



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:40 AM UTC

PDB ID : 1VIW / pdb_00001viw
Title : TENEBRIO MOLITOR ALPHA-AMYLASE-INHIBITOR COMPLEX
Authors : Nahoum, V.; Egloff, M.P.; Payan, F.
Deposited on : 1998-07-21
Resolution : 3.00 Å(reported)

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

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

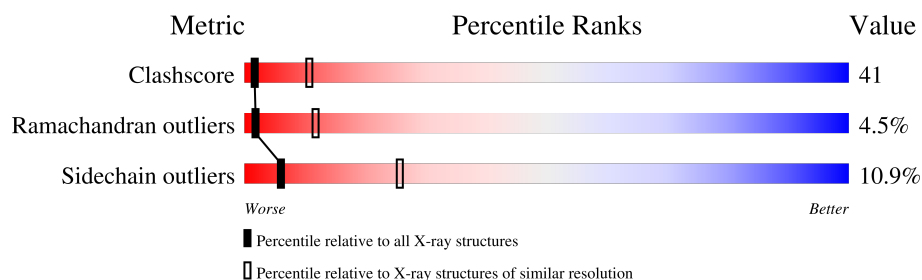
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	471	
2	B	205	
3	C	2	
3	D	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	A	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5218 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 ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3604	2240	627	717	20			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ASN	ASP	conflict	UNP P56634
A	158	ALA	GLN	conflict	UNP P56634
A	200	ASP	SER	conflict	UNP P56634

- Molecule 2 is a protein called ALPHA-AMYLASE-INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	198	Total	C	N	O	S	0	0	0
			1556	976	255	323	2			

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



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

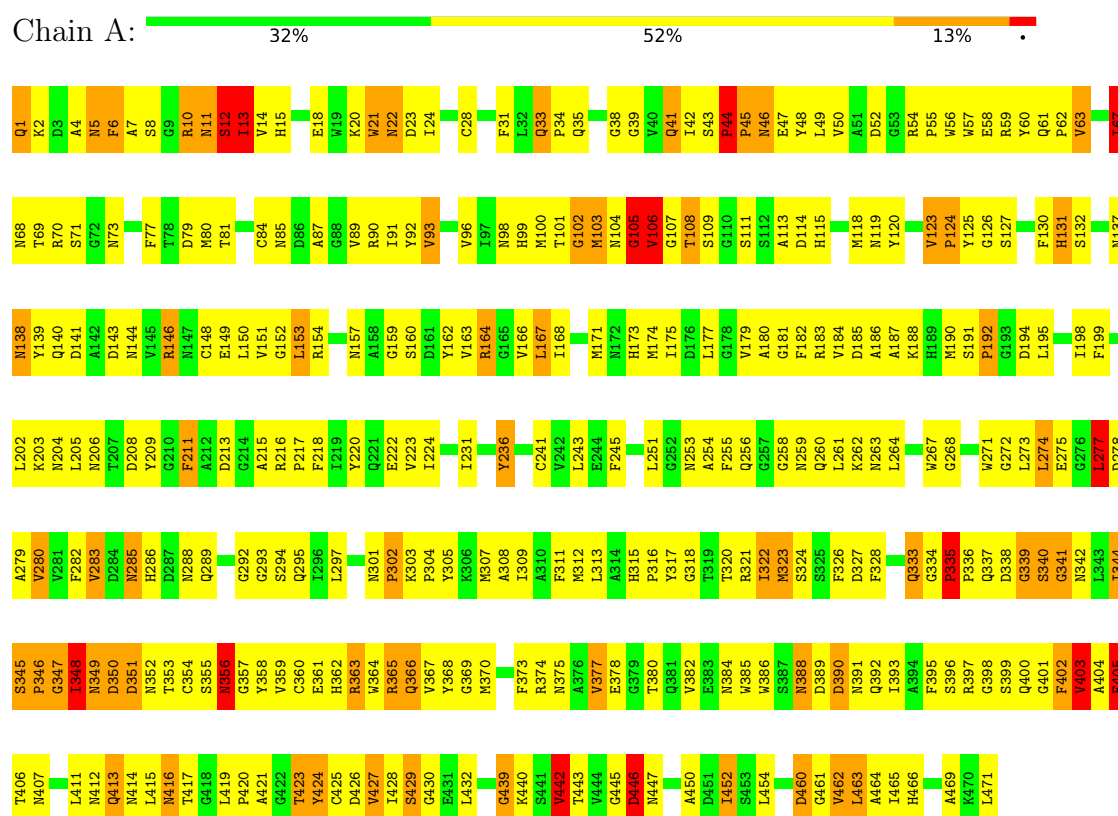
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

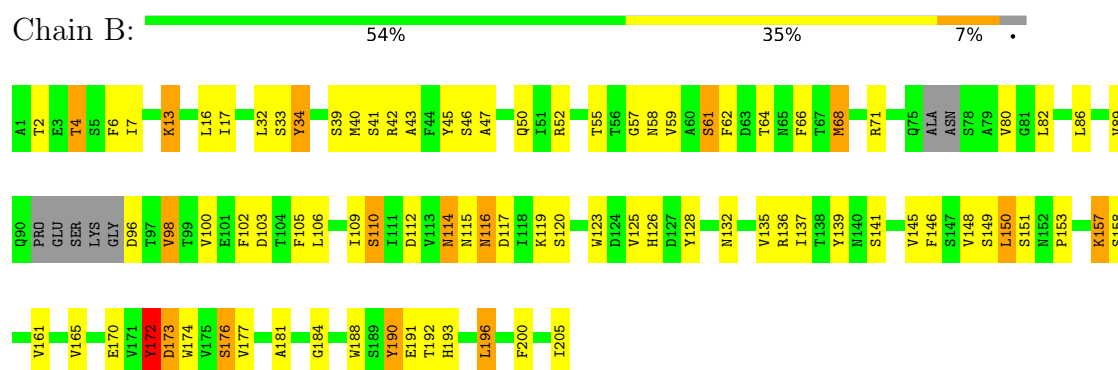
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: ALPHA-AMYLASE



• Molecule 2: ALPHA-AMYLASE-INHIBITOR



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

Chain C:  50% 50%

MAG1
MAG2

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

Chain D:  100%

MAG1
MAG2

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.47Å 75.91Å 61.99Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.2 (10.00-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.230 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, NAG, CA, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.21	31/3682 (0.8%)	1.53	88/5001 (1.8%)
2	B	0.92	3/1588 (0.2%)	1.19	10/2162 (0.5%)
All	All	1.13	34/5270 (0.6%)	1.44	98/7163 (1.4%)

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	A	1	2
2	B	0	2
All	All	1	4

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	N-CA	-17.67	1.24	1.46
1	A	182	PHE	CA-C	-14.66	1.34	1.52
1	A	349	ASN	C-N	-13.42	1.15	1.33
1	A	442	VAL	C-O	-13.15	1.06	1.24
1	A	424	TYR	C-N	11.45	1.49	1.33
1	A	123	VAL	CA-CB	10.85	1.68	1.54
1	A	349	ASN	N-CA	-10.22	1.33	1.46
1	A	443	THR	CA-C	9.70	1.65	1.52
1	A	423	THR	CA-C	-8.48	1.42	1.52
2	B	116	ASN	C-O	8.12	1.33	1.23
1	A	424	TYR	N-CA	-7.96	1.36	1.46
1	A	443	THR	CA-CB	-7.83	1.41	1.53
2	B	61	SER	C-O	-7.46	1.14	1.24
1	A	12	SER	N-CA	7.29	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	VAL	N-CA	7.14	1.56	1.47
1	A	377	VAL	C-N	-6.76	1.24	1.33
1	A	348	ILE	C-N	6.73	1.43	1.33
1	A	429	SER	CA-C	-6.43	1.44	1.52
1	A	423	THR	C-N	-6.41	1.23	1.33
1	A	425	CYS	N-CA	6.21	1.54	1.46
1	A	439	GLY	N-CA	6.20	1.54	1.45
1	A	347	GLY	CA-C	-6.11	1.46	1.51
1	A	10	ARG	C-N	6.08	1.41	1.33
1	A	124	PRO	C-N	-6.05	1.25	1.33
1	A	346	PRO	C-N	-5.96	1.30	1.33
1	A	337	GLN	CA-C	5.92	1.59	1.52
1	A	192	PRO	C-N	-5.84	1.26	1.33
1	A	413	GLN	C-N	-5.61	1.25	1.33
2	B	61	SER	C-N	-5.61	1.25	1.33
1	A	411	LEU	C-N	-5.36	1.27	1.33
1	A	335	PRO	C-N	-5.31	1.27	1.33
1	A	412	ASN	CA-C	-5.24	1.48	1.53
1	A	439	GLY	C-N	5.18	1.40	1.33
1	A	280	VAL	C-O	-5.05	1.18	1.24

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLY	N-CA-C	-16.56	88.67	110.69
1	A	294	SER	N-CA-C	13.10	133.41	109.32
1	A	351	ASP	N-CA-C	-12.45	95.39	112.94
1	A	63	VAL	N-CA-C	-12.10	101.41	111.81
1	A	183	ARG	N-CA-C	-10.81	86.60	107.57
1	A	442	VAL	CA-C-O	-9.79	109.60	121.54
1	A	104	ASN	O-C-N	9.59	135.66	123.19
1	A	443	THR	N-CA-CB	-9.18	96.24	110.56
1	A	132	SER	CA-C-N	-8.42	111.34	119.76
1	A	132	SER	C-N-CA	-8.42	111.34	119.76
2	B	61	SER	O-C-N	-8.42	113.45	123.13
1	A	442	VAL	CB-CA-C	-8.33	100.14	111.63
1	A	123	VAL	N-CA-C	8.12	126.41	108.88
1	A	337	GLN	CA-C-N	8.10	137.01	121.54
1	A	337	GLN	C-N-CA	8.10	137.01	121.54
1	A	44	PRO	CA-C-N	7.99	127.71	119.64
1	A	44	PRO	C-N-CA	7.99	127.71	119.64
1	A	349	ASN	O-C-N	-7.98	111.98	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASN	CA-C-N	7.94	136.98	121.41
1	A	104	ASN	C-N-CA	7.94	136.98	121.41
1	A	294	SER	CB-CA-C	-7.78	106.54	115.79
1	A	345	SER	CA-C-N	-7.75	112.01	119.76
1	A	345	SER	C-N-CA	-7.75	112.01	119.76
1	A	388	ASN	N-CA-C	-7.68	103.23	112.59
1	A	106	VAL	CB-CA-C	-7.66	103.95	112.68
1	A	295	GLN	N-CA-C	7.48	123.72	111.37
1	A	106	VAL	N-CA-C	7.39	117.27	106.55
1	A	217	PRO	CB-CA-C	-7.23	102.71	111.46
1	A	104	ASN	N-CA-C	7.13	121.13	109.72
1	A	347	GLY	CA-C-N	-7.02	109.33	121.97
1	A	347	GLY	C-N-CA	-7.02	109.33	121.97
1	A	11	ASN	O-C-N	6.93	131.38	123.48
1	A	341	GLY	CA-C-N	-6.90	112.98	122.30
1	A	341	GLY	C-N-CA	-6.90	112.98	122.30
1	A	105	GLY	N-CA-C	6.88	129.47	113.18
2	B	176	SER	O-C-N	-6.80	112.04	122.93
1	A	102	GLY	CA-C-N	6.72	134.38	121.54
1	A	102	GLY	C-N-CA	6.72	134.38	121.54
1	A	344	ILE	CB-CA-C	-6.68	102.65	111.13
1	A	378	GLU	N-CA-C	6.66	119.41	110.35
1	A	412	ASN	N-CA-C	-6.64	99.68	109.11
1	A	41	GLN	N-CA-C	-6.55	96.45	107.99
2	B	190	TYR	N-CA-C	6.42	121.11	113.28
2	B	145	VAL	N-CA-C	6.41	117.06	107.51
1	A	289	GLN	N-CA-C	-6.38	105.25	113.16
1	A	294	SER	CA-C-N	6.38	130.39	120.82
1	A	294	SER	C-N-CA	6.38	130.39	120.82
2	B	61	SER	N-CA-C	-6.33	98.89	108.96
1	A	11	ASN	CA-C-N	6.32	133.60	121.54
1	A	11	ASN	C-N-CA	6.32	133.60	121.54
1	A	301	ASN	CA-C-N	6.27	127.67	119.84
1	A	301	ASN	C-N-CA	6.27	127.67	119.84
2	B	89	VAL	N-CA-C	6.27	117.51	107.73
1	A	131	HIS	N-CA-C	-6.25	102.72	110.41
2	B	176	SER	CA-C-O	-6.24	108.66	120.69
1	A	182	PHE	CA-C-N	6.23	131.99	122.77
1	A	182	PHE	C-N-CA	6.23	131.99	122.77
1	A	341	GLY	O-C-N	6.20	130.76	122.70
1	A	348	ILE	N-CA-C	6.14	122.11	109.34
1	A	357	GLY	N-CA-C	6.14	123.79	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLN	N-CA-C	6.11	119.47	112.57
1	A	349	ASN	N-CA-C	-6.10	97.81	110.80
2	B	100	VAL	CA-C-N	-6.09	114.40	122.99
2	B	100	VAL	C-N-CA	-6.09	114.40	122.99
1	A	183	ARG	N-CA-CB	6.00	120.48	110.53
1	A	292	GLY	CA-C-N	5.94	129.11	120.91
1	A	292	GLY	C-N-CA	5.94	129.11	120.91
1	A	139	TYR	N-CA-C	-5.88	106.15	113.15
1	A	348	ILE	CA-C-N	-5.83	110.41	121.54
1	A	348	ILE	C-N-CA	-5.83	110.41	121.54
1	A	424	TYR	O-C-N	5.75	130.29	123.27
1	A	351	ASP	O-C-N	5.58	128.94	122.19
1	A	13	ILE	N-CA-CB	-5.57	105.41	112.60
1	A	429	SER	CA-C-N	-5.50	114.99	122.03
1	A	429	SER	C-N-CA	-5.50	114.99	122.03
1	A	347	GLY	O-C-N	-5.48	119.89	123.35
1	A	377	VAL	O-C-N	-5.46	117.18	122.09
2	B	57	GLY	N-CA-C	-5.45	107.16	114.25
1	A	268	GLY	CA-C-N	5.45	126.65	119.84
1	A	268	GLY	C-N-CA	5.45	126.65	119.84
1	A	348	ILE	O-C-N	5.38	129.30	122.57
1	A	378	GLU	O-C-N	5.35	129.39	122.81
1	A	146	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	405	PHE	N-CA-C	5.22	115.24	107.88
1	A	211	PHE	N-CA-C	5.18	117.75	110.23
1	A	149	GLU	N-CA-C	5.18	117.14	108.23
1	A	164	ARG	N-CA-C	-5.18	105.64	111.28
1	A	356	ASN	N-CA-C	5.16	118.32	111.30
1	A	446	ASP	N-CA-C	5.13	121.73	110.80
1	A	348	ILE	CA-CB-CG1	-5.12	101.69	110.40
1	A	280	VAL	N-CA-C	-5.12	99.15	107.28
1	A	316	PRO	N-CA-C	5.11	120.27	113.57
1	A	403	VAL	CB-CA-C	-5.09	104.22	111.40
1	A	429	SER	O-C-N	5.08	128.83	122.23
1	A	93	VAL	N-CA-C	5.05	116.09	109.58
1	A	423	THR	O-C-N	5.05	129.43	123.27
1	A	377	VAL	CB-CA-C	-5.03	104.99	111.88
1	A	469	ALA	N-CA-C	-5.01	105.28	113.19

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
1	A	1	PCA	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	GLY	Mainchain
1	A	442	VAL	Mainchain
2	B	116	ASN	Mainchain
2	B	176	SER	Mainchain

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	3604	0	3330	351	0
2	B	1556	0	1463	66	0
3	C	28	0	25	3	0
3	D	28	0	25	0	0
4	A	1	0	0	1	0
5	A	1	0	0	0	0
All	All	5218	0	4843	413	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 41.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG11	1:A:125:TYR:CE2	1.59	1.38
1:A:123:VAL:HG21	1:A:125:TYR:CD2	1.74	1.22
1:A:123:VAL:HG11	1:A:125:TYR:CD2	1.76	1.19
1:A:123:VAL:HG21	1:A:125:TYR:CE2	1.87	1.09
1:A:61:GLN:HB3	1:A:101:THR:HG22	1.31	1.09
1:A:432:LEU:O	1:A:432:LEU:HD12	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:HD12	1:A:349:ASN:N	1.74	1.03
1:A:345:SER:HB3	1:A:358:TYR:CD2	1.95	1.00
1:A:123:VAL:CG1	1:A:125:TYR:CE2	2.46	0.99
1:A:123:VAL:CG2	1:A:125:TYR:CD2	2.45	0.98
1:A:123:VAL:CG1	1:A:125:TYR:CD2	2.47	0.97
1:A:274:LEU:HD21	1:A:279:ALA:HB2	1.46	0.97
1:A:349:ASN:O	1:A:350:ASP:HB2	1.66	0.94
1:A:421:ALA:HB2	1:A:446:ASP:HA	1.47	0.94
1:A:123:VAL:CG2	1:A:125:TYR:HD2	1.80	0.94
1:A:70:ARG:HH21	1:A:342:ASN:HD21	1.15	0.93
1:A:313:LEU:HD23	1:A:370:MET:HB3	1.50	0.90
1:A:364:TRP:HB3	1:A:366:GLN:HE22	1.37	0.89
1:A:102:GLY:HA2	1:A:115:HIS:CD2	2.08	0.88
1:A:442:VAL:HG23	1:A:442:VAL:O	1.72	0.88
1:A:338:ASP:OD1	1:A:338:ASP:O	1.90	0.88
2:B:86:LEU:HB2	2:B:98:VAL:HG13	1.56	0.88
1:A:123:VAL:CB	1:A:125:TYR:CD2	2.57	0.86
1:A:47:GLU:HG3	1:A:108:THR:HG22	1.57	0.86
1:A:349:ASN:O	1:A:350:ASP:CB	2.18	0.86
1:A:123:VAL:CB	1:A:125:TYR:HD2	1.89	0.85
1:A:432:LEU:O	1:A:432:LEU:CD1	2.23	0.85
1:A:346:PRO:HD2	1:A:356:ASN:HD21	1.43	0.83
1:A:427:VAL:HA	1:A:430:GLY:O	1.77	0.82
1:A:426:ASP:O	1:A:430:GLY:O	1.96	0.82
1:A:420:PRO:O	1:A:424:TYR:OH	1.98	0.81
2:B:110:SER:HB3	2:B:120:SER:HB3	1.61	0.80
1:A:42:ILE:HD12	1:A:80:MET:HE1	1.63	0.80
1:A:262:LYS:HA	1:A:393:ILE:HD11	1.65	0.79
1:A:364:TRP:HB3	1:A:366:GLN:NE2	1.95	0.79
1:A:77:PHE:CZ	1:A:174:MET:HE1	2.18	0.79
1:A:452:ILE:HD13	1:A:452:ILE:H	1.45	0.79
1:A:364:TRP:HB2	1:A:367:VAL:HG12	1.65	0.79
1:A:114:ASP:HB3	1:A:119:ASN:HB2	1.65	0.78
1:A:347:GLY:HA2	1:A:354:CYS:HA	1.66	0.77
1:A:93:VAL:HG23	1:A:179:VAL:HG11	1.64	0.77
1:A:348:ILE:O	1:A:349:ASN:C	2.26	0.77
2:B:136:ARG:NH2	3:C:1:NAG:H3	1.99	0.76
1:A:335:PRO:HB2	1:A:336:PRO:HD2	1.67	0.76
1:A:424:TYR:O	1:A:442:VAL:HG22	1.84	0.76
1:A:120:TYR:HB2	1:A:125:TYR:HB2	1.68	0.76
2:B:109:ILE:HG13	2:B:123:TRP:CD1	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ALA:CB	1:A:446:ASP:HA	2.16	0.75
1:A:12:SER:O	1:A:38:GLY:N	2.19	0.74
1:A:442:VAL:O	1:A:442:VAL:CG2	2.32	0.74
1:A:348:ILE:CD1	1:A:349:ASN:N	2.50	0.73
1:A:370:MET:HE1	1:A:464:ALA:HB2	1.71	0.73
1:A:10:ARG:HA	1:A:375:ASN:ND2	2.04	0.73
2:B:68:MET:SD	2:B:82:LEU:HD23	2.29	0.72
1:A:70:ARG:NH2	1:A:342:ASN:HD21	1.85	0.72
1:A:63:VAL:HG21	1:A:107:GLY:HA2	1.71	0.72
1:A:123:VAL:CG2	1:A:125:TYR:CE2	2.67	0.72
1:A:402:PHE:HD1	1:A:465:ILE:HG12	1.55	0.72
1:A:366:GLN:HE21	1:A:366:GLN:N	1.88	0.71
1:A:348:ILE:HD12	1:A:349:ASN:H	1.55	0.71
2:B:86:LEU:HD23	2:B:177:VAL:HG12	1.71	0.71
1:A:151:VAL:HG12	1:A:151:VAL:O	1.89	0.71
1:A:377:VAL:O	1:A:380:THR:HG23	1.89	0.71
1:A:413:GLN:HB3	1:A:452:ILE:HD11	1.73	0.70
1:A:307:MET:HE3	1:A:461:GLY:HA3	1.72	0.70
1:A:124:PRO:HD2	1:A:162:TYR:OH	1.92	0.70
1:A:440:LYS:HE3	1:A:442:VAL:HG12	1.71	0.70
1:A:380:THR:OG1	1:A:397:ARG:HB3	1.91	0.70
1:A:33:GLN:HE21	1:A:87:ALA:HB1	1.56	0.70
1:A:338:ASP:O	1:A:340:SER:N	2.24	0.70
1:A:286:HIS:HA	1:A:323:MET:HE1	1.74	0.70
1:A:335:PRO:CB	1:A:336:PRO:HD2	2.21	0.69
1:A:11:ASN:HB2	1:A:375:ASN:OD1	1.93	0.69
1:A:370:MET:O	1:A:373:PHE:HB3	1.93	0.68
1:A:274:LEU:N	1:A:274:LEU:HD22	2.06	0.68
2:B:110:SER:HB3	2:B:120:SER:CB	2.24	0.68
1:A:137:ASN:HB2	1:A:144:ASN:ND2	2.09	0.68
1:A:192:PRO:HA	1:A:195:LEU:HB2	1.75	0.67
2:B:146:PHE:HB2	2:B:165:VAL:HG12	1.75	0.67
1:A:31:PHE:CD2	1:A:363:ARG:HD3	2.30	0.67
1:A:63:VAL:HG11	1:A:107:GLY:HA3	1.77	0.67
1:A:70:ARG:HH21	1:A:342:ASN:ND2	1.89	0.67
1:A:137:ASN:HB2	1:A:144:ASN:HD21	1.58	0.66
1:A:4:ALA:O	1:A:5:ASN:HB2	1.95	0.66
1:A:348:ILE:CG1	1:A:349:ASN:H	2.08	0.66
1:A:348:ILE:CD1	1:A:349:ASN:H	2.09	0.66
1:A:262:LYS:HD2	1:A:389:ASP:HA	1.78	0.66
1:A:423:THR:HG23	1:A:442:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:O	1:A:164:ARG:HG3	1.95	0.66
1:A:49:LEU:HD12	1:A:106:VAL:O	1.95	0.66
1:A:271:TRP:HB2	1:A:273:LEU:HD13	1.77	0.65
1:A:340:SER:O	1:A:340:SER:OG	2.09	0.65
1:A:362:HIS:CD2	1:A:363:ARG:HG2	2.32	0.65
1:A:96:VAL:HA	1:A:185:ASP:HB3	1.79	0.65
1:A:81:THR:O	1:A:85:ASN:HB2	1.97	0.65
1:A:336:PRO:HG2	1:A:358:TYR:CZ	2.33	0.64
2:B:136:ARG:HH21	3:C:1:NAG:H3	1.60	0.64
1:A:204:ASN:HD22	1:A:216:ARG:HH11	1.45	0.64
1:A:366:GLN:NE2	1:A:366:GLN:H	1.96	0.64
1:A:267:TRP:CD1	1:A:311:PHE:HE2	2.16	0.64
1:A:328:PHE:HB2	1:A:333:GLN:HE22	1.63	0.64
1:A:31:PHE:O	1:A:34:PRO:HD2	1.98	0.64
1:A:392:GLN:HG2	1:A:406:THR:HB	1.80	0.64
2:B:151:SER:HA	2:B:157:LYS:O	1.98	0.64
1:A:274:LEU:HD22	1:A:274:LEU:H	1.63	0.64
1:A:105:GLY:HA2	1:A:113:ALA:O	1.97	0.63
1:A:347:GLY:O	1:A:348:ILE:HD13	1.98	0.63
1:A:396:SER:HB2	1:A:401:GLY:O	1.99	0.63
1:A:272:GLY:C	1:A:273:LEU:HD12	2.23	0.63
1:A:138:ASN:OD1	1:A:140:GLN:HB2	1.98	0.63
1:A:348:ILE:HG23	1:A:349:ASN:N	2.14	0.63
2:B:52:ARG:CZ	2:B:170:GLU:HA	2.29	0.63
1:A:361:GLU:O	1:A:367:VAL:HG11	1.98	0.63
1:A:283:VAL:HG21	1:A:309:ILE:HG22	1.80	0.62
1:A:164:ARG:O	1:A:168:ILE:HG13	1.98	0.62
1:A:370:MET:HE1	1:A:464:ALA:CB	2.29	0.62
2:B:146:PHE:HD2	2:B:165:VAL:HG11	1.65	0.62
1:A:324:SER:OG	1:A:360:CYS:HA	1.98	0.62
1:A:452:ILE:HD13	1:A:452:ILE:N	2.15	0.62
1:A:48:TYR:OH	1:A:70:ARG:HG3	2.00	0.62
1:A:253:ASN:OD1	1:A:258:GLY:HA3	2.00	0.62
1:A:102:GLY:HA2	1:A:115:HIS:HD2	1.63	0.61
1:A:93:VAL:CG2	1:A:179:VAL:HG11	2.29	0.61
1:A:364:TRP:HB2	1:A:367:VAL:CG1	2.31	0.61
1:A:427:VAL:CA	1:A:430:GLY:O	2.47	0.61
1:A:93:VAL:HG21	1:A:174:MET:HE3	1.82	0.60
1:A:55:PRO:O	1:A:58:GLU:HG2	2.01	0.60
1:A:304:PRO:HA	1:A:307:MET:SD	2.42	0.60
2:B:146:PHE:CD2	2:B:165:VAL:HG11	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:CB	1:A:101:THR:HG22	2.19	0.60
1:A:163:VAL:O	1:A:167:LEU:HD22	2.01	0.60
1:A:335:PRO:CB	1:A:336:PRO:CD	2.80	0.60
1:A:220:TYR:CD2	1:A:243:LEU:HD21	2.36	0.60
1:A:386:TRP:CD2	1:A:415:LEU:HD21	2.37	0.60
2:B:196:LEU:HD23	2:B:196:LEU:N	2.16	0.60
1:A:397:ARG:HG3	1:A:397:ARG:HH11	1.67	0.60
1:A:322:ILE:HD12	1:A:322:ILE:N	2.17	0.60
2:B:150:LEU:O	2:B:158:SER:HA	2.01	0.60
1:A:31:PHE:CE1	1:A:352:ASN:ND2	2.70	0.59
1:A:93:VAL:HG21	1:A:174:MET:CE	2.33	0.59
1:A:402:PHE:CD1	1:A:465:ILE:HG12	2.37	0.59
2:B:62:PHE:CZ	2:B:86:LEU:HD11	2.37	0.59
1:A:13:ILE:HG12	1:A:321:ARG:HG3	1.83	0.59
1:A:405:PHE:HB3	1:A:461:GLY:O	2.01	0.59
1:A:49:LEU:HD12	1:A:50:VAL:H	1.68	0.58
1:A:313:LEU:HD23	1:A:370:MET:CB	2.28	0.58
1:A:461:GLY:O	1:A:462:VAL:HB	2.04	0.58
2:B:146:PHE:HB2	2:B:165:VAL:CG1	2.34	0.58
1:A:348:ILE:HD12	1:A:348:ILE:C	2.25	0.57
2:B:181:ALA:HB1	2:B:193:HIS:ND1	2.19	0.57
1:A:42:ILE:CD1	1:A:80:MET:HE1	2.32	0.57
1:A:262:LYS:HD2	1:A:389:ASP:CA	2.34	0.57
1:A:39:GLY:HA2	1:A:89:VAL:HG13	1.86	0.57
1:A:328:PHE:CB	1:A:333:GLN:HE22	2.17	0.57
1:A:131:HIS:CE1	1:A:157:ASN:HA	2.40	0.57
1:A:205:LEU:HD13	1:A:211:PHE:CD1	2.39	0.56
1:A:243:LEU:HD23	1:A:280:VAL:HB	1.87	0.56
1:A:399:SER:O	1:A:419:LEU:HG	2.05	0.56
1:A:426:ASP:O	1:A:430:GLY:C	2.47	0.56
2:B:86:LEU:CD2	2:B:177:VAL:HG12	2.34	0.56
1:A:427:VAL:HG22	1:A:464:ALA:HB3	1.87	0.56
2:B:96:ASP:N	2:B:114:ASN:ND2	2.53	0.56
1:A:465:ILE:O	1:A:465:ILE:HG13	2.06	0.56
1:A:130:PHE:CE2	1:A:154:ARG:HB3	2.41	0.55
1:A:302:PRO:O	1:A:305:TYR:HB3	2.06	0.55
1:A:348:ILE:CG1	1:A:349:ASN:N	2.69	0.55
1:A:31:PHE:C	1:A:34:PRO:HD2	2.31	0.55
1:A:123:VAL:HB	1:A:125:TYR:HD2	1.69	0.55
1:A:181:GLY:HA2	1:A:218:PHE:O	2.06	0.55
1:A:391:ASN:HB3	1:A:407:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:CD2	1:A:279:ALA:HB2	2.30	0.55
1:A:359:VAL:HB	1:A:361:GLU:OE1	2.07	0.55
1:A:7:ALA:HB3	1:A:10:ARG:HD2	1.88	0.54
1:A:391:ASN:O	1:A:406:THR:HA	2.07	0.54
1:A:166:VAL:HG23	1:A:167:LEU:N	2.23	0.54
1:A:272:GLY:O	1:A:273:LEU:HD12	2.07	0.54
1:A:338:ASP:O	1:A:339:GLY:C	2.51	0.54
2:B:148:VAL:HB	2:B:161:VAL:HG12	1.90	0.54
1:A:164:ARG:NH2	1:A:194:ASP:HB3	2.23	0.54
1:A:243:LEU:HB3	1:A:282:PHE:CE1	2.43	0.54
1:A:344:ILE:HG22	1:A:345:SER:N	2.23	0.54
1:A:123:VAL:HG21	1:A:125:TYR:HE2	1.63	0.54
2:B:109:ILE:HD11	2:B:150:LEU:HD12	1.90	0.54
2:B:126:HIS:O	2:B:126:HIS:CD2	2.60	0.54
1:A:385:TRP:CZ2	1:A:393:ILE:HD12	2.43	0.53
1:A:103:MET:H	1:A:115:HIS:CD2	2.27	0.53
2:B:151:SER:O	2:B:153:PRO:HD3	2.08	0.53
1:A:21:TRP:HZ2	1:A:45:PRO:HA	1.72	0.53
1:A:346:PRO:HG2	1:A:355:SER:OG	2.08	0.53
2:B:17:ILE:O	2:B:43:ALA:HA	2.08	0.53
2:B:50:GLN:HB2	2:B:174:TRP:CZ3	2.44	0.53
1:A:102:GLY:HA2	1:A:115:HIS:NE2	2.24	0.53
1:A:251:LEU:O	1:A:255:PHE:HD1	1.91	0.53
1:A:328:PHE:HB2	1:A:333:GLN:NE2	2.24	0.53
2:B:135:VAL:HA	2:B:149:SER:O	2.08	0.53
1:A:415:LEU:HD12	1:A:452:ILE:CD1	2.39	0.53
1:A:220:TYR:CE2	1:A:243:LEU:HD21	2.44	0.53
2:B:128:TYR:CE1	2:B:150:LEU:HD22	2.44	0.52
1:A:24:ILE:HG22	1:A:28:CYS:SG	2.50	0.52
1:A:336:PRO:CG	1:A:358:TYR:CZ	2.93	0.52
1:A:62:PRO:HD2	1:A:100:MET:O	2.09	0.52
1:A:243:LEU:HB3	1:A:282:PHE:HE1	1.75	0.52
1:A:12:SER:CB	1:A:320:THR:OG1	2.58	0.51
2:B:6:PHE:C	2:B:7:ILE:HD12	2.36	0.51
1:A:84:CYS:SG	1:A:91:ILE:HD11	2.51	0.51
1:A:15:HIS:HD2	1:A:323:MET:SD	2.34	0.51
1:A:254:ALA:HA	1:A:259:ASN:HB3	1.91	0.51
1:A:428:ILE:HG13	1:A:462:VAL:HG13	1.93	0.51
2:B:114:ASN:O	2:B:115:ASN:HB2	2.10	0.50
1:A:336:PRO:HG2	1:A:358:TYR:OH	2.11	0.50
1:A:429:SER:OG	1:A:430:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:ARG:HH21	3:C:1:NAG:C3	2.25	0.50
1:A:60:TYR:O	1:A:99:HIS:HE1	1.94	0.50
1:A:2:LYS:HB3	1:A:241:CYS:SG	2.52	0.50
1:A:107:GLY:HA3	1:A:111:SER:O	2.12	0.50
2:B:13:LYS:HD2	2:B:13:LYS:N	2.27	0.50
1:A:150:LEU:O	1:A:153:LEU:HB2	2.12	0.50
1:A:138:ASN:C	1:A:140:GLN:H	2.19	0.50
1:A:198:ILE:O	1:A:202:LEU:HD13	2.12	0.50
1:A:366:GLN:NE2	1:A:366:GLN:N	2.53	0.49
2:B:196:LEU:HD23	2:B:196:LEU:H	1.76	0.49
1:A:123:VAL:HB	1:A:124:PRO:C	2.37	0.49
1:A:364:TRP:CB	1:A:367:VAL:HG12	2.40	0.49
1:A:384:ASN:O	1:A:395:PHE:HA	2.12	0.49
1:A:67:ILE:HD11	1:A:173:HIS:HE1	1.76	0.49
1:A:123:VAL:HG12	1:A:124:PRO:O	2.11	0.49
2:B:128:TYR:CZ	2:B:150:LEU:HD13	2.47	0.49
1:A:419:LEU:HB3	1:A:420:PRO:HD2	1.94	0.49
1:A:98:ASN:HB2	1:A:190:MET:SD	2.52	0.49
2:B:112:ASP:HA	2:B:117:ASP:HA	1.93	0.49
2:B:139:TYR:CE1	2:B:165:VAL:HG13	2.48	0.49
1:A:373:PHE:HA	1:A:466:HIS:CE1	2.48	0.49
1:A:402:PHE:CD1	1:A:402:PHE:C	2.89	0.49
1:A:48:TYR:CE2	1:A:59:ARG:HD2	2.47	0.49
1:A:67:ILE:HD12	1:A:67:ILE:H	1.77	0.49
1:A:47:GLU:CD	1:A:109:SER:HB3	2.38	0.49
1:A:335:PRO:HB2	1:A:336:PRO:CD	2.39	0.49
1:A:203:LYS:NZ	1:A:203:LYS:HB3	2.28	0.48
1:A:388:ASN:OD1	1:A:392:GLN:HB2	2.13	0.48
1:A:397:ARG:HG3	1:A:397:ARG:NH1	2.26	0.48
1:A:423:THR:CG2	1:A:424:TYR:N	2.76	0.48
2:B:137:ILE:HD12	2:B:148:VAL:HG22	1.94	0.48
1:A:151:VAL:O	1:A:151:VAL:CG1	2.60	0.48
1:A:11:ASN:ND2	1:A:375:ASN:HA	2.29	0.48
1:A:273:LEU:HB3	1:A:317:TYR:OH	2.14	0.48
1:A:141:ASP:OD2	1:A:144:ASN:HB2	2.13	0.47
1:A:348:ILE:O	1:A:350:ASP:N	2.46	0.47
2:B:71:ARG:HB2	2:B:192:THR:OG1	2.13	0.47
1:A:20:LYS:HE3	1:A:342:ASN:O	2.13	0.47
1:A:419:LEU:CB	1:A:420:PRO:HD2	2.45	0.47
1:A:46:ASN:C	1:A:46:ASN:ND2	2.71	0.47
1:A:338:ASP:O	1:A:338:ASP:CG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CH2	1:A:42:ILE:HD11	2.50	0.47
1:A:313:LEU:HB3	1:A:370:MET:HG3	1.94	0.47
1:A:454:LEU:HD11	1:A:460:ASP:O	2.13	0.47
1:A:58:GLU:HG3	1:A:59:ARG:N	2.28	0.47
1:A:286:HIS:CA	1:A:323:MET:HE1	2.45	0.47
1:A:137:ASN:CB	1:A:144:ASN:HD21	2.26	0.47
1:A:424:TYR:N	1:A:424:TYR:CD1	2.83	0.47
1:A:18:GLU:HG3	1:A:335:PRO:HG3	1.97	0.47
1:A:415:LEU:HB2	1:A:452:ILE:HD12	1.97	0.47
1:A:92:TYR:HD1	1:A:181:GLY:HA3	1.80	0.47
1:A:21:TRP:CZ3	1:A:42:ILE:HD11	2.49	0.47
1:A:346:PRO:HD2	1:A:356:ASN:ND2	2.22	0.47
1:A:18:GLU:CG	1:A:335:PRO:HG3	2.45	0.46
1:A:103:MET:O	1:A:115:HIS:HB2	2.15	0.46
1:A:166:VAL:HG23	1:A:167:LEU:H	1.79	0.46
2:B:7:ILE:HD12	2:B:7:ILE:N	2.30	0.46
1:A:21:TRP:CE3	1:A:71:SER:HB3	2.50	0.46
2:B:2:THR:HG22	2:B:4:THR:HG22	1.97	0.46
1:A:307:MET:HG2	1:A:461:GLY:O	2.15	0.46
1:A:351:ASP:CG	1:A:353:THR:HG23	2.40	0.46
2:B:52:ARG:HB3	2:B:173:ASP:HA	1.97	0.46
1:A:22:ASN:HD22	1:A:23:ASP:N	2.12	0.46
1:A:49:LEU:HD12	1:A:50:VAL:N	2.31	0.46
1:A:415:LEU:O	1:A:450:ALA:N	2.49	0.46
2:B:177:VAL:HG11	2:B:200:PHE:CZ	2.51	0.46
1:A:125:TYR:OH	1:A:166:VAL:HG21	2.16	0.46
2:B:59:VAL:HG23	2:B:141:SER:HB3	1.97	0.46
1:A:151:VAL:O	1:A:153:LEU:N	2.48	0.46
1:A:188:LYS:HG3	1:A:231:ILE:HG21	1.98	0.46
1:A:417:THR:O	1:A:419:LEU:HD13	2.16	0.46
2:B:64:THR:CG2	2:B:137:ILE:HB	2.45	0.46
1:A:33:GLN:HE21	1:A:87:ALA:CB	2.24	0.46
1:A:236:TYR:CD1	1:A:236:TYR:N	2.84	0.46
1:A:285:ASN:O	1:A:286:HIS:C	2.58	0.46
1:A:130:PHE:CD2	1:A:154:ARG:HB3	2.51	0.45
1:A:277:LEU:HD13	1:A:277:LEU:H	1.81	0.45
2:B:71:ARG:O	2:B:191:GLU:HG3	2.16	0.45
1:A:328:PHE:HA	1:A:333:GLN:HE22	1.82	0.45
1:A:180:ALA:HB2	1:A:211:PHE:CZ	2.51	0.45
1:A:43:SER:OG	1:A:44:PRO:HD2	2.17	0.45
1:A:123:VAL:HB	1:A:125:TYR:CD2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:CD1	1:A:6:PHE:N	2.83	0.45
1:A:80:MET:O	1:A:84:CYS:HB2	2.17	0.45
1:A:92:TYR:CD1	1:A:181:GLY:HA3	2.52	0.45
1:A:404:ALA:O	1:A:462:VAL:HA	2.16	0.45
2:B:32:LEU:HD12	2:B:32:LEU:N	2.32	0.45
1:A:1:PCA:HB3	1:A:216:ARG:HB2	1.97	0.45
1:A:12:SER:HB2	1:A:320:THR:OG1	2.16	0.45
1:A:80:MET:HB3	1:A:80:MET:HE2	1.81	0.45
1:A:286:HIS:HA	1:A:323:MET:CE	2.45	0.45
1:A:177:LEU:O	1:A:209:TYR:CZ	2.70	0.45
1:A:31:PHE:CG	1:A:363:ARG:HD3	2.52	0.45
1:A:48:TYR:CZ	1:A:59:ARG:HD2	2.52	0.45
1:A:321:ARG:NH2	4:A:498:CL:CL	2.86	0.45
2:B:109:ILE:HG13	2:B:123:TRP:CG	2.52	0.45
1:A:205:LEU:HD12	1:A:215:ALA:HB3	1.99	0.45
2:B:32:LEU:HB3	2:B:41:SER:OG	2.16	0.45
1:A:13:ILE:O	1:A:321:ARG:HA	2.18	0.44
1:A:303:LYS:HE3	1:A:460:ASP:HA	1.99	0.44
1:A:366:GLN:H	1:A:366:GLN:CD	2.25	0.44
1:A:184:VAL:HG21	1:A:199:PHE:CZ	2.53	0.44
1:A:274:LEU:N	1:A:274:LEU:CD2	2.78	0.44
2:B:132:ASN:O	2:B:153:PRO:HD2	2.17	0.44
1:A:187:ALA:HA	1:A:190:MET:HE2	1.99	0.44
1:A:256:GLN:OE1	1:A:297:LEU:HD21	2.18	0.44
1:A:328:PHE:CA	1:A:333:GLN:HE22	2.29	0.44
1:A:61:GLN:HA	1:A:100:MET:O	2.17	0.44
1:A:174:MET:O	1:A:179:VAL:HG22	2.18	0.44
1:A:68:ASN:HA	1:A:73:ASN:HA	1.99	0.44
1:A:285:ASN:OD1	1:A:285:ASN:C	2.61	0.44
1:A:386:TRP:CE2	1:A:415:LEU:HD21	2.52	0.44
1:A:403:VAL:HA	1:A:463:LEU:O	2.18	0.44
1:A:415:LEU:HD12	1:A:452:ILE:HD11	2.00	0.44
1:A:47:GLU:CG	1:A:108:THR:HG22	2.40	0.43
2:B:172:TYR:O	2:B:173:ASP:C	2.60	0.43
1:A:102:GLY:CA	1:A:115:HIS:HD2	2.30	0.43
1:A:206:ASN:ND2	1:A:209:TYR:CE1	2.87	0.43
1:A:224:ILE:HG21	2:B:39:SER:HB3	1.99	0.43
1:A:151:VAL:HG11	2:B:188:TRP:CD1	2.53	0.43
1:A:187:ALA:HB3	1:A:223:VAL:CG2	2.48	0.43
1:A:220:TYR:CB	1:A:280:VAL:HG21	2.49	0.43
1:A:368:TYR:CD1	1:A:369:GLY:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LEU:HD23	1:A:471:LEU:H	1.84	0.43
1:A:144:ASN:O	1:A:148:CYS:HB2	2.18	0.43
1:A:323:MET:O	1:A:361:GLU:HB2	2.19	0.43
2:B:34:TYR:CE1	2:B:192:THR:HB	2.54	0.43
2:B:45:TYR:CE2	2:B:47:ALA:HB3	2.54	0.43
1:A:20:LYS:HE3	1:A:342:ASN:HB2	2.00	0.42
1:A:423:THR:HG22	1:A:424:TYR:N	2.33	0.42
1:A:206:ASN:ND2	1:A:209:TYR:HE1	2.17	0.42
1:A:206:ASN:HD22	1:A:209:TYR:HE1	1.67	0.42
1:A:315:HIS:O	1:A:374:ARG:NH1	2.50	0.42
1:A:405:PHE:CD1	1:A:405:PHE:N	2.87	0.42
1:A:224:ILE:HA	1:A:245:PHE:CD2	2.54	0.42
1:A:305:TYR:O	1:A:308:ALA:HB3	2.19	0.42
2:B:80:VAL:HG22	2:B:184:GLY:HA3	2.01	0.42
1:A:118:MET:O	1:A:126:GLY:HA2	2.20	0.42
1:A:324:SER:HB2	1:A:362:HIS:ND1	2.33	0.42
1:A:333:GLN:HE21	1:A:333:GLN:HB3	1.39	0.42
1:A:113:ALA:HB1	1:A:120:TYR:CE1	2.54	0.42
1:A:146:ARG:HD3	1:A:191:SER:HA	2.01	0.42
1:A:271:TRP:CB	1:A:273:LEU:HD13	2.47	0.42
1:A:398:GLY:C	1:A:400:GLN:H	2.27	0.42
1:A:416:ASN:CG	1:A:417:THR:N	2.77	0.42
1:A:326:PHE:CD1	1:A:326:PHE:C	2.98	0.42
1:A:367:VAL:HG13	1:A:368:TYR:H	1.84	0.42
1:A:24:ILE:HD12	1:A:80:MET:SD	2.58	0.42
1:A:54:ARG:CZ	1:A:70:ARG:HD3	2.49	0.42
1:A:373:PHE:CD2	1:A:464:ALA:HB1	2.55	0.42
1:A:141:ASP:HB2	2:B:115:ASN:HD21	1.83	0.42
1:A:171:MET:O	1:A:174:MET:HB2	2.20	0.42
1:A:388:ASN:HD21	1:A:390:ASP:HB3	1.85	0.42
2:B:114:ASN:N	2:B:114:ASN:HD22	2.17	0.42
1:A:334:GLY:C	1:A:335:PRO:O	2.63	0.42
1:A:348:ILE:CG2	1:A:349:ASN:N	2.77	0.42
1:A:406:THR:HG22	1:A:454:LEU:HD23	2.01	0.42
2:B:82:LEU:O	2:B:102:PHE:HB2	2.20	0.42
1:A:220:TYR:HA	1:A:241:CYS:O	2.20	0.42
1:A:220:TYR:HD2	1:A:243:LEU:HD21	1.82	0.42
1:A:174:MET:C	1:A:179:VAL:HG22	2.45	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.91	0.41
2:B:52:ARG:NE	2:B:170:GLU:HA	2.34	0.41
1:A:90:ARG:HB3	1:A:92:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PHE:HA	1:A:466:HIS:ND1	2.35	0.41
1:A:31:PHE:HZ	1:A:368:TYR:CD2	2.39	0.41
1:A:84:CYS:SG	1:A:89:VAL:HB	2.61	0.41
2:B:103:ASP:OD2	2:B:106:LEU:HG	2.21	0.41
1:A:151:VAL:HA	2:B:105:PHE:CE2	2.55	0.41
1:A:157:ASN:C	1:A:159:GLY:H	2.28	0.41
1:A:186:ALA:H	1:A:222:GLU:HB3	1.85	0.41
1:A:338:ASP:C	1:A:340:SER:N	2.76	0.41
2:B:128:TYR:CE2	2:B:150:LEU:HD13	2.54	0.41
1:A:56:TRP:CG	1:A:57:TRP:N	2.88	0.41
1:A:175:ILE:HD11	1:A:202:LEU:HG	2.03	0.41
1:A:260:GLN:HB2	1:A:263:ASN:OD1	2.20	0.41
1:A:52:ASP:C	1:A:54:ARG:H	2.28	0.41
1:A:59:ARG:NH1	1:A:70:ARG:HB2	2.35	0.41
1:A:118:MET:HE3	1:A:127:SER:OG	2.21	0.41
1:A:138:ASN:C	1:A:140:GLN:N	2.78	0.41
1:A:166:VAL:HG23	1:A:167:LEU:HD13	2.02	0.41
1:A:311:PHE:O	1:A:315:HIS:HB2	2.21	0.41
1:A:392:GLN:HG2	1:A:406:THR:CB	2.49	0.41
1:A:392:GLN:HA	1:A:405:PHE:O	2.21	0.41
1:A:402:PHE:CG	1:A:403:VAL:N	2.88	0.41
1:A:423:THR:C	1:A:424:TYR:CD1	2.99	0.41
2:B:177:VAL:O	2:B:177:VAL:HG23	2.20	0.41
1:A:120:TYR:O	1:A:125:TYR:N	2.55	0.41
1:A:202:LEU:O	1:A:216:ARG:NH1	2.54	0.41
1:A:275:GLU:O	1:A:278:ASP:HB2	2.20	0.41
1:A:33:GLN:HB2	1:A:87:ALA:O	2.21	0.40
1:A:41:GLN:HA	1:A:92:TYR:HB2	2.02	0.40
1:A:42:ILE:O	1:A:42:ILE:HG23	2.21	0.40
1:A:59:ARG:HH12	1:A:70:ARG:HB2	1.87	0.40
1:A:377:VAL:HG21	1:A:397:ARG:NH1	2.37	0.40
2:B:40:MET:HE3	2:B:42:ARG:HD3	2.02	0.40
1:A:264:LEU:O	1:A:267:TRP:HB2	2.21	0.40
1:A:364:TRP:O	1:A:365:ARG:C	2.65	0.40
1:A:77:PHE:O	1:A:81:THR:HG23	2.21	0.40
1:A:452:ILE:N	1:A:452:ILE:CD1	2.83	0.40
2:B:126:HIS:O	2:B:126:HIS:CG	2.74	0.40
2:B:191:GLU:HG2	2:B:193:HIS:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/471 (100%)	361 (77%)	83 (18%)	25 (5%)	1	9
2	B	192/205 (94%)	166 (86%)	21 (11%)	5 (3%)	4	23
All	All	661/676 (98%)	527 (80%)	104 (16%)	30 (4%)	2	12

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	MET
1	A	105	GLY
1	A	340	SER
1	A	446	ASP
2	B	172	TYR
2	B	173	ASP
1	A	8	SER
1	A	152	GLY
1	A	213	ASP
1	A	339	GLY
1	A	350	ASP
1	A	462	VAL
1	A	12	SER
1	A	67	ILE
1	A	312	MET
1	A	390	ASP
2	B	34	TYR
1	A	318	GLY
1	A	5	ASN
1	A	44	PRO
1	A	208	ASP
1	A	277	LEU
1	A	302	PRO
1	A	447	ASN
2	B	58	ASN

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Mol	Chain	Res	Type
2	B	66	PHE
1	A	335	PRO
1	A	445	GLY
1	A	283	VAL
1	A	439	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/380 (100%)	338 (89%)	42 (11%)	6	25
2	B	180/185 (97%)	161 (89%)	19 (11%)	6	27
All	All	560/565 (99%)	499 (89%)	61 (11%)	6	26

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	13	ILE
1	A	14	VAL
1	A	21	TRP
1	A	22	ASN
1	A	33	GLN
1	A	45	PRO
1	A	46	ASN
1	A	67	ILE
1	A	69	THR
1	A	79	ASP
1	A	106	VAL
1	A	108	THR
1	A	138	ASN
1	A	143	ASP
1	A	153	LEU
1	A	167	LEU
1	A	236	TYR

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Mol	Chain	Res	Type
1	A	261	LEU
1	A	274	LEU
1	A	277	LEU
1	A	285	ASN
1	A	288	ASN
1	A	322	ILE
1	A	323	MET
1	A	327	ASP
1	A	333	GLN
1	A	348	ILE
1	A	356	ASN
1	A	363	ARG
1	A	365	ARG
1	A	366	GLN
1	A	382	VAL
1	A	402	PHE
1	A	403	VAL
1	A	405	PHE
1	A	414	ASN
1	A	416	ASN
1	A	427	VAL
1	A	452	ILE
1	A	460	ASP
1	A	463	LEU
2	B	4	THR
2	B	13	LYS
2	B	16	LEU
2	B	33	SER
2	B	46	SER
2	B	55	THR
2	B	61	SER
2	B	68	MET
2	B	98	VAL
2	B	110	SER
2	B	114	ASN
2	B	119	LYS
2	B	125	VAL
2	B	150	LEU
2	B	157	LYS
2	B	172	TYR
2	B	190	TYR
2	B	196	LEU

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Mol	Chain	Res	Type
2	B	205	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	22	ASN
1	A	33	GLN
1	A	46	ASN
1	A	99	HIS
1	A	115	HIS
1	A	137	ASN
1	A	140	GLN
1	A	173	HIS
1	A	204	ASN
1	A	259	ASN
1	A	260	GLN
1	A	286	HIS
1	A	331	ASN
1	A	333	GLN
1	A	342	ASN
1	A	356	ASN
1	A	366	GLN
1	A	384	ASN
1	A	392	GLN
1	A	416	ASN
2	B	27	ASN
2	B	31	GLN
2	B	114	ASN
2	B	115	ASN
2	B	126	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	PCA	A	1	1	7,8,9	1.37	1 (14%)	9,10,12	8.47	7 (77%)

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
1	PCA	A	1	1	1/1/2/4	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	3.19	1.59	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	20.44	140.69	112.66
1	A	1	PCA	OE-CD-N	9.96	146.52	124.96
1	A	1	PCA	CG-CD-N	-6.31	92.93	108.39
1	A	1	PCA	CB-CG-CD	-6.26	94.73	104.41
1	A	1	PCA	CB-CA-N	-4.90	89.75	103.24
1	A	1	PCA	OE-CD-CG	-3.50	120.48	126.72
1	A	1	PCA	CG-CB-CA	-2.68	93.88	104.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	PCA	CA

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	C	1	3,2	14,14,15	0.77	1 (7%)	17,19,21	1.22	1 (5%)
3	NAG	C	2	3	14,14,15	0.52	0	17,19,21	1.19	1 (5%)
3	NAG	D	1	3,2	14,14,15	0.92	1 (7%)	17,19,21	1.51	2 (11%)
3	NAG	D	2	3	14,14,15	1.15	1 (7%)	17,19,21	1.12	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
3	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	3.55	1.57	1.52
3	D	1	NAG	C1-C2	2.19	1.55	1.52
3	C	1	NAG	C1-C2	2.15	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	1	NAG	C1-O5-C5	-5.08	105.38	112.19
3	C	1	NAG	C1-O5-C5	-4.07	106.73	112.19
3	C	2	NAG	C1-O5-C5	-3.97	106.87	112.19
3	D	2	NAG	C1-O5-C5	-3.70	107.23	112.19
3	D	1	NAG	C2-N2-C7	-2.33	119.78	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

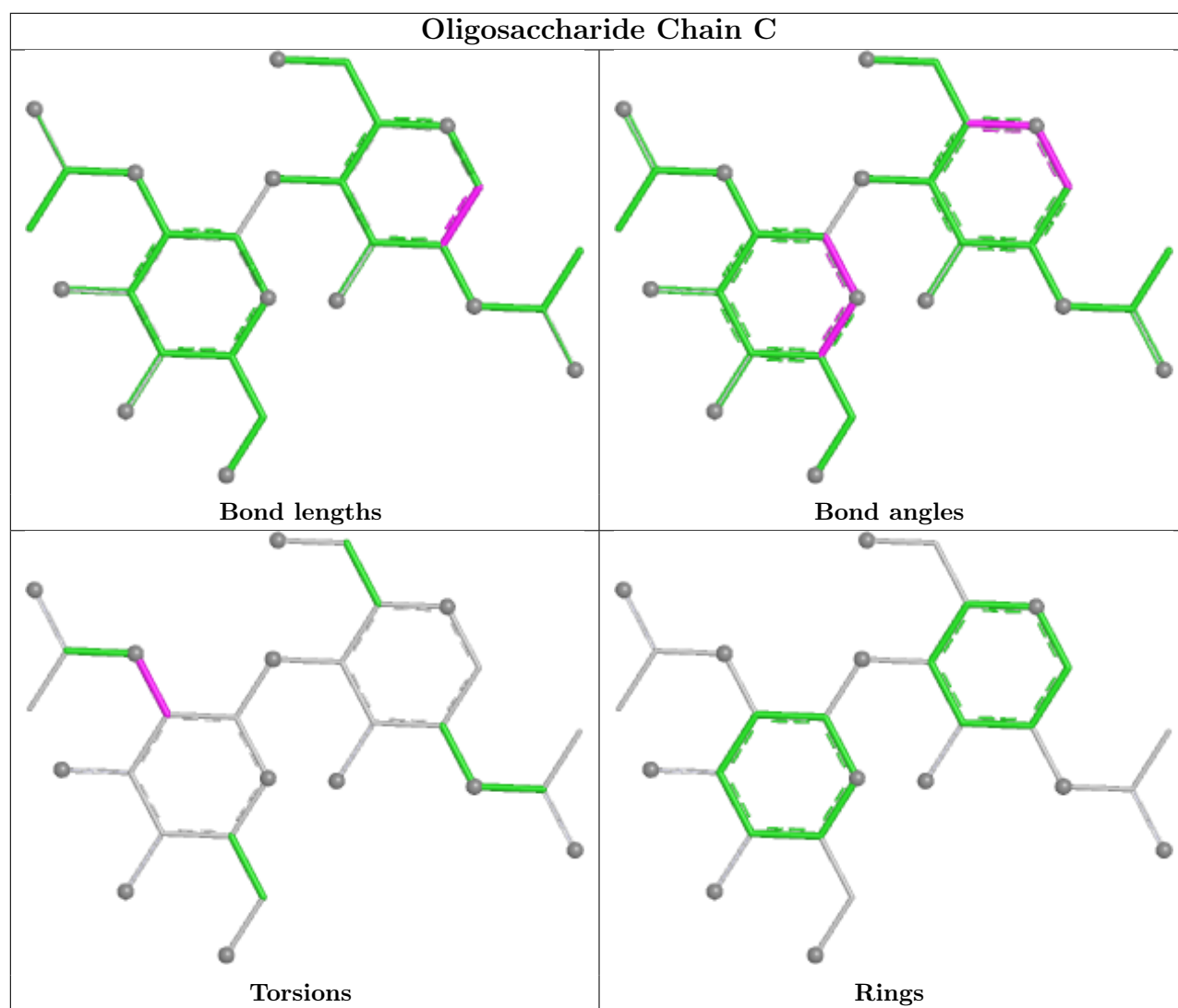
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7

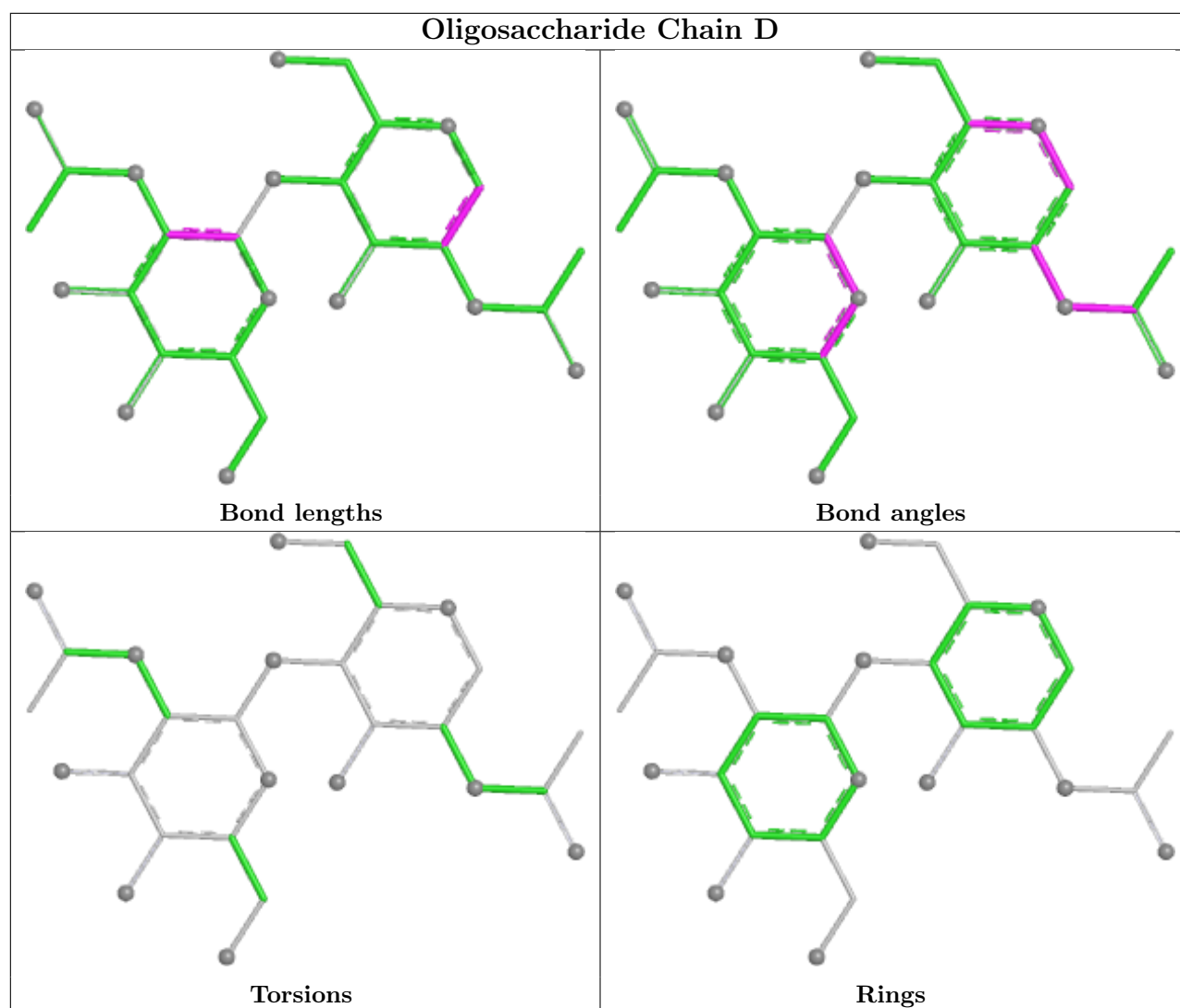
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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 [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	349:ASN	C	350:ASP	N	1.14

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.