(A)	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	767(A)	NAG	O7-C7-N2-C2
4	A	768(A)	NAG	C8-C7-N2-C2
4	A	768(A)	NAG	O7-C7-N2-C2
4	A	771(A)	NAG	C8-C7-N2-C2
4	A	771(A)	NAG	O7-C7-N2-C2
4	B	767(A)	NAG	C8-C7-N2-C2
4	B	767(A)	NAG	O7-C7-N2-C2
4	B	772(A)	NAG	C8-C7-N2-C2
4	B	772(A)	NAG	O7-C7-N2-C2
4	C	768(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	O7-C7-N2-C2
4	C	770(A)	NAG	C8-C7-N2-C2
4	C	770(A)	NAG	O7-C7-N2-C2
4	C	771(A)	NAG	C8-C7-N2-C2
4	C	771(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O7-C7-N2-C2
4	C	771(A)	NAG	C4-C5-C6-O6
4	C	767(A)	NAG	O5-C5-C6-O6
4	A	772(A)	NAG	O5-C5-C6-O6
4	C	767(A)	NAG	C4-C5-C6-O6
4	A	772(A)	NAG	C4-C5-C6-O6
4	C	771(A)	NAG	O5-C5-C6-O6
4	C	768(A)	NAG	C4-C5-C6-O6
4	C	768(A)	NAG	O5-C5-C6-O6
4	D	773(A)	NAG	O5-C5-C6-O6
4	C	770(A)	NAG	C4-C5-C6-O6
4	D	767(A)	NAG	C4-C5-C6-O6
4	C	770(A)	NAG	O5-C5-C6-O6
4	A	768(A)	NAG	O5-C5-C6-O6
4	D	767(A)	NAG	O5-C5-C6-O6
4	A	772(A)	NAG	C8-C7-N2-C2
4	B	773(A)	NAG	O5-C5-C6-O6
4	D	773(A)	NAG	C4-C5-C6-O6
4	A	771(A)	NAG	O5-C5-C6-O6
4	A	772(A)	NAG	O7-C7-N2-C2
4	C	769(A)	NAG	C4-C5-C6-O6
4	B	773(A)	NAG	C8-C7-N2-C2
4	C	767(A)	NAG	C8-C7-N2-C2
4	B	767(A)	NAG	C4-C5-C6-O6
4	A	768(A)	NAG	C4-C5-C6-O6
4	B	773(A)	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	C	767(A)	NAG	O7-C7-N2-C2
4	B	767(A)	NAG	O5-C5-C6-O6
4	C	769(A)	NAG	O5-C5-C6-O6
6	D	801	BPR	O-C-N1-C1
4	B	772(A)	NAG	O5-C5-C6-O6
4	B	773(A)	NAG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	767(A)	NAG	3	0
4	C	768(A)	NAG	1	0
4	A	768(A)	NAG	1	0
6	D	801	BPR	1	0
6	A	801	BPR	2	0
6	B	801	BPR	3	0
4	D	773(A)	NAG	1	0
4	C	769(A)	NAG	2	0
6	C	801	BPR	4	0
4	B	767(A)	NAG	2	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

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	724/728 (99%)	0.44	23 (3%)	50	51	9, 35, 60, 94	13 (1%)
1	B	728/728 (100%)	0.24	17 (2%)	61	62	7, 31, 58, 76	12 (1%)
1	C	723/728 (99%)	0.92	120 (16%)	4	3	12, 43, 85, 108	12 (1%)
1	D	728/728 (100%)	0.36	28 (3%)	44	45	12, 33, 66, 86	10 (1%)
All	All	2903/2912 (99%)	0.49	188 (6%)	25	25	7, 35, 69, 108	47 (1%)

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	LEU	6.4
1	A	101	SER	5.2
1	C	83	TYR	5.1
1	C	90	LEU	5.0
1	D	82	GLU	4.6
1	C	417	TYR	4.5
1	A	102	THR	4.5
1	C	468	TYR	4.4
1	D	83	TYR	4.2
1	C	70	TYR	4.0
1	C	116	PHE	3.9
1	D	101	SER	3.9
1	C	39	SER	3.9
1	C	79	PHE	3.9
1	C	88	ILE	3.9
1	C	506	ASP	3.8
1	C	461	PHE	3.7
1	C	81	ALA	3.7
1	C	766	PRO	3.6
1	D	99	GLY	3.5
1	B	103	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	134	ILE	3.5
1	A	103	ASN	3.4
1	A	93	SER	3.4
1	A	96	ASP	3.4
1	B	83	TYR	3.4
1	C	137	LEU	3.4
1	D	81	ALA	3.4
1	B	487	SER	3.4
1	C	414	TYR	3.3
1	C	76	ILE	3.3
1	C	388	GLN	3.3
1	C	438	ASP	3.2
1	C	84	GLY	3.2
1	A	377	ASN	3.2
1	C	69	LEU	3.2
1	C	487	SER	3.2
1	C	94	THR	3.2
1	C	95	PHE	3.2
1	B	99	GLY	3.1
1	C	395	THR	3.1
1	C	141	GLN	3.1
1	C	492	ARG	3.1
1	C	384	ILE	3.1
1	A	83	TYR	3.0
1	C	439	TYR	3.0
1	C	77	LEU	3.0
1	C	486	SER	3.0
1	C	143	ILE	3.0
1	C	115	LEU	3.0
1	B	39	SER	3.0
1	C	467	TYR	2.9
1	C	93	SER	2.9
1	C	97	GLU	2.9
1	B	41	ARG	2.9
1	C	140	ARG	2.9
1	D	100	TYR	2.9
1	A	450	ASN	2.9
1	A	765	LEU	2.9
1	C	449	LEU	2.9
1	C	385	CYS	2.9
1	C	73	GLU	2.9
1	B	488	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	96	ASP	2.8
1	C	135	TYR	2.8
1	C	416	TYR	2.8
1	C	432	TYR	2.8
1	C	494	LEU	2.8
1	C	472	CYS	2.8
1	C	380	GLY	2.7
1	C	181	SER	2.7
1	C	412	SER	2.7
1	C	451	PRO	2.7
1	C	491	LEU	2.7
1	C	490	GLU	2.7
1	C	505	GLN	2.7
1	C	89	PHE	2.7
1	C	148	ILE	2.7
1	C	139	LYS	2.7
1	C	574	ILE	2.6
1	C	415	LEU	2.6
1	C	42	THR	2.6
1	D	102	THR	2.6
1	C	434	ILE	2.6
1	C	78	LEU	2.6
1	C	394	CYS	2.6
1	C	445	LEU	2.6
1	D	103	ASN	2.6
1	A	39	SER	2.6
1	C	113	PHE	2.6
1	D	79	PHE	2.6
1	C	91	GLU	2.6
1	C	179	ASN	2.6
1	C	493	VAL	2.6
1	D	84	GLY	2.5
1	D	90	LEU	2.5
1	C	435	GLN	2.5
1	C	480	TYR	2.5
1	D	379	GLU	2.5
1	C	450	ASN	2.5
1	C	389	THR	2.5
1	C	398	THR	2.5
1	C	41	ARG	2.5
1	C	136	ASP	2.5
1	C	386	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	ALA	2.5
1	C	465	ALA	2.5
1	C	537	SER	2.5
1	B	617	GLY	2.5
1	C	410	LEU	2.5
1	C	305	TRP	2.5
1	B	101	SER	2.5
1	D	39	SER	2.5
1	C	138	ASN	2.4
1	A	378	GLU	2.4
1	C	396	PHE	2.4
1	C	85	ASN	2.4
1	A	379	GLU	2.4
1	C	538	LYS	2.4
1	C	72	GLN	2.4
1	B	498	SER	2.4
1	C	180	LEU	2.4
1	C	105	TYR	2.4
1	B	697	GLN	2.3
1	C	762	CYS	2.3
1	D	138	ASN	2.3
1	C	419	SER	2.3
1	D	485	SER	2.3
1	D	487	SER	2.3
1	C	114	ILE	2.3
1	A	116	PHE	2.3
1	C	120	TYR	2.3
1	C	149	PRO	2.3
1	C	86	SER	2.3
1	C	488	ASP	2.3
1	A	439	TYR	2.3
1	A	491	LEU	2.3
1	C	504	LEU	2.3
1	D	143	ILE	2.3
1	C	387	PHE	2.3
1	C	401	ALA	2.2
1	B	503	MET	2.2
1	C	479	LEU	2.2
1	A	79	PHE	2.2
1	C	437	ASN	2.2
1	C	536	LYS	2.2
1	C	119	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	483	HIS	2.2
1	D	726	ALA	2.2
1	C	761	GLN	2.2
1	C	436	LEU	2.2
1	C	477	LEU	2.2
1	D	491	LEU	2.2
1	C	409	ALA	2.1
1	C	470	LEU	2.1
1	A	492	ARG	2.1
1	B	40	ARG	2.1
1	B	145	GLU	2.1
1	D	537	SER	2.1
1	D	757	HIS	2.1
1	C	459	ALA	2.1
1	C	75	ASN	2.1
1	D	377	ASN	2.1
1	A	70	TYR	2.1
1	B	489	LYS	2.1
1	D	538	LYS	2.1
1	C	422	HIS	2.1
1	D	95	PHE	2.1
1	C	107	VAL	2.1
1	C	442	VAL	2.1
1	C	482	LEU	2.1
1	A	94	THR	2.1
1	C	443	THR	2.1
1	D	547	TYR	2.1
1	C	535	ASP	2.1
1	B	143	ILE	2.1
1	D	295	ILE	2.1
1	C	132	TYR	2.1
1	C	191	GLU	2.0
1	C	421	GLU	2.0
1	D	88	ILE	2.0
1	C	456	TYR	2.0
1	D	388	GLN	2.0
1	A	77	LEU	2.0
1	B	399	LYS	2.0
1	C	307	THR	2.0
1	A	766	PRO	2.0
1	A	87	SER	2.0

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

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

6.3 Carbohydrates ⓘ

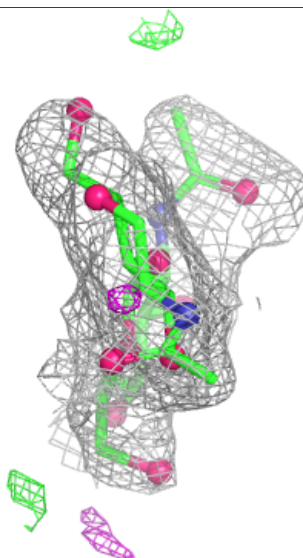
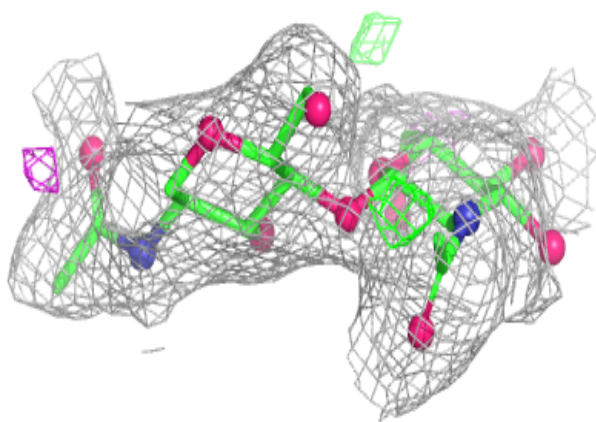
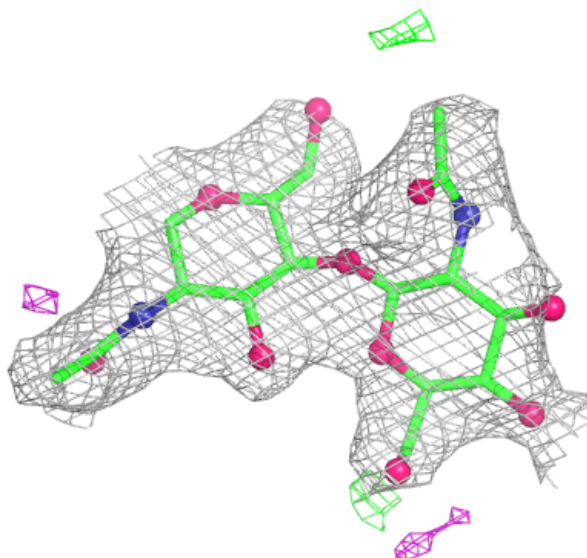
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.36	0.19	82,84,85,86	0
3	BMA	J	3	11/12	0.44	0.20	103,104,105,105	0
3	NAG	J	2	14/15	0.55	0.19	96,98,100,102	0
2	NAG	M	2	14/15	0.58	0.16	55,58,64,67	0
3	NAG	J	1	14/15	0.61	0.20	84,87,91,92	0
2	NAG	K	2	14/15	0.66	0.14	52,55,56,58	0
3	NAG	G	2	14/15	0.68	0.15	71,72,74,78	0
2	NAG	I	2	14/15	0.70	0.13	48,53,55,56	0
2	NAG	H	2	14/15	0.74	0.14	57,59,60,60	0
3	NAG	G	1	14/15	0.76	0.14	62,65,66,67	0
2	NAG	E	2	14/15	0.76	0.13	50,54,56,58	0
2	NAG	L	2	14/15	0.77	0.16	59,64,66,67	0
2	NAG	F	2	14/15	0.80	0.11	49,51,53,54	0
2	NAG	I	1	14/15	0.80	0.12	44,47,50,51	0
2	NAG	L	1	14/15	0.82	0.14	43,46,50,57	0
2	NAG	M	1	14/15	0.84	0.11	35,41,45,50	0
2	NAG	H	1	14/15	0.84	0.11	46,51,54,54	0
2	NAG	F	1	14/15	0.87	0.10	40,44,47,48	0
2	NAG	E	1	14/15	0.88	0.10	32,39,44,48	0
2	NAG	K	1	14/15	0.91	0.08	29,36,41,46	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.

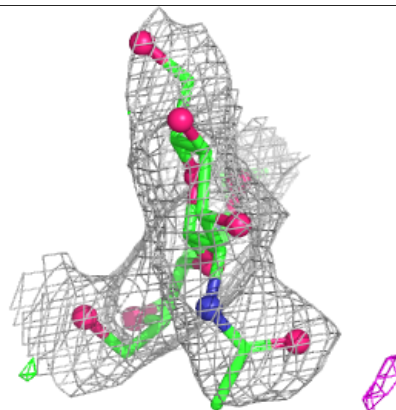
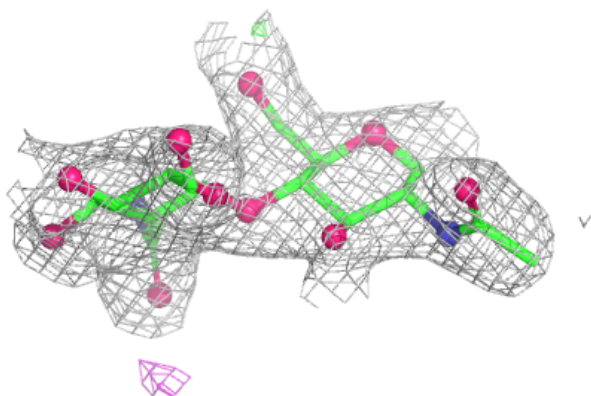
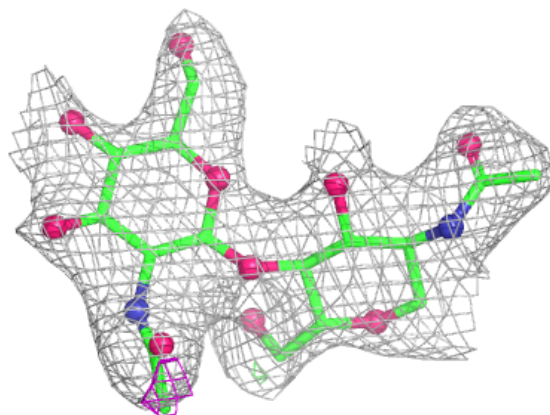
Electron density around Chain E:

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



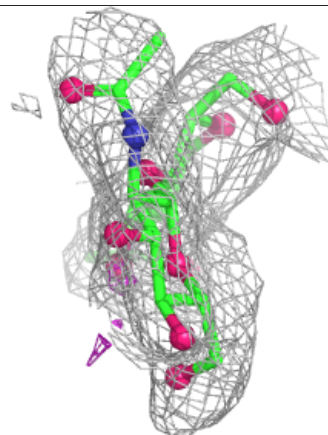
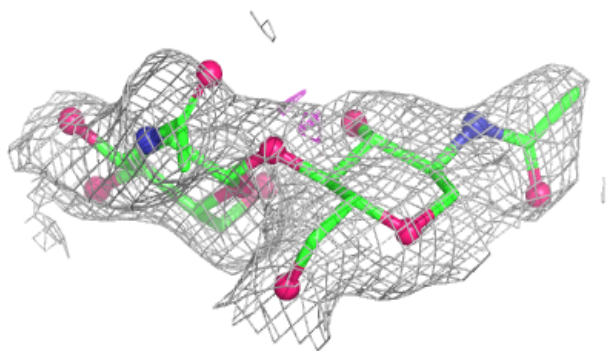
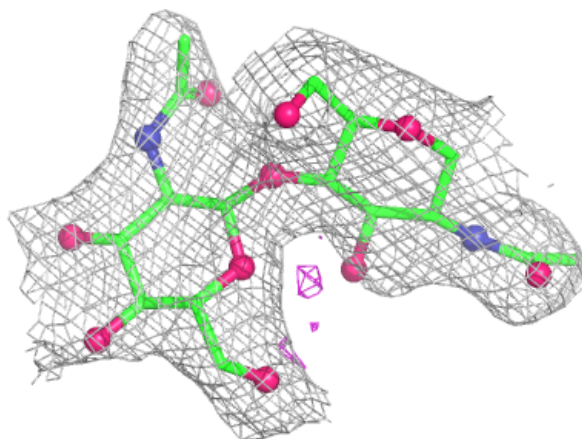
Electron density around Chain F:

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



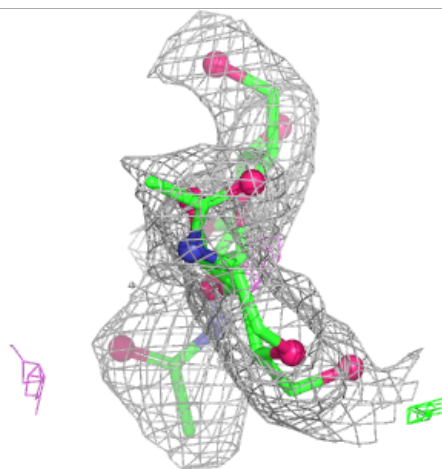
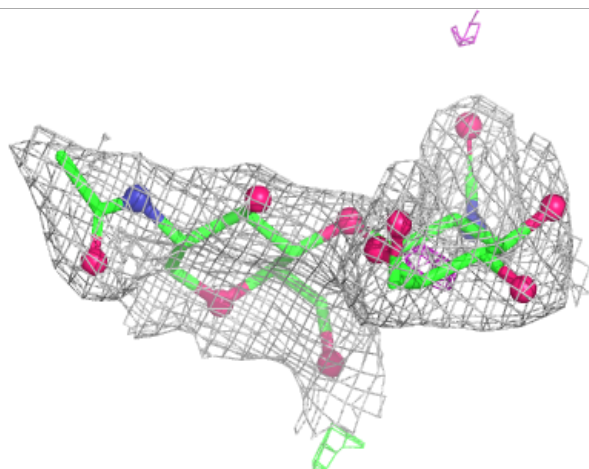
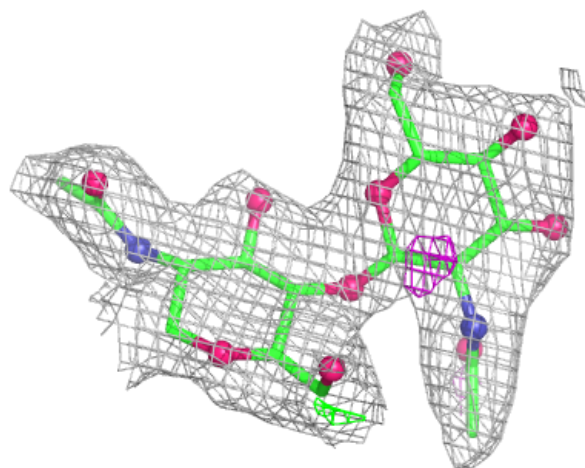
Electron density around Chain H:

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



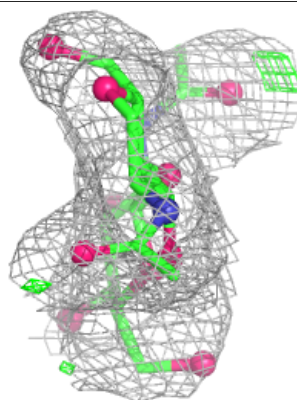
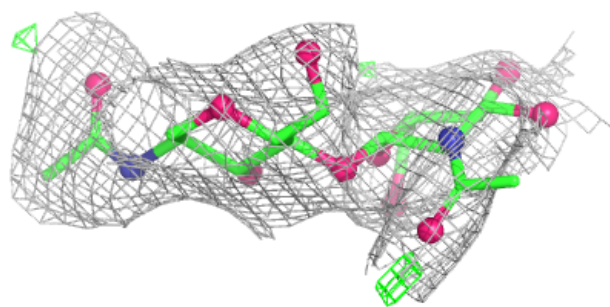
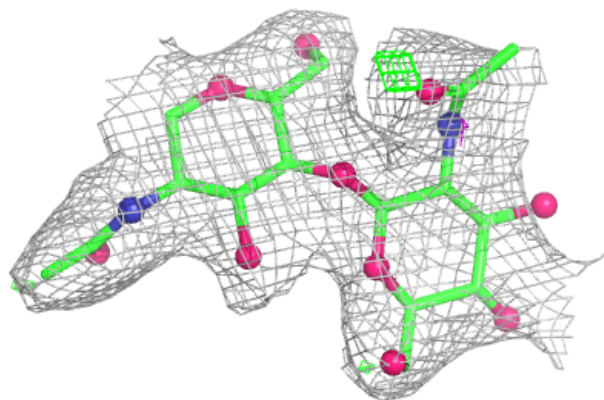
Electron density around Chain I:

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

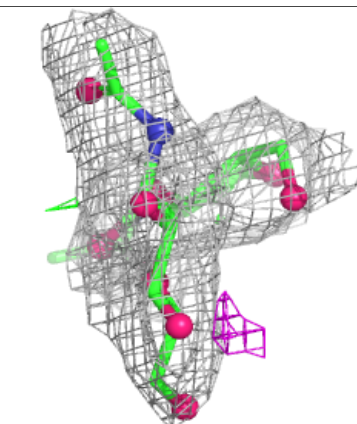
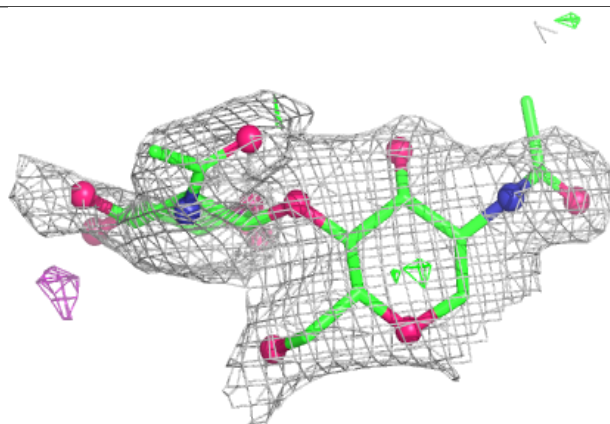
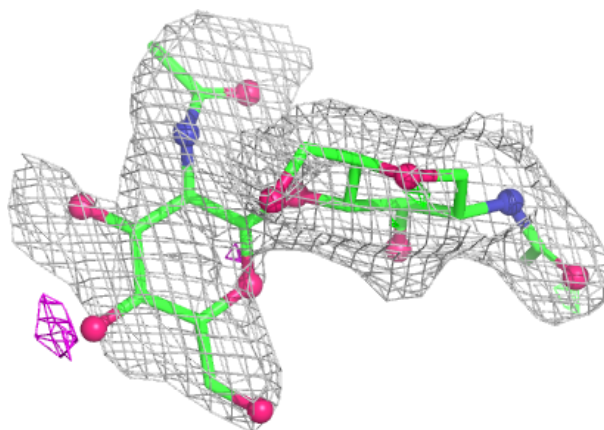


Electron density around Chain K:

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

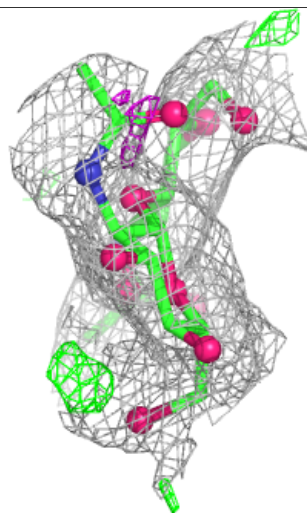
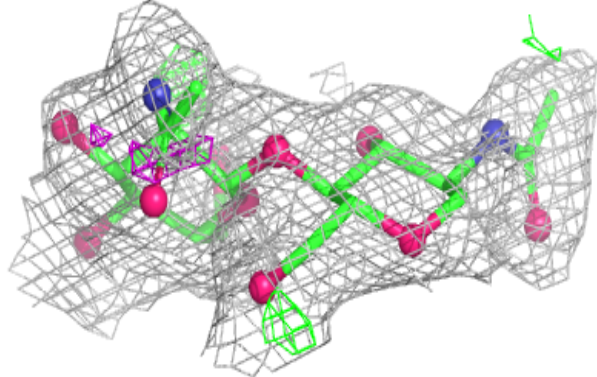
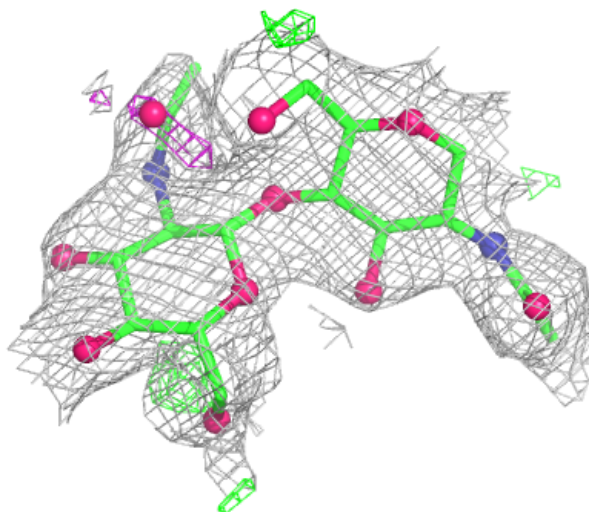
**Electron density around Chain L:**

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



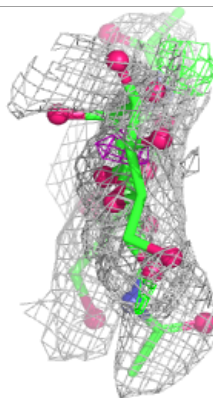
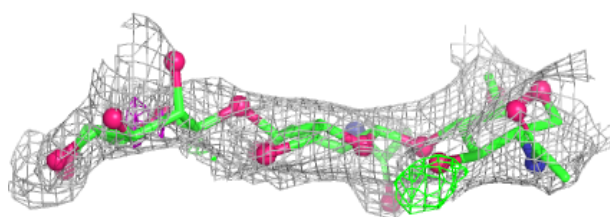
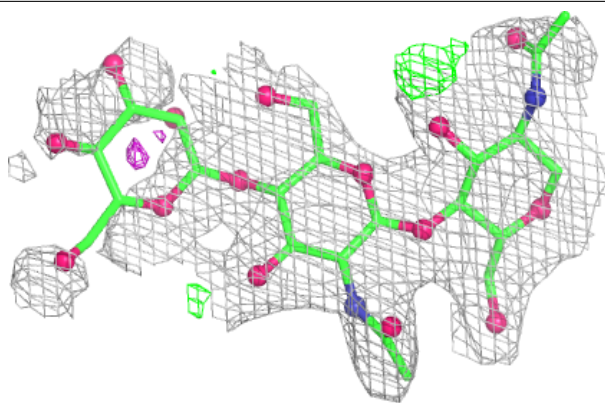
Electron density around Chain M:

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

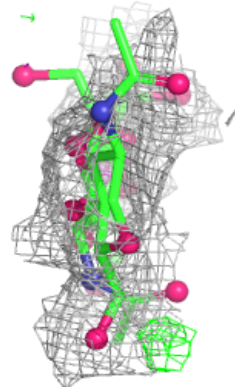
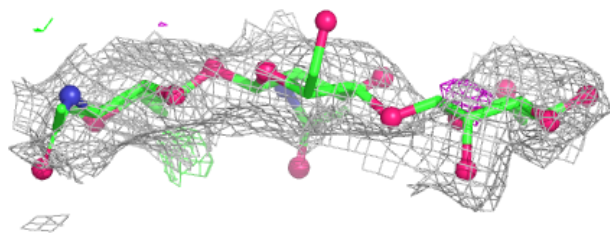
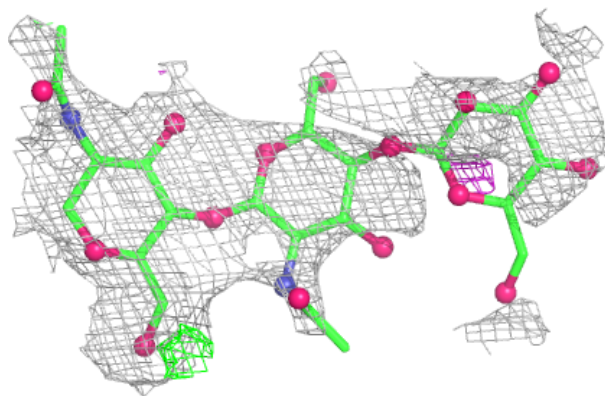


Electron density around Chain G:

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

**Electron density around Chain J:**

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	767(A)	14/15	0.20	0.23	97,99,101,102	0
4	NAG	D	773(A)	14/15	0.54	0.18	55,58,66,66	0
4	NAG	C	768(A)	14/15	0.55	0.18	100,101,101,101	0
4	NAG	C	767(A)	14/15	0.56	0.16	93,95,96,96	0
4	NAG	A	771(A)	14/15	0.57	0.16	47,50,53,53	3
4	NAG	A	767(A)	14/15	0.59	0.16	84,86,87,88	0
4	NAG	B	767(A)	14/15	0.59	0.18	76,77,79,79	0
4	NAG	A	768(A)	14/15	0.65	0.17	82,83,85,85	0
4	NAG	C	771(A)	14/15	0.69	0.14	56,59,62,62	0
4	NAG	B	772(A)	14/15	0.72	0.14	50,53,58,59	0
4	NAG	C	770(A)	14/15	0.76	0.13	55,58,60,61	0
4	NAG	A	772(A)	14/15	0.85	0.10	44,46,48,51	0
5	SO4	C	1502	5/5	0.85	0.13	44,46,49,49	0
4	NAG	C	769(A)	14/15	0.86	0.11	33,35,38,39	0
4	NAG	B	773(A)	14/15	0.86	0.10	38,41,42,43	0
6	BPR	B	801	15/15	0.90	0.10	14,17,20,21	0
6	BPR	A	801	15/15	0.91	0.10	26,28,30,30	0
4	NAG	B	771(A)	14/15	0.91	0.08	23,30,34,37	0
6	BPR	D	801	15/15	0.92	0.09	22,25,27,28	0
6	BPR	C	801	15/15	0.94	0.07	16,21,22,22	0
5	SO4	A	1500	5/5	0.94	0.09	45,45,46,46	0
5	SO4	D	1503	5/5	0.96	0.07	46,46,47,47	0
5	SO4	B	1501	5/5	0.98	0.06	37,38,40,40	0

6.5 Other polymers

There are no such residues in this entry.