



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 02:16 AM EDT

PDB ID : 1U8C
Title : A novel adaptation of the integrin PSI domain revealed from its crystal structure
Authors : Xiong, J.P.; Stehle, T.; Goodman, S.L.; Arnaout, M.A.
Deposited on : 2004-08-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

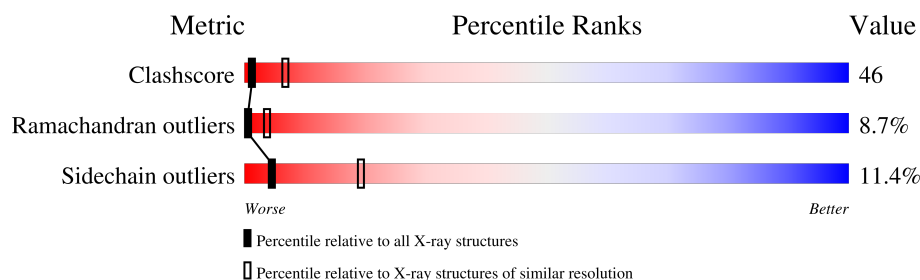
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	
2	B	692	
3	C	2	
3	D	2	
3	E	2	
3	G	2	
4	F	2	
4	H	2	

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Mol	Chain	Length	Quality of chain
4	I	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	-	-	X	-
3	NAG	C	2	-	-	X	-
3	NAG	E	1	X	-	-	-
5	NAG	A	2821	X	-	-	-
5	NAG	B	3320	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12115 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	753	VAL	ILE	SEE REMARK 999	UNP P06756

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	599	Total	C	N	O	S	0	0	0
			4627	2864	777	930	56			

- 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			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

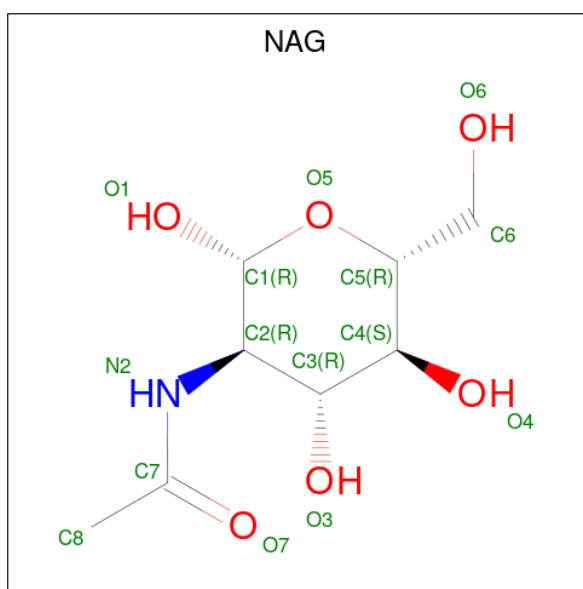
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

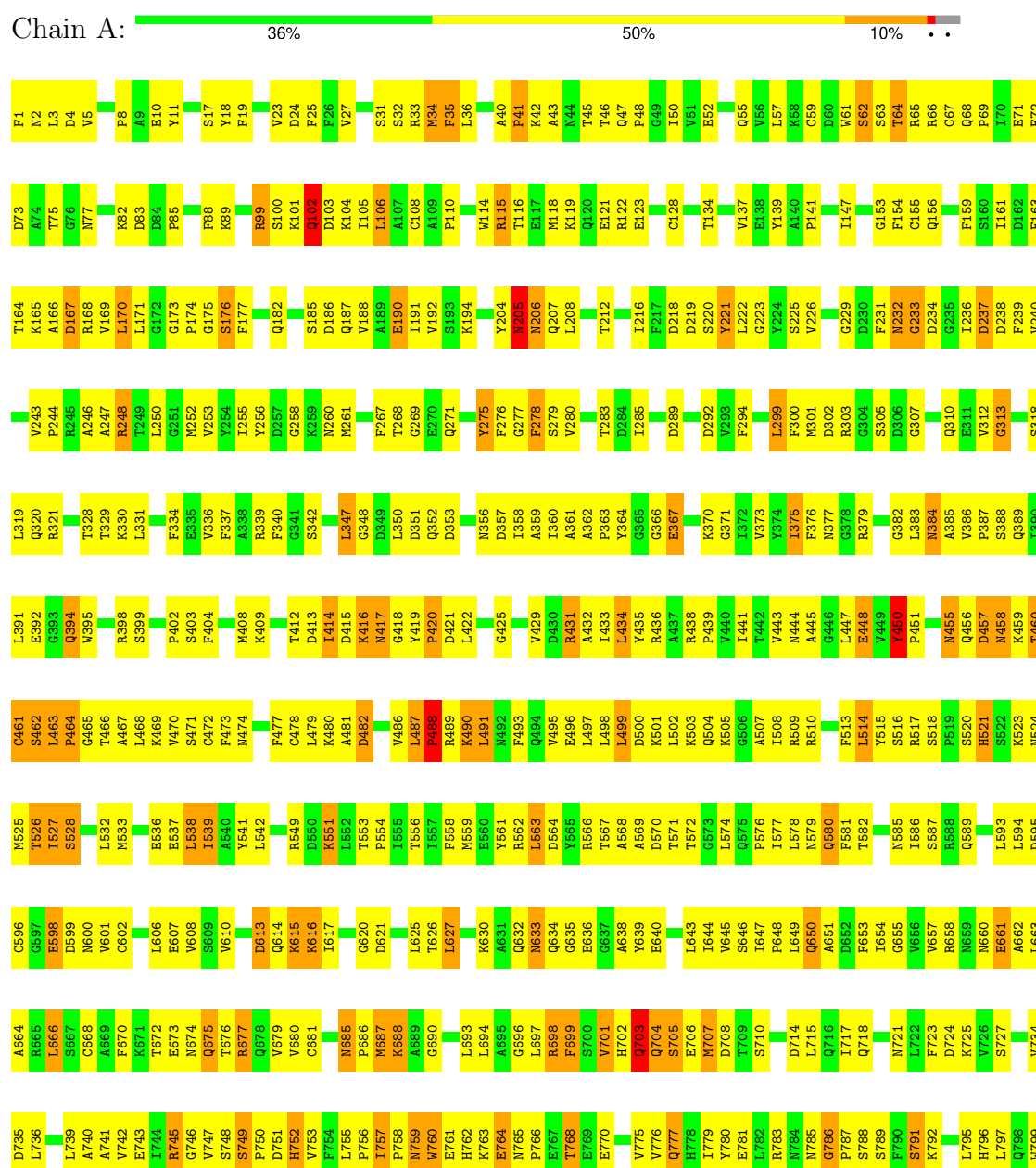
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total 5	Ca 5	0	0
6	B	1	Total 1	Ca 1	0	0

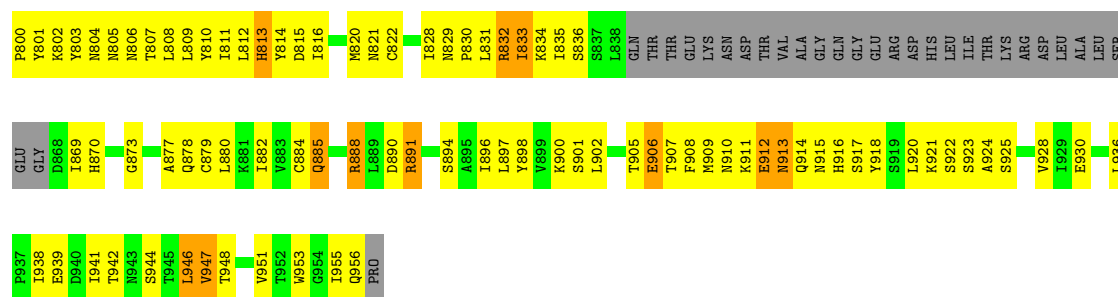
3 Residue-property plots

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. 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.

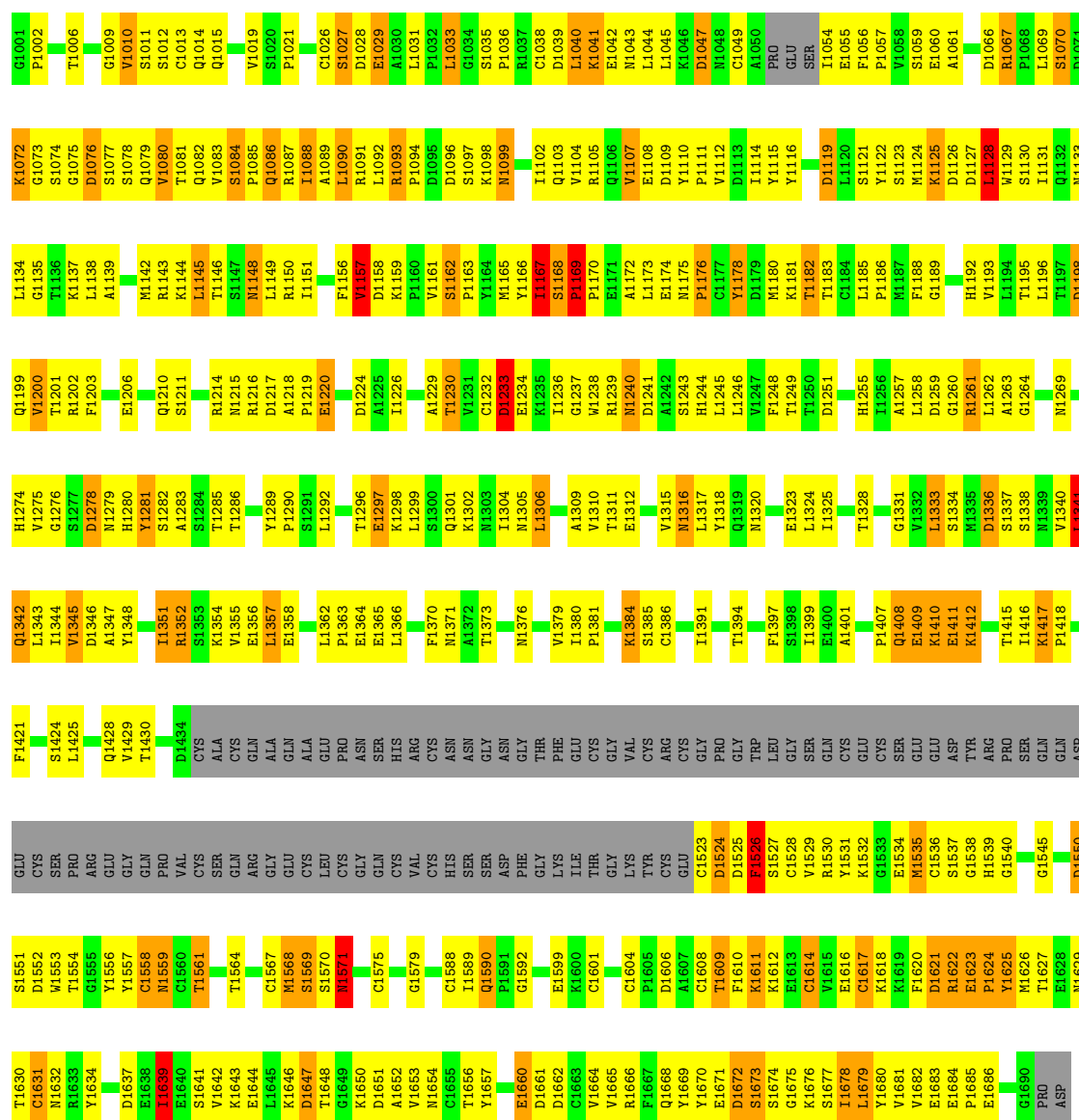
Note EDS was not executed.

• Molecule 1: Integrin alpha-V





• Molecule 2: Integrin beta-3




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

Chain C:  100%


NAG1
NAG2

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

Chain D:  100%

NAG1
NAG2

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

Chain E:  50% 50%


NAG1
NAG2

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

Chain G:  50% 50%

NAG1
NAG2

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

Chain F:  100%

NAG1
NDG2

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

Chain H:  100%

NAG1
NDG2

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

Chain I:  100%

NAG1
NDG2

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.00Å 130.00Å 307.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.293 , 0.367	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12115	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/7372	0.71	0/9994
2	B	0.43	0/4708	0.71	1/6367 (0.0%)
All	All	0.45	0/12080	0.71	1/16361 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1169	PRO	C-N-CD	6.01	141.02	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7216	0	7033	637	0
2	B	4627	0	4449	450	0
3	C	28	0	25	8	0
3	D	28	0	25	0	0
3	E	28	0	25	2	0
3	G	28	0	25	2	0
4	F	28	0	24	0	0
4	H	28	0	24	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	24	5	0
5	A	42	0	39	9	0
5	B	28	0	26	3	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	12115	0	11719	1100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

All (1100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:LYS:HE2	2:B:1075:GLY:HA3	1.30	1.14
1:A:487:LEU:HD23	1:A:488:PRO:HD3	1.24	1.11
2:B:1041:LYS:HD2	2:B:1045:LEU:CD1	1.80	1.11
2:B:1040:LEU:O	2:B:1042:GLU:N	1.86	1.09
2:B:1611:LYS:HG3	2:B:1669:TYR:HE2	1.17	1.08
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.33	1.07
2:B:1041:LYS:HD3	2:B:1044:LEU:HD22	1.35	1.04
1:A:828:ILE:HD12	1:A:829:ASN:H	1.21	1.03
2:B:1341:LEU:HD12	2:B:1342:GLN:H	1.23	1.02
1:A:617:ILE:HD11	1:A:625:LEU:HD22	1.43	0.99
2:B:1040:LEU:HD13	2:B:1043:ASN:HD22	1.24	0.98
1:A:438:ARG:HH12	1:A:577:ILE:HB	1.27	0.97
2:B:1611:LYS:HG3	2:B:1669:TYR:CE2	1.99	0.97
2:B:1218:ALA:HB3	2:B:1219:PRO:HD3	1.45	0.96
1:A:463:LEU:HB3	1:A:464:PRO:HD2	1.44	0.95
1:A:921:LYS:HD2	1:A:946:LEU:HD12	1.49	0.94
2:B:1345:VAL:HG23	2:B:1346:ASP:H	1.34	0.93
2:B:1391:ILE:H	2:B:1391:ILE:HD12	1.29	0.93
2:B:1041:LYS:O	2:B:1045:LEU:HB2	1.67	0.93
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.50	0.92
2:B:1157:VAL:HG23	2:B:1189:GLY:H	1.34	0.92
1:A:664:ALA:HB2	1:A:693:LEU:HD11	1.51	0.92
1:A:783:ARG:HB2	1:A:894:SER:HB3	1.51	0.92
2:B:1110:TYR:CD1	2:B:1111:PRO:HD2	2.04	0.92
1:A:416:LYS:H	1:A:416:LYS:HD2	1.33	0.91
2:B:1333:LEU:HG	2:B:1334:SER:H	1.33	0.91
1:A:580:GLN:HG3	1:A:581:PHE:H	1.34	0.91
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1067:ARG:HH21	2:B:1081:THR:HG22	1.35	0.91
1:A:455:ASN:C	1:A:455:ASN:HD22	1.75	0.91
1:A:789:SER:HB3	1:A:890:ASP:HA	1.52	0.90
2:B:1408:GLN:HE21	2:B:1408:GLN:HA	1.33	0.90
1:A:749:SER:HB3	1:A:750:PRO:HD3	1.51	0.90
1:A:640:GLU:H	1:A:685:ASN:HD22	1.19	0.90
1:A:617:ILE:HD13	1:A:701:VAL:HG11	1.54	0.90
1:A:650:GLN:HE21	1:A:650:GLN:N	1.68	0.90
1:A:464:PRO:HG2	1:A:465:GLY:H	1.37	0.90
1:A:741:ALA:H	1:A:786:GLY:HA3	1.37	0.89
2:B:1041:LYS:HD2	2:B:1045:LEU:HD13	1.51	0.88
2:B:1040:LEU:HD12	2:B:1040:LEU:H	1.36	0.88
2:B:1088:ILE:HG22	2:B:1425:LEU:HD11	1.53	0.88
1:A:438:ARG:NH1	1:A:577:ILE:HB	1.88	0.88
2:B:1199:GLN:HE21	2:B:1199:GLN:HA	1.34	0.88
1:A:563:LEU:HD23	1:A:564:ASP:H	1.38	0.87
2:B:1087:ARG:NH2	2:B:1428:GLN:HE22	1.71	0.86
1:A:463:LEU:HB3	1:A:464:PRO:CD	2.05	0.86
2:B:1646:LYS:NZ	2:B:1646:LYS:HB3	1.89	0.86
1:A:909:MET:O	1:A:915:ASN:HB3	1.76	0.86
2:B:1041:LYS:HD2	2:B:1045:LEU:HD12	1.53	0.86
1:A:2:ASN:HA	1:A:389:GLN:OE1	1.76	0.86
1:A:384:ASN:HD22	1:A:385:ALA:N	1.73	0.85
2:B:1087:ARG:HH22	2:B:1428:GLN:HE22	1.22	0.85
2:B:1093:ARG:HB2	2:B:1094:PRO:HD2	1.58	0.85
1:A:688:LYS:HA	1:A:688:LYS:NZ	1.91	0.85
2:B:1185:LEU:HD12	2:B:1186:PRO:HD2	1.56	0.84
1:A:828:ILE:HD12	1:A:829:ASN:N	1.92	0.84
1:A:101:LYS:HB3	1:A:104:LYS:HE2	1.60	0.83
1:A:458:ASN:ND2	5:A:2458:NAG:H61	1.91	0.83
2:B:1128:LEU:HD11	2:B:1210:GLN:HB3	1.59	0.83
2:B:1157:VAL:CG2	2:B:1189:GLY:H	1.92	0.83
2:B:1642:VAL:HG11	2:B:1680:TYR:HB3	1.61	0.82
1:A:495:VAL:HG12	1:A:496:GLU:H	1.43	0.82
2:B:1244:HIS:O	2:B:1245:LEU:HD23	1.80	0.82
1:A:630:LYS:HE3	1:A:694:LEU:HD21	1.62	0.81
1:A:451:PRO:HD2	1:A:473:PHE:HB2	1.59	0.81
2:B:1061:ALA:HB1	2:B:1088:ILE:HD11	1.62	0.81
2:B:1646:LYS:HB3	2:B:1646:LYS:HZ2	1.45	0.81
2:B:1087:ARG:NH2	2:B:1428:GLN:NE2	2.27	0.81
2:B:1084:SER:HB3	2:B:1085:PRO:HD3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HG	1:A:59:CYS:HB2	1.64	0.80
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.12	0.80
2:B:1110:TYR:HD1	2:B:1111:PRO:HD2	1.40	0.80
3:C:1:NAG:H61	3:C:2:NAG:C7	2.12	0.80
1:A:27:VAL:HG22	1:A:34:MET:HG2	1.63	0.79
2:B:1169:PRO:CG	2:B:1173:LEU:HD23	2.12	0.79
1:A:384:ASN:HD21	1:A:386:VAL:HG23	1.48	0.79
1:A:436:ARG:HH12	1:A:571:THR:HB	1.48	0.79
2:B:1356:GLU:HG2	2:B:1385:SER:HB2	1.63	0.79
1:A:487:LEU:CD2	1:A:488:PRO:HD3	2.10	0.79
1:A:801:TYR:HB3	1:A:878:GLN:O	1.83	0.78
2:B:1169:PRO:HB2	2:B:1170:PRO:HD3	1.65	0.78
2:B:1646:LYS:HZ3	2:B:1647:ASP:H	1.28	0.78
1:A:459:LYS:HB2	1:A:470:VAL:C	2.04	0.78
3:C:1:NAG:H61	3:C:2:NAG:C2	2.13	0.78
2:B:1125:LYS:HD2	2:B:1126:ASP:N	1.98	0.78
4:H:1:NAG:H3	4:H:2:NDG:N2	1.99	0.78
5:A:2458:NAG:O7	5:A:2458:NAG:H3	1.84	0.78
1:A:487:LEU:H	1:A:488:PRO:HD2	1.49	0.77
2:B:1648:THR:HA	4:I:1:NAG:H62	1.66	0.77
1:A:523:LYS:HG2	1:A:524:ASN:H	1.48	0.77
1:A:450:TYR:CB	1:A:451:PRO:HD3	2.14	0.77
2:B:1622:ARG:HH11	2:B:1660:GLU:HB3	1.48	0.77
2:B:1041:LYS:HD3	2:B:1044:LEU:CD2	2.13	0.77
1:A:688:LYS:HA	1:A:688:LYS:HZ3	1.47	0.76
1:A:946:LEU:H	1:A:946:LEU:HD23	1.48	0.76
2:B:1622:ARG:NH1	2:B:1660:GLU:HB3	2.00	0.76
1:A:510:ARG:O	1:A:542:LEU:HD12	1.86	0.76
5:A:2260:NAG:O7	5:A:2260:NAG:H3	1.85	0.76
2:B:1167:ILE:N	2:B:1167:ILE:HD12	2.00	0.76
1:A:499:LEU:N	1:A:499:LEU:HD22	2.01	0.76
1:A:436:ARG:NH2	1:A:574:LEU:HD13	2.01	0.76
1:A:414:ILE:HG21	1:A:434:LEU:HD11	1.68	0.76
2:B:1623:GLU:CD	2:B:1624:PRO:HD2	2.06	0.75
1:A:760:TRP:CZ2	1:A:905:THR:HB	2.21	0.75
1:A:672:THR:OG1	1:A:677:ARG:HA	1.86	0.75
2:B:1646:LYS:HE2	2:B:1668:GLN:OE1	1.87	0.75
1:A:835:ILE:HG12	1:A:836:SER:H	1.52	0.75
2:B:1673:SER:HB2	2:B:1676:LYS:HG2	1.68	0.75
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.69	0.75
1:A:749:SER:CB	1:A:750:PRO:HD3	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1040:LEU:C	2:B:1042:GLU:H	1.88	0.75
2:B:1417:LYS:HB3	2:B:1424:SER:CB	2.16	0.75
1:A:789:SER:CB	1:A:890:ASP:HA	2.17	0.75
1:A:447:LEU:HB2	1:A:559:MET:SD	2.27	0.74
2:B:1202:ARG:O	2:B:1206:GLU:HG2	1.87	0.74
1:A:675:GLN:H	1:A:675:GLN:CD	1.90	0.74
2:B:1060:GLU:HA	2:B:1098:LYS:HE3	1.67	0.74
1:A:640:GLU:H	1:A:685:ASN:ND2	1.84	0.74
2:B:1041:LYS:CD	2:B:1045:LEU:HD13	2.17	0.74
1:A:3:LEU:HD12	1:A:391:LEU:HD21	1.70	0.74
2:B:1664:VAL:HG22	2:B:1686:GLU:HB2	1.70	0.74
1:A:450:TYR:CD1	1:A:474:ASN:HB2	2.23	0.74
1:A:554:PRO:HG2	1:A:685:ASN:OD1	1.88	0.73
2:B:1345:VAL:HG23	2:B:1346:ASP:N	2.04	0.73
1:A:749:SER:HB3	1:A:750:PRO:CD	2.17	0.73
1:A:602:CYS:HA	1:A:636:GLU:OE2	1.87	0.73
2:B:1119:ASP:O	2:B:1124:MET:HG3	1.89	0.73
1:A:487:LEU:H	1:A:488:PRO:CD	2.02	0.73
2:B:1072:LYS:CE	2:B:1075:GLY:HA3	2.15	0.73
1:A:260:ASN:ND2	5:A:2260:NAG:H62	2.04	0.73
2:B:1166:TYR:CE2	2:B:1216:ARG:HB2	2.24	0.73
2:B:1347:ALA:O	2:B:1351:ILE:HG23	1.88	0.73
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.16	0.72
1:A:463:LEU:HD12	1:A:468:LEU:HB3	1.70	0.72
2:B:1157:VAL:HG23	2:B:1158:ASP:H	1.53	0.72
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.72	0.72
1:A:634:GLN:OE1	1:A:690:GLY:HA2	1.89	0.72
2:B:1088:ILE:CG2	2:B:1425:LEU:HD11	2.18	0.72
1:A:647:ILE:HD11	1:A:677:ARG:HB3	1.70	0.72
1:A:3:LEU:HD21	1:A:350:LEU:HD21	1.72	0.72
2:B:1112:VAL:HG13	2:B:1149:LEU:HD12	1.72	0.72
2:B:1131:ILE:HG23	2:B:1134:LEU:HD23	1.71	0.72
1:A:514:LEU:HD23	1:A:515:TYR:CE1	2.25	0.71
1:A:526:THR:O	1:A:527:ILE:HG23	1.89	0.71
1:A:593:LEU:HD11	1:A:600:ASN:HB3	1.71	0.71
1:A:3:LEU:CD2	1:A:350:LEU:HD11	2.21	0.71
1:A:55:GLN:HE21	1:A:57:LEU:HD11	1.56	0.71
1:A:450:TYR:HB3	1:A:451:PRO:CD	2.19	0.70
1:A:710:SER:HB3	1:A:735:ASP:HA	1.73	0.70
1:A:137:VAL:HG11	1:A:192:VAL:HA	1.74	0.70
1:A:795:LEU:HD23	1:A:884:CYS:SG	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1590:GLN:HE21	2:B:1590:GLN:HA	1.56	0.70
2:B:1622:ARG:HH12	2:B:1661:ASP:H	1.40	0.70
1:A:509:ARG:HG3	1:A:509:ARG:HH11	1.57	0.70
1:A:167:ASP:OD1	1:A:188:VAL:HG21	1.91	0.70
1:A:539:ILE:N	1:A:539:ILE:HD12	2.07	0.70
2:B:1199:GLN:HA	2:B:1199:GLN:NE2	2.05	0.70
2:B:1202:ARG:NH1	2:B:1202:ARG:HB3	2.06	0.69
1:A:490:LYS:HB3	1:A:567:THR:HG23	1.74	0.69
1:A:674:ASN:O	1:A:676:THR:N	2.24	0.69
2:B:1159:LYS:HE2	2:B:1289:TYR:CE2	2.27	0.69
2:B:1553:TRP:CZ3	2:B:1561:THR:HG22	2.27	0.69
1:A:802:LYS:HA	1:A:808:LEU:HD13	1.73	0.69
1:A:474:ASN:OD1	1:A:539:ILE:HG23	1.93	0.69
1:A:501:LYS:O	1:A:504:GLN:HG3	1.92	0.69
1:A:55:GLN:HG3	1:A:57:LEU:HD11	1.75	0.69
1:A:271:GLN:HE22	1:A:301:MET:H	1.39	0.69
1:A:57:LEU:N	1:A:57:LEU:HD12	2.07	0.68
1:A:580:GLN:HG3	1:A:581:PHE:N	2.06	0.68
1:A:906:GLU:C	1:A:908:PHE:H	1.94	0.68
1:A:499:LEU:HD21	1:A:513:PHE:CZ	2.29	0.68
2:B:1666:ARG:HB2	2:B:1682:VAL:HG21	1.76	0.68
2:B:1410:LYS:C	2:B:1412:LYS:H	1.97	0.68
1:A:432:ALA:C	1:A:433:ILE:HD12	2.14	0.68
1:A:650:GLN:HE21	1:A:650:GLN:H	1.38	0.68
1:A:721:ASN:O	1:A:725:LYS:HB3	1.93	0.68
2:B:1157:VAL:HG21	2:B:1188:PHE:H	1.58	0.68
1:A:487:LEU:O	1:A:488:PRO:O	2.12	0.68
1:A:650:GLN:H	1:A:650:GLN:NE2	1.92	0.68
2:B:1169:PRO:HG2	2:B:1173:LEU:HD23	1.74	0.67
1:A:222:LEU:HD12	1:A:223:GLY:H	1.59	0.67
1:A:447:LEU:HD22	1:A:559:MET:HG2	1.75	0.67
1:A:633:ASN:ND2	1:A:635:GLY:H	1.92	0.67
1:A:643:LEU:HB3	1:A:681:CYS:HB2	1.77	0.67
2:B:1647:ASP:HB2	2:B:1668:GLN:OE1	1.94	0.67
3:C:1:NAG:H61	3:C:2:NAG:H2	1.76	0.67
1:A:104:LYS:HE3	1:A:167:ASP:OD1	1.94	0.67
1:A:955:ILE:N	1:A:955:ILE:HD12	2.10	0.67
2:B:1352:ARG:HH12	2:B:1391:ILE:HG23	1.58	0.67
3:G:1:NAG:H61	3:G:2:NAG:O5	1.95	0.67
2:B:1067:ARG:NH2	2:B:1081:THR:HG22	2.09	0.67
2:B:1075:GLY:O	2:B:1076:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:O	1:A:65:ARG:HG2	1.94	0.67
1:A:123:GLU:HB3	1:A:153:GLY:O	1.95	0.67
1:A:462:SER:OG	1:A:469:LYS:HD2	1.95	0.67
1:A:761:GLU:HB2	1:A:763:LYS:NZ	2.10	0.67
1:A:190:GLU:CD	1:A:205:ASN:HB2	2.15	0.67
1:A:621:ASP:HA	1:A:891:ARG:NH1	2.10	0.66
2:B:1257:ALA:O	2:B:1258:LEU:HB2	1.94	0.66
2:B:1590:GLN:HE21	2:B:1590:GLN:CA	2.08	0.66
4:H:1:NAG:H3	4:H:2:NDG:HA	1.58	0.66
1:A:873:GLY:O	1:A:877:ALA:HB3	1.95	0.66
1:A:82:LYS:O	1:A:83:ASP:HB2	1.96	0.66
1:A:222:LEU:HD12	1:A:223:GLY:N	2.09	0.66
2:B:1249:THR:HA	2:B:1309:ALA:O	1.96	0.66
2:B:1166:TYR:HE2	2:B:1216:ARG:HB2	1.60	0.66
2:B:1653:VAL:HG13	2:B:1669:TYR:HB3	1.78	0.66
1:A:556:THR:HG22	1:A:589:GLN:HE21	1.61	0.65
1:A:714:ASP:C	1:A:715:LEU:HD12	2.16	0.65
1:A:759:ASN:O	1:A:760:TRP:HB2	1.95	0.65
2:B:1067:ARG:HH21	2:B:1081:THR:CG2	2.05	0.65
2:B:1661:ASP:O	2:B:1662:ASP:HB2	1.96	0.65
3:C:1:NAG:H61	3:C:2:NAG:O7	1.97	0.65
1:A:563:LEU:HD23	1:A:564:ASP:N	2.11	0.65
2:B:1173:LEU:HD22	2:B:1178:TYR:CE1	2.31	0.65
2:B:1169:PRO:HG3	2:B:1173:LEU:HD23	1.79	0.65
1:A:664:ALA:CB	1:A:693:LEU:HD11	2.26	0.65
2:B:1084:SER:O	2:B:1086:GLN:NE2	2.30	0.65
1:A:33:ARG:HE	1:A:35:PHE:HZ	1.45	0.65
1:A:614:GLN:OE1	1:A:625:LEU:HA	1.96	0.65
2:B:1333:LEU:HD21	2:B:1337:SER:OG	1.97	0.65
2:B:1588:CYS:C	2:B:1590:GLN:H	2.00	0.64
1:A:83:ASP:O	1:A:85:PRO:HD3	1.97	0.64
2:B:1617:CYS:SG	2:B:1618:LYS:N	2.70	0.64
1:A:607:GLU:HG3	1:A:632:GLN:CG	2.28	0.64
1:A:715:LEU:HD12	1:A:715:LEU:N	2.12	0.64
1:A:551:LYS:HD3	1:A:551:LYS:N	2.13	0.64
1:A:946:LEU:HD23	1:A:946:LEU:N	2.12	0.64
2:B:1134:LEU:HD12	2:B:1135:GLY:N	2.13	0.64
1:A:755:LEU:O	1:A:756:PRO:C	2.33	0.64
1:A:768:THR:HG22	1:A:836:SER:HA	1.79	0.64
2:B:1115:TYR:CE1	2:B:1236:ILE:HG13	2.33	0.64
1:A:367:GLU:HG2	1:A:370:LYS:NZ	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1333:LEU:HG	2:B:1334:SER:N	2.10	0.64
2:B:1409:GLU:O	2:B:1410:LYS:HB2	1.98	0.64
2:B:1417:LYS:HB3	2:B:1424:SER:HB3	1.80	0.64
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.80	0.63
1:A:429:VAL:HG23	1:A:431:ARG:CG	2.28	0.63
2:B:1590:GLN:C	2:B:1592:GLY:H	2.02	0.63
2:B:1664:VAL:CG2	2:B:1686:GLU:HB2	2.28	0.63
1:A:451:PRO:CD	1:A:473:PHE:HB2	2.29	0.63
1:A:704:GLN:HE21	1:A:707:MET:HG2	1.63	0.63
1:A:509:ARG:HG3	1:A:509:ARG:NH1	2.13	0.63
1:A:703:GLN:NE2	1:A:704:GLN:N	2.47	0.63
1:A:119:LYS:HE3	1:A:121:GLU:OE2	1.99	0.63
2:B:1015:GLN:O	2:B:1019:VAL:HG23	1.99	0.63
2:B:1116:TYR:OH	2:B:1340:VAL:HG21	1.99	0.63
1:A:220:SER:O	1:A:221:TYR:HB2	1.99	0.63
1:A:1:PHE:HB3	1:A:377:ASN:HD21	1.64	0.63
1:A:99:ARG:NH2	1:A:409:LYS:HE3	2.14	0.63
1:A:116:THR:HG21	1:A:147:ILE:HG21	1.80	0.63
2:B:1148:ASN:ND2	2:B:1239:ARG:HH12	1.96	0.62
2:B:1650:LYS:O	2:B:1651:ASP:HB3	1.98	0.62
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.34	0.62
1:A:780:TYR:OH	1:A:922:SER:OG	2.18	0.62
1:A:687:MET:O	1:A:687:MET:HG3	1.98	0.62
1:A:745:ARG:HA	1:A:745:ARG:NE	2.14	0.62
2:B:1134:LEU:HD12	2:B:1135:GLY:H	1.64	0.62
2:B:1137:LYS:NZ	2:B:1341:LEU:HD22	2.13	0.62
2:B:1341:LEU:CD1	2:B:1342:GLN:H	2.06	0.62
1:A:472:CYS:HA	1:A:541:TYR:HA	1.80	0.62
2:B:1041:LYS:HA	2:B:1044:LEU:HB3	1.82	0.62
1:A:640:GLU:HG3	1:A:685:ASN:HD21	1.64	0.62
1:A:880:LEU:C	1:A:880:LEU:HD23	2.20	0.62
1:A:394:GLN:H	1:A:394:GLN:HE21	1.47	0.62
2:B:1173:LEU:HD13	2:B:1178:TYR:CD1	2.34	0.62
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.80	0.62
1:A:801:TYR:CE2	1:A:802:LYS:HE2	2.35	0.62
2:B:1162:SER:HB3	2:B:1163:PRO:HD3	1.81	0.62
2:B:1275:VAL:HG12	2:B:1276:GLY:N	2.15	0.62
2:B:1373:THR:OG1	2:B:1379:VAL:HG12	2.00	0.62
1:A:596:CYS:HB3	1:A:601:VAL:C	2.20	0.62
2:B:1297:GLU:O	2:B:1301:GLN:HG3	2.00	0.62
1:A:750:PRO:C	1:A:752:HIS:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PRO:HG2	1:A:651:ALA:HB3	1.82	0.61
2:B:1159:LYS:HE2	2:B:1289:TYR:CZ	2.34	0.61
2:B:1642:VAL:CG1	2:B:1680:TYR:HB3	2.30	0.61
1:A:114:TRP:CZ3	1:A:116:THR:HG22	2.34	0.61
1:A:481:ALA:O	1:A:482:ASP:HB3	1.99	0.61
2:B:1041:LYS:CD	2:B:1045:LEU:CD1	2.69	0.61
1:A:414:ILE:HG22	1:A:421:ASP:OD1	2.00	0.61
1:A:455:ASN:C	1:A:455:ASN:ND2	2.48	0.61
4:H:1:NAG:C7	4:H:2:NDG:H8C1	2.30	0.61
1:A:441:ILE:HD11	1:A:576:PRO:CG	2.30	0.61
2:B:1083:VAL:HA	2:B:1103:GLN:O	2.01	0.61
1:A:1:PHE:HA	1:A:388:SER:OG	2.00	0.61
2:B:1086:GLN:HE21	2:B:1086:GLN:CA	2.12	0.61
1:A:139:TYR:CE1	1:A:141:PRO:HD3	2.36	0.61
1:A:170:LEU:HD13	1:A:226:VAL:HG21	1.82	0.61
1:A:675:GLN:H	1:A:675:GLN:NE2	1.99	0.61
2:B:1557:TYR:O	2:B:1558:CYS:HB2	2.01	0.61
1:A:460:THR:O	1:A:461:CYS:HB3	2.01	0.60
1:A:25:PHE:CD1	1:A:412:THR:HB	2.35	0.60
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.83	0.60
2:B:1669:TYR:HE1	2:B:1671:GLU:HG3	1.67	0.60
1:A:551:LYS:HD3	1:A:551:LYS:H	1.66	0.60
1:A:154:PHE:O	1:A:175:GLY:HA3	2.01	0.60
2:B:1590:GLN:C	2:B:1592:GLY:N	2.54	0.60
2:B:1173:LEU:HA	2:B:1176:PRO:HD2	1.83	0.60
2:B:1671:GLU:O	2:B:1672:ASP:HB3	1.99	0.60
1:A:477:PHE:O	1:A:477:PHE:CD1	2.55	0.60
2:B:1041:LYS:HG3	2:B:1045:LEU:HD13	1.83	0.60
2:B:1059:SER:HA	2:B:1091:ARG:O	2.02	0.60
1:A:741:ALA:N	1:A:786:GLY:HA3	2.15	0.60
1:A:745:ARG:HE	1:A:745:ARG:CA	2.13	0.60
1:A:828:ILE:CD1	1:A:829:ASN:N	2.65	0.60
2:B:1090:LEU:HD21	2:B:1401:ALA:HB3	1.84	0.60
1:A:741:ALA:H	1:A:786:GLY:CA	2.11	0.60
2:B:1142:MET:HB3	2:B:1149:LEU:HD13	1.83	0.60
1:A:946:LEU:N	1:A:946:LEU:CD2	2.65	0.59
2:B:1168:SER:H	2:B:1169:PRO:CD	2.15	0.59
2:B:1315:VAL:HG13	2:B:1316:ASN:N	2.17	0.59
1:A:238:ASP:HB3	1:A:256:TYR:O	2.01	0.59
2:B:1041:LYS:CG	2:B:1045:LEU:HD13	2.33	0.59
2:B:1169:PRO:HG2	2:B:1170:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD23	1:A:350:LEU:HD11	1.84	0.59
1:A:187:GLN:O	1:A:191:ILE:HG13	2.02	0.59
1:A:646:SER:HB2	1:A:714:ASP:HB2	1.83	0.59
1:A:925:SER:CB	1:A:944:SER:HB3	2.32	0.59
2:B:1026:CYS:O	2:B:1027:SER:HB2	2.01	0.59
2:B:1299:LEU:HD11	2:B:1306:LEU:HD12	1.84	0.59
2:B:1399:ILE:HD13	2:B:1416:ILE:HD13	1.85	0.59
2:B:1408:GLN:HA	2:B:1408:GLN:NE2	2.12	0.59
1:A:549:ARG:HH11	1:A:549:ARG:HG3	1.66	0.59
2:B:1129:TRP:C	2:B:1131:ILE:H	2.06	0.59
2:B:1292:LEU:HD22	2:B:1325:ILE:HD11	1.83	0.59
2:B:1683:GLU:O	2:B:1684:GLU:HB3	2.02	0.59
2:B:1673:SER:C	2:B:1675:GLY:H	2.04	0.59
2:B:1557:TYR:HB2	2:B:1559:ASN:OD1	2.02	0.59
1:A:1:PHE:HD2	1:A:2:ASN:ND2	2.01	0.59
1:A:768:THR:CG2	1:A:836:SER:HA	2.33	0.59
1:A:43:ALA:HB3	1:A:55:GLN:HG2	1.84	0.59
1:A:271:GLN:HE22	1:A:301:MET:N	2.00	0.59
1:A:756:PRO:O	1:A:757:ILE:HG22	2.01	0.59
1:A:648:PRO:HG2	1:A:651:ALA:CB	2.34	0.58
1:A:707:MET:SD	1:A:708:ASP:N	2.67	0.58
2:B:1429:VAL:HG12	2:B:1430:THR:N	2.18	0.58
1:A:613:ASP:O	1:A:615:LYS:HG2	2.03	0.58
1:A:171:LEU:C	1:A:171:LEU:HD23	2.24	0.58
2:B:1653:VAL:CG1	2:B:1669:TYR:HB3	2.33	0.58
1:A:25:PHE:CE1	1:A:412:THR:HB	2.39	0.58
1:A:375:ILE:C	1:A:375:ILE:HD12	2.24	0.58
2:B:1040:LEU:HD13	2:B:1043:ASN:ND2	2.08	0.58
1:A:384:ASN:HD22	1:A:384:ASN:C	2.06	0.58
1:A:271:GLN:NE2	1:A:301:MET:H	2.02	0.58
1:A:40:ALA:O	1:A:42:LYS:N	2.37	0.58
1:A:231:PHE:HA	1:A:320:GLN:HE22	1.68	0.58
1:A:444:ASN:HB2	1:A:480:LYS:HD2	1.85	0.58
1:A:514:LEU:HB2	1:A:539:ILE:HB	1.85	0.58
1:A:781:GLU:HG3	1:A:896:ILE:HG12	1.85	0.57
1:A:909:MET:HB2	1:A:915:ASN:ND2	2.19	0.57
2:B:1198:ASP:O	2:B:1200:VAL:HG13	2.04	0.57
1:A:1:PHE:CD2	1:A:2:ASN:ND2	2.72	0.57
1:A:745:ARG:HA	1:A:745:ARG:HE	1.69	0.57
2:B:1168:SER:HB3	2:B:1174:GLU:OE1	2.03	0.57
2:B:1169:PRO:HB2	2:B:1170:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1371:ASN:OD1	2:B:1381:PRO:HA	2.04	0.57
2:B:1529:VAL:O	2:B:1530:ARG:HB2	2.04	0.57
2:B:1040:LEU:HD12	2:B:1040:LEU:N	2.15	0.57
2:B:1169:PRO:HG2	2:B:1170:PRO:HD2	1.87	0.57
2:B:1259:ASP:O	2:B:1261:ARG:N	2.37	0.57
2:B:1678:ILE:C	2:B:1679:LEU:HD23	2.25	0.57
1:A:43:ALA:CB	1:A:55:GLN:HG2	2.34	0.57
1:A:394:GLN:HE22	1:A:395:TRP:HE1	1.52	0.57
2:B:1002:PRO:HA	2:B:1006:THR:OG1	2.05	0.57
1:A:229:GLY:N	1:A:237:ASP:HB3	2.20	0.57
1:A:956:GLN:CD	1:A:956:GLN:H	2.08	0.57
2:B:1666:ARG:HB2	2:B:1682:VAL:CG2	2.35	0.57
1:A:115:ARG:O	1:A:116:THR:OG1	2.16	0.57
1:A:647:ILE:CD1	1:A:677:ARG:HB3	2.35	0.57
2:B:1612:LYS:C	2:B:1614:CYS:N	2.58	0.57
2:B:1093:ARG:CB	2:B:1094:PRO:HD2	2.29	0.57
1:A:431:ARG:HG2	1:A:431:ARG:HH11	1.69	0.56
1:A:443:VAL:HG21	1:A:561:TYR:HE1	1.70	0.56
1:A:450:TYR:HB2	1:A:474:ASN:H	1.69	0.56
1:A:501:LYS:C	1:A:503:LYS:H	2.07	0.56
1:A:748:SER:O	1:A:749:SER:C	2.41	0.56
1:A:73:ASP:OD1	1:A:75:THR:HB	2.06	0.56
1:A:391:LEU:HD12	1:A:435:TYR:CE2	2.39	0.56
1:A:491:LEU:HD12	1:A:567:THR:HG21	1.88	0.56
1:A:813:HIS:C	1:A:813:HIS:CD2	2.78	0.56
2:B:1226:ILE:HD11	2:B:1248:PHE:CD1	2.40	0.56
2:B:1551:SER:O	2:B:1552:ASP:HB2	2.05	0.56
1:A:340:PHE:O	1:A:361:ALA:O	2.23	0.56
3:C:1:NAG:H61	3:C:2:NAG:N2	2.20	0.56
1:A:66:ARG:HG2	1:A:67:CYS:N	2.19	0.56
1:A:654:ILE:HG13	1:A:699:PHE:HA	1.88	0.56
1:A:757:ILE:O	1:A:757:ILE:HG23	2.06	0.56
1:A:810:TYR:OH	1:A:831:LEU:HB2	2.05	0.56
2:B:1218:ALA:CB	2:B:1219:PRO:HD3	2.27	0.56
1:A:116:THR:CG2	1:A:147:ILE:HG21	2.36	0.56
1:A:487:LEU:N	1:A:488:PRO:CD	2.65	0.56
5:A:2260:NAG:O7	5:A:2260:NAG:C3	2.54	0.56
2:B:1105:ARG:HG3	2:B:1105:ARG:HH11	1.71	0.56
1:A:606:LEU:HB3	1:A:717:ILE:HD12	1.88	0.56
1:A:607:GLU:HG3	1:A:632:GLN:HG3	1.86	0.56
2:B:1126:ASP:CG	2:B:1127:ASP:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1121:SER:HB3	2:B:1220:GLU:OE2	2.05	0.55
2:B:1612:LYS:C	2:B:1614:CYS:H	2.09	0.55
1:A:351:ASP:OD2	1:A:353:ASP:HB3	2.05	0.55
1:A:710:SER:HB2	1:A:734:VAL:O	2.05	0.55
2:B:1678:ILE:HD13	2:B:1678:ILE:H	1.70	0.55
1:A:348:GLY:O	1:A:356:ASN:HA	2.06	0.55
1:A:414:ILE:HG12	1:A:414:ILE:O	2.06	0.55
1:A:260:ASN:ND2	5:A:2260:NAG:C6	2.66	0.55
2:B:1031:LEU:HD23	2:B:1031:LEU:H	1.71	0.55
2:B:1608:CYS:O	2:B:1610:PHE:N	2.40	0.55
1:A:450:TYR:CG	1:A:474:ASN:HB2	2.41	0.55
1:A:816:ILE:HD11	1:A:822:CYS:SG	2.47	0.55
2:B:1124:MET:HA	2:B:1127:ASP:OD1	2.06	0.55
2:B:1411:GLU:O	2:B:1412:LYS:C	2.45	0.55
1:A:225:SER:OG	1:A:280:VAL:HG22	2.07	0.55
1:A:447:LEU:O	1:A:448:GLU:OE2	2.25	0.55
1:A:835:ILE:HG12	1:A:836:SER:N	2.20	0.55
2:B:1681:VAL:HG12	2:B:1682:VAL:O	2.07	0.55
1:A:462:SER:HA	1:A:469:LYS:HA	1.88	0.55
2:B:1138:LEU:CD2	2:B:1151:ILE:HG21	2.37	0.55
2:B:1199:GLN:O	2:B:1201:THR:N	2.39	0.55
2:B:1354:LYS:HB2	2:B:1386:CYS:O	2.07	0.55
1:A:502:LEU:HD23	1:A:553:THR:HG22	1.88	0.55
2:B:1127:ASP:C	2:B:1129:TRP:H	2.10	0.55
2:B:1315:VAL:HG13	2:B:1316:ASN:H	1.72	0.55
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.89	0.55
1:A:441:ILE:HG12	1:A:487:LEU:CD1	2.37	0.55
1:A:645:VAL:CG1	1:A:679:VAL:HB	2.37	0.55
2:B:1115:TYR:OH	2:B:1192:HIS:ND1	2.39	0.55
2:B:1417:LYS:HB3	2:B:1424:SER:HB2	1.89	0.55
1:A:155:CYS:O	1:A:156:GLN:HB2	2.05	0.55
1:A:299:LEU:HD22	2:B:1258:LEU:HD22	1.89	0.55
1:A:707:MET:CE	1:A:708:ASP:H	2.19	0.55
2:B:1086:GLN:NE2	2:B:1086:GLN:N	2.56	0.55
1:A:458:ASN:ND2	5:A:2458:NAG:C6	2.66	0.54
1:A:416:LYS:HD3	1:A:571:THR:HG22	1.89	0.54
1:A:482:ASP:HB2	1:A:528:SER:O	2.06	0.54
1:A:909:MET:O	1:A:915:ASN:CB	2.51	0.54
2:B:1045:LEU:C	2:B:1047:ASP:H	2.11	0.54
1:A:108:CYS:HA	1:A:128:CYS:HA	1.89	0.54
1:A:523:LYS:HE3	1:A:536:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ILE:O	2:B:1530:ARG:HB2	2.07	0.54
1:A:765:ASN:N	1:A:766:PRO:HD3	2.22	0.54
2:B:1622:ARG:HH12	2:B:1661:ASP:N	2.04	0.54
1:A:328:THR:HG22	1:A:329:THR:H	1.73	0.54
1:A:672:THR:HG23	1:A:677:ARG:H	1.72	0.54
2:B:1105:ARG:NH1	2:B:1394:THR:OG1	2.40	0.54
1:A:416:LYS:HD2	1:A:416:LYS:N	2.14	0.54
1:A:650:GLN:N	1:A:650:GLN:NE2	2.44	0.54
1:A:657:VAL:HG12	1:A:698:ARG:CZ	2.37	0.54
2:B:1356:GLU:HG2	2:B:1385:SER:CB	2.33	0.54
2:B:1230:THR:O	2:B:1302:LYS:HG3	2.07	0.54
1:A:578:LEU:HD12	1:A:578:LEU:N	2.23	0.54
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.90	0.54
2:B:1069:LEU:O	2:B:1070:SER:O	2.25	0.54
2:B:1144:LYS:O	2:B:1145:LEU:HB2	2.06	0.54
1:A:61:TRP:O	1:A:62:SER:HB3	2.08	0.54
1:A:101:LYS:O	1:A:101:LYS:HD3	2.08	0.54
1:A:376:PHE:HB3	1:A:383:LEU:HD11	1.90	0.54
1:A:464:PRO:HG2	1:A:465:GLY:N	2.15	0.54
1:A:799:TRP:CG	1:A:800:PRO:HD2	2.43	0.54
5:A:2458:NAG:O7	5:A:2458:NAG:C3	2.55	0.54
2:B:1281:TYR:CE1	2:B:1283:ALA:HB3	2.43	0.54
1:A:620:GLY:H	1:A:703:GLN:HG2	1.73	0.53
2:B:1608:CYS:O	2:B:1611:LYS:N	2.41	0.53
1:A:433:ILE:HD12	1:A:433:ILE:N	2.23	0.53
1:A:614:GLN:O	1:A:616:LYS:HG2	2.08	0.53
1:A:743:GLU:HG2	1:A:785:ASN:ND2	2.24	0.53
2:B:1202:ARG:HB3	2:B:1202:ARG:HH11	1.74	0.53
1:A:161:ILE:HA	1:A:170:LEU:O	2.08	0.53
1:A:100:SER:HB2	1:A:105:ILE:HG22	1.91	0.53
1:A:739:LEU:O	1:A:788:SER:OG	2.27	0.53
2:B:1240:ASN:C	2:B:1240:ASN:HD22	2.12	0.53
2:B:1341:LEU:C	2:B:1343:LEU:H	2.11	0.53
2:B:1166:TYR:O	2:B:1168:SER:N	2.42	0.53
2:B:1251:ASP:HA	2:B:1311:THR:OG1	2.09	0.53
1:A:3:LEU:HD21	1:A:350:LEU:CD2	2.39	0.53
1:A:62:SER:O	1:A:64:THR:N	2.33	0.53
1:A:101:LYS:CB	1:A:104:LYS:HE2	2.35	0.53
2:B:1076:ASP:O	2:B:1078:SER:N	2.38	0.53
2:B:1196:LEU:HD12	2:B:1237:GLY:C	2.30	0.53
1:A:514:LEU:HD22	1:A:539:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:GLU:O	1:A:765:ASN:HB2	2.09	0.53
1:A:340:PHE:C	1:A:342:SER:H	2.13	0.53
1:A:436:ARG:NH1	1:A:571:THR:HB	2.20	0.53
2:B:1090:LEU:HD21	2:B:1401:ALA:CB	2.39	0.53
1:A:24:ASP:OD1	1:A:99:ARG:NE	2.35	0.52
1:A:300:PHE:HB3	1:A:313:GLY:HA2	1.90	0.52
1:A:579:ASN:O	1:A:582:THR:HB	2.09	0.52
1:A:644:ILE:HG13	1:A:718:GLN:NE2	2.25	0.52
1:A:761:GLU:HB2	1:A:763:LYS:HZ1	1.72	0.52
1:A:955:ILE:HG22	1:A:955:ILE:O	2.08	0.52
2:B:1102:ILE:HG21	2:B:1357:LEU:HD21	1.91	0.52
2:B:1180:MET:O	2:B:1181:LYS:HB3	2.09	0.52
2:B:1630:THR:O	2:B:1632:ASN:N	2.41	0.52
1:A:513:PHE:CE1	1:A:521:HIS:HB3	2.45	0.52
1:A:45:THR:C	1:A:47:GLN:H	2.11	0.52
1:A:239:PHE:O	1:A:256:TYR:N	2.43	0.52
1:A:710:SER:HA	1:A:736:LEU:HG	1.92	0.52
2:B:1418:PRO:HB2	2:B:1421:PHE:CG	2.44	0.52
1:A:384:ASN:ND2	1:A:386:VAL:H	2.07	0.52
1:A:747:VAL:HG12	1:A:779:ILE:HB	1.91	0.52
2:B:1391:ILE:H	2:B:1391:ILE:CD1	2.07	0.52
1:A:246:ALA:HB3	1:A:252:MET:N	2.25	0.52
1:A:363:PRO:HB2	1:A:364:TYR:CD1	2.45	0.52
2:B:1673:SER:O	2:B:1675:GLY:N	2.43	0.52
1:A:169:VAL:O	1:A:185:SER:HA	2.09	0.52
1:A:415:ASP:HB2	1:A:416:LYS:HD2	1.91	0.52
1:A:436:ARG:CZ	1:A:574:LEU:HD13	2.39	0.52
1:A:663:LEU:N	1:A:663:LEU:HD22	2.24	0.52
2:B:1044:LEU:HD23	2:B:1045:LEU:N	2.25	0.52
1:A:177:PHE:CD1	1:A:212:THR:HA	2.45	0.52
1:A:450:TYR:HB2	1:A:474:ASN:HB2	1.92	0.52
1:A:645:VAL:HG13	1:A:645:VAL:O	2.09	0.52
2:B:1352:ARG:HB3	2:B:1352:ARG:HH11	1.74	0.52
2:B:1429:VAL:CG1	2:B:1430:THR:N	2.73	0.52
1:A:187:GLN:HE21	1:A:206:ASN:HB2	1.74	0.52
1:A:444:ASN:O	1:A:479:LEU:HD12	2.10	0.52
1:A:493:PHE:CD1	1:A:493:PHE:N	2.77	0.52
2:B:1666:ARG:HG3	2:B:1666:ARG:HH11	1.74	0.52
1:A:558:PHE:CZ	3:E:1:NAG:H82	2.45	0.52
2:B:1296:THR:O	2:B:1297:GLU:C	2.47	0.52
1:A:811:ILE:HA	1:A:901:SER:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1653:VAL:CG2	2:B:1654:ASN:N	2.73	0.51
2:B:1673:SER:C	2:B:1675:GLY:N	2.64	0.51
1:A:61:TRP:CH2	1:A:415:ASP:HB3	2.45	0.51
1:A:459:LYS:HD3	1:A:470:VAL:HA	1.92	0.51
1:A:608:VAL:CG2	1:A:717:ILE:HG13	2.40	0.51
1:A:615:LYS:HG3	1:A:615:LYS:O	2.10	0.51
1:A:653:PHE:HA	1:A:699:PHE:HB3	1.92	0.51
1:A:746:GLY:HA2	1:A:779:ILE:O	2.10	0.51
1:A:905:THR:HG22	1:A:905:THR:O	2.09	0.51
2:B:1114:ILE:HB	2:B:1151:ILE:HG22	1.92	0.51
2:B:1170:PRO:HG2	2:B:1178:TYR:CE2	2.45	0.51
2:B:1418:PRO:HG2	2:B:1421:PHE:CD2	2.46	0.51
1:A:246:ALA:HB3	1:A:252:MET:H	1.76	0.51
1:A:516:SER:OG	1:A:518:SER:HB3	2.11	0.51
2:B:1099:ASN:N	2:B:1099:ASN:HD22	2.09	0.51
2:B:1126:ASP:O	2:B:1129:TRP:N	2.43	0.51
2:B:1408:GLN:HE21	2:B:1408:GLN:CA	2.08	0.51
2:B:1410:LYS:C	2:B:1412:LYS:N	2.63	0.51
1:A:439:PRO:O	1:A:576:PRO:HB2	2.10	0.51
1:A:740:ALA:O	1:A:742:VAL:HG23	2.10	0.51
1:A:776:VAL:HG12	1:A:777:GLN:N	2.25	0.51
2:B:1666:ARG:NH2	4:I:1:NAG:O7	2.41	0.51
1:A:363:PRO:HB2	1:A:364:TYR:CE1	2.45	0.51
1:A:441:ILE:HD11	1:A:576:PRO:HG3	1.93	0.51
1:A:672:THR:HG23	1:A:676:THR:H	1.76	0.51
1:A:810:TYR:CE2	1:A:833:ILE:HD12	2.45	0.51
2:B:1073:GLY:HA3	2:B:1109:ASP:O	2.11	0.51
1:A:394:GLN:H	1:A:394:GLN:NE2	2.07	0.51
1:A:599:ASP:CG	1:A:601:VAL:HG12	2.31	0.51
1:A:607:GLU:HG3	1:A:632:GLN:HG2	1.92	0.51
2:B:1033:LEU:HD12	2:B:1035:SER:O	2.10	0.51
2:B:1557:TYR:O	2:B:1558:CYS:CB	2.58	0.51
1:A:577:ILE:HG13	1:A:578:LEU:N	2.25	0.51
1:A:650:GLN:O	1:A:702:HIS:N	2.43	0.51
1:A:830:PRO:HG2	1:A:831:LEU:HD13	1.92	0.51
1:A:928:VAL:CG2	1:A:941:ILE:HB	2.41	0.51
2:B:1066:ASP:O	2:B:1067:ARG:HB2	2.11	0.51
2:B:1079:GLN:O	2:B:1080:VAL:C	2.46	0.51
2:B:1275:VAL:HG12	2:B:1276:GLY:H	1.76	0.51
1:A:586:ILE:HG13	1:A:587:SER:N	2.26	0.51
1:A:755:LEU:C	1:A:757:ILE:N	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1219:PRO:HB2	2:B:1255:HIS:CE1	2.45	0.51
1:A:743:GLU:HG2	1:A:785:ASN:HD21	1.76	0.50
1:A:906:GLU:CA	1:A:906:GLU:OE1	2.59	0.50
2:B:1040:LEU:H	2:B:1040:LEU:CD1	2.17	0.50
2:B:1119:ASP:HB2	2:B:1156:PHE:CZ	2.46	0.50
1:A:339:ARG:O	1:A:362:ALA:HA	2.11	0.50
1:A:347:LEU:HD12	1:A:357:ASP:C	2.31	0.50
1:A:415:ASP:OD2	1:A:417:ASN:OD1	2.29	0.50
1:A:441:ILE:HG12	1:A:487:LEU:HD11	1.92	0.50
1:A:639:TYR:HA	1:A:685:ASN:O	2.11	0.50
1:A:715:LEU:N	1:A:715:LEU:CD1	2.74	0.50
2:B:1102:ILE:HG22	2:B:1397:PHE:HB2	1.94	0.50
2:B:1244:HIS:O	2:B:1305:ASN:HB2	2.11	0.50
2:B:1380:ILE:HG13	2:B:1380:ILE:O	2.11	0.50
1:A:328:THR:HG22	1:A:329:THR:N	2.26	0.50
1:A:384:ASN:ND2	1:A:385:ALA:N	2.53	0.50
2:B:1529:VAL:HG21	2:B:1556:TYR:CE1	2.46	0.50
2:B:1621:ASP:O	2:B:1626:MET:SD	2.70	0.50
1:A:85:PRO:O	1:A:115:ARG:HG2	2.10	0.50
2:B:1021:PRO:HA	2:B:1093:ARG:HD2	1.94	0.50
2:B:1526:PHE:O	2:B:1528:CYS:SG	2.70	0.50
1:A:247:ALA:HB3	1:A:250:LEU:HB2	1.92	0.50
1:A:616:LYS:O	1:A:616:LYS:HG3	2.12	0.50
2:B:1262:LEU:HD12	2:B:1262:LEU:N	2.27	0.50
2:B:1564:THR:O	2:B:1567:CYS:N	2.45	0.50
1:A:384:ASN:C	1:A:384:ASN:ND2	2.65	0.50
2:B:1033:LEU:CD1	2:B:1035:SER:H	2.24	0.50
2:B:1410:LYS:O	2:B:1412:LYS:N	2.44	0.50
1:A:275:TYR:CE2	2:B:1258:LEU:HB3	2.47	0.50
1:A:459:LYS:HB2	1:A:471:SER:N	2.26	0.50
1:A:626:THR:HA	1:A:698:ARG:HA	1.94	0.50
1:A:908:PHE:O	1:A:909:MET:HG2	2.11	0.50
1:A:938:ILE:O	1:A:939:GLU:HG3	2.11	0.50
2:B:1134:LEU:HD22	2:B:1340:VAL:HG11	1.93	0.50
2:B:1269:ASN:ND2	2:B:1290:PRO:HB3	2.26	0.50
1:A:236:ILE:HG13	1:A:237:ASP:N	2.27	0.50
2:B:1215:ASN:ND2	2:B:1217:ASP:O	2.45	0.50
2:B:1229:ALA:HA	2:B:1236:ILE:CD1	2.42	0.50
2:B:1564:THR:O	2:B:1567:CYS:HB2	2.12	0.50
1:A:114:TRP:CE3	1:A:116:THR:HG22	2.47	0.49
1:A:413:ASP:O	1:A:415:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:GLU:C	1:A:908:PHE:N	2.63	0.49
2:B:1102:ILE:CG2	2:B:1397:PHE:HB2	2.41	0.49
2:B:1166:TYR:C	2:B:1167:ILE:HD12	2.32	0.49
2:B:1185:LEU:CD1	2:B:1186:PRO:HD2	2.35	0.49
1:A:176:SER:CB	1:A:182:GLN:HB2	2.42	0.49
2:B:1059:SER:HB3	2:B:1092:LEU:HD23	1.94	0.49
2:B:1620:PHE:C	2:B:1622:ARG:H	2.15	0.49
1:A:283:THR:O	1:A:292:ASP:HB2	2.12	0.49
1:A:413:ASP:C	1:A:415:ASP:H	2.16	0.49
1:A:705:SER:O	1:A:707:MET:N	2.46	0.49
2:B:1249:THR:HB	2:B:1309:ALA:HB3	1.94	0.49
2:B:1345:VAL:CG2	2:B:1346:ASP:N	2.75	0.49
5:B:3371:NAG:H5	5:B:3371:NAG:N2	2.27	0.49
1:A:244:PRO:HA	1:A:276:PHE:O	2.11	0.49
2:B:1226:ILE:HD11	2:B:1248:PHE:CG	2.47	0.49
2:B:1653:VAL:HG22	2:B:1654:ASN:N	2.27	0.49
1:A:443:VAL:HG21	1:A:561:TYR:CE1	2.48	0.49
1:A:497:LEU:O	1:A:498:LEU:HD23	2.13	0.49
2:B:1079:GLN:O	2:B:1081:THR:HG22	2.13	0.49
2:B:1157:VAL:HG23	2:B:1189:GLY:N	2.16	0.49
2:B:1601:CYS:O	2:B:1604:CYS:HB2	2.12	0.49
1:A:747:VAL:HG13	1:A:747:VAL:O	2.13	0.49
1:A:916:HIS:HA	1:A:953:TRP:CD1	2.48	0.49
2:B:1173:LEU:HD13	2:B:1178:TYR:HB3	1.94	0.49
1:A:312:VAL:HG12	1:A:336:VAL:HA	1.94	0.49
1:A:710:SER:CB	1:A:735:ASP:HA	2.40	0.49
1:A:736:LEU:HB2	1:A:936:LEU:HD11	1.93	0.49
1:A:18:TYR:HB2	1:A:41:PRO:HG2	1.94	0.49
1:A:450:TYR:CB	1:A:451:PRO:CD	2.87	0.49
1:A:466:THR:O	1:A:468:LEU:N	2.45	0.49
1:A:781:GLU:HG3	1:A:896:ILE:CG1	2.42	0.49
1:A:367:GLU:HG2	1:A:370:LYS:HZ2	1.77	0.49
1:A:384:ASN:HD22	1:A:385:ALA:H	1.58	0.49
1:A:496:GLU:C	1:A:497:LEU:HD12	2.33	0.49
2:B:1169:PRO:CB	2:B:1170:PRO:CD	2.90	0.49
2:B:1173:LEU:HD13	2:B:1178:TYR:CG	2.47	0.49
2:B:1199:GLN:C	2:B:1201:THR:H	2.16	0.49
1:A:165:LYS:C	1:A:167:ASP:H	2.15	0.48
1:A:499:LEU:N	1:A:499:LEU:CD2	2.72	0.48
2:B:1351:ILE:CG1	2:B:1352:ARG:N	2.75	0.48
1:A:489:ARG:N	1:A:528:SER:OG	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:VAL:HG21	1:A:809:LEU:HD21	1.95	0.48
2:B:1114:ILE:HD13	2:B:1344:ILE:HG21	1.95	0.48
2:B:1122:TYR:C	2:B:1124:MET:H	2.16	0.48
2:B:1362:LEU:HD12	2:B:1363:PRO:HD2	1.94	0.48
1:A:447:LEU:HD22	1:A:559:MET:CG	2.43	0.48
1:A:673:GLU:OE2	1:A:673:GLU:HA	2.13	0.48
2:B:1170:PRO:C	2:B:1172:ALA:N	2.66	0.48
1:A:186:ASP:OD1	1:A:207:GLN:HB2	2.12	0.48
2:B:1085:PRO:C	2:B:1086:GLN:NE2	2.66	0.48
2:B:1146:THR:C	2:B:1148:ASN:H	2.15	0.48
2:B:1262:LEU:C	2:B:1264:GLY:N	2.66	0.48
1:A:748:SER:HB2	1:A:947:VAL:HG23	1.96	0.48
1:A:804:ASN:C	1:A:806:ASN:N	2.66	0.48
2:B:1317:LEU:HD23	2:B:1318:TYR:CE1	2.48	0.48
2:B:1262:LEU:C	2:B:1264:GLY:H	2.16	0.48
1:A:75:THR:O	1:A:89:LYS:NZ	2.44	0.48
1:A:361:ALA:O	1:A:363:PRO:HD3	2.13	0.48
2:B:1009:GLY:HA3	2:B:1038:CYS:HB3	1.94	0.48
2:B:1168:SER:H	2:B:1169:PRO:HD3	1.78	0.48
1:A:367:GLU:HG2	1:A:370:LYS:HZ3	1.78	0.48
2:B:1232:CYS:O	2:B:1234:GLU:N	2.47	0.48
1:A:336:VAL:O	1:A:337:PHE:HB2	2.14	0.48
1:A:570:ASP:C	1:A:572:THR:H	2.17	0.48
2:B:1198:ASP:O	2:B:1200:VAL:N	2.46	0.48
2:B:1575:CYS:HB2	2:B:1579:GLY:O	2.14	0.48
1:A:1:PHE:HB3	1:A:377:ASN:ND2	2.29	0.48
1:A:527:ILE:O	1:A:528:SER:HB2	2.13	0.48
1:A:606:LEU:CB	1:A:727:SER:HB3	2.44	0.48
1:A:704:GLN:HG3	1:A:707:MET:HG3	1.96	0.48
1:A:828:ILE:O	1:A:830:PRO:HD2	2.14	0.48
1:A:907:THR:HG22	1:A:907:THR:O	2.14	0.48
2:B:1126:ASP:N	2:B:1126:ASP:OD2	2.46	0.48
2:B:1158:ASP:OD1	2:B:1159:LYS:N	2.39	0.48
2:B:1336:ASP:C	2:B:1338:SER:H	2.17	0.48
2:B:1616:GLU:O	2:B:1616:GLU:HG3	2.13	0.48
1:A:614:GLN:OE1	1:A:626:THR:N	2.42	0.47
2:B:1057:PRO:N	2:B:1093:ARG:HH21	2.12	0.47
2:B:1060:GLU:CA	2:B:1098:LYS:HE3	2.41	0.47
2:B:1082:GLN:HG2	2:B:1107:VAL:HG23	1.96	0.47
2:B:1623:GLU:CD	2:B:1624:PRO:CD	2.81	0.47
1:A:35:PHE:CD1	1:A:35:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LYS:O	1:A:469:LYS:HB3	2.14	0.47
1:A:723:PHE:N	1:A:723:PHE:CD1	2.83	0.47
2:B:1066:ASP:O	2:B:1086:GLN:OE1	2.32	0.47
2:B:1069:LEU:HB3	2:B:1105:ARG:HE	1.79	0.47
2:B:1568:MET:HG3	2:B:1569:SER:H	1.79	0.47
1:A:489:ARG:O	1:A:528:SER:HB2	2.14	0.47
1:A:928:VAL:HB	1:A:941:ILE:HB	1.97	0.47
2:B:1666:ARG:O	2:B:1682:VAL:HG23	2.13	0.47
1:A:3:LEU:CD2	1:A:350:LEU:HD21	2.43	0.47
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.44	0.47
2:B:1087:ARG:CZ	2:B:1428:GLN:NE2	2.77	0.47
2:B:1126:ASP:O	2:B:1127:ASP:C	2.53	0.47
2:B:1306:LEU:O	2:B:1328:THR:HG23	2.14	0.47
2:B:1312:GLU:O	2:B:1315:VAL:HG12	2.13	0.47
2:B:1399:ILE:CD1	2:B:1416:ILE:HD13	2.44	0.47
1:A:439:PRO:HB2	1:A:487:LEU:HD13	1.95	0.47
1:A:594:LEU:O	1:A:595:ASP:HB2	2.14	0.47
2:B:1262:LEU:O	2:B:1264:GLY:N	2.47	0.47
2:B:1333:LEU:CG	2:B:1334:SER:H	2.17	0.47
2:B:1571:ASN:HD22	2:B:1571:ASN:HA	1.56	0.47
1:A:436:ARG:HH12	1:A:571:THR:CB	2.25	0.47
1:A:514:LEU:HD22	1:A:539:ILE:CB	2.44	0.47
1:A:556:THR:HA	1:A:589:GLN:HA	1.97	0.47
1:A:909:MET:HB3	1:A:912:GLU:OE2	2.14	0.47
1:A:285:ILE:N	1:A:292:ASP:OD1	2.42	0.47
2:B:1015:GLN:HA	2:B:1015:GLN:NE2	2.30	0.47
2:B:1156:PHE:HA	2:B:1189:GLY:O	2.14	0.47
2:B:1159:LYS:HE2	2:B:1289:TYR:CD2	2.49	0.47
2:B:1166:TYR:O	2:B:1167:ILE:C	2.52	0.47
2:B:1185:LEU:HD22	2:B:1211:SER:OG	2.14	0.47
2:B:1348:TYR:O	2:B:1351:ILE:HG12	2.14	0.47
2:B:1536:CYS:HB2	2:B:1540:GLY:O	2.14	0.47
2:B:1617:CYS:SG	2:B:1618:LYS:HG2	2.54	0.47
2:B:1652:ALA:HB2	2:B:1670:TYR:CD2	2.49	0.47
1:A:101:LYS:HD2	1:A:104:LYS:NZ	2.30	0.47
1:A:139:TYR:CZ	1:A:141:PRO:HD3	2.50	0.47
1:A:815:ASP:HB2	1:A:898:TYR:HB2	1.96	0.47
1:A:906:GLU:OE1	1:A:906:GLU:HA	2.15	0.47
2:B:1015:GLN:HA	2:B:1015:GLN:HE21	1.80	0.47
2:B:1320:ASN:O	2:B:1324:LEU:HD23	2.14	0.47
1:A:261:MET:O	1:A:261:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:HB2	1:A:370:LYS:HG3	1.97	0.47
1:A:525:MET:O	1:A:526:THR:HB	2.15	0.47
2:B:1161:VAL:HG13	2:B:1285:THR:HG22	1.97	0.47
2:B:1671:GLU:HG2	2:B:1677:SER:CB	2.45	0.47
1:A:168:ARG:NH2	1:A:208:LEU:HG	2.30	0.47
1:A:759:ASN:O	1:A:760:TRP:CB	2.63	0.47
2:B:1670:TYR:HE1	2:B:1672:ASP:OD1	1.98	0.47
1:A:329:THR:O	1:A:330:LYS:HD3	2.15	0.46
1:A:633:ASN:HD22	1:A:634:GLN:N	2.12	0.46
2:B:1218:ALA:HB3	2:B:1219:PRO:CD	2.31	0.46
1:A:394:GLN:NE2	1:A:395:TRP:NE1	2.62	0.46
1:A:402:PRO:O	1:A:403:SER:HB2	2.15	0.46
1:A:421:ASP:HB3	1:A:434:LEU:HD21	1.96	0.46
1:A:539:ILE:N	1:A:539:ILE:CD1	2.74	0.46
1:A:802:LYS:CA	1:A:808:LEU:HD13	2.44	0.46
2:B:1623:GLU:OE2	2:B:1624:PRO:N	2.48	0.46
1:A:294:PHE:CE2	1:A:358:ILE:HD13	2.50	0.46
1:A:567:THR:O	1:A:567:THR:HG22	2.16	0.46
2:B:1150:ARG:HG3	2:B:1239:ARG:CZ	2.46	0.46
1:A:1:PHE:O	1:A:2:ASN:CG	2.53	0.46
1:A:170:LEU:HD11	1:A:239:PHE:HB3	1.96	0.46
1:A:205:ASN:HD22	1:A:205:ASN:HA	1.55	0.46
1:A:490:LYS:CB	1:A:567:THR:HG23	2.43	0.46
1:A:644:ILE:HD13	1:A:680:VAL:HG23	1.98	0.46
2:B:1031:LEU:HD23	2:B:1031:LEU:N	2.31	0.46
2:B:1358:GLU:HG2	2:B:1417:LYS:O	2.15	0.46
2:B:1648:THR:HA	4:I:2:NDG:C1	2.45	0.46
1:A:33:ARG:HG3	1:A:35:PHE:CE1	2.50	0.46
1:A:163:PHE:HA	1:A:168:ARG:O	2.16	0.46
1:A:232:ASN:O	1:A:233:GLY:C	2.53	0.46
1:A:429:VAL:HG23	1:A:431:ARG:HG3	1.97	0.46
1:A:792:LYS:HB2	1:A:930:GLU:HB2	1.98	0.46
2:B:1559:ASN:OD1	2:B:1559:ASN:N	2.38	0.46
1:A:24:ASP:OD2	1:A:25:PHE:N	2.49	0.46
1:A:239:PHE:O	1:A:255:ILE:HA	2.15	0.46
1:A:660:ASN:OD1	1:A:661:GLU:N	2.48	0.46
1:A:666:LEU:HD13	1:A:681:CYS:HB3	1.97	0.46
2:B:1363:PRO:HD2	2:B:1366:LEU:HD23	1.96	0.46
1:A:110:PRO:O	1:A:156:GLN:HG2	2.15	0.46
1:A:339:ARG:O	1:A:342:SER:HB2	2.16	0.46
2:B:1054:ILE:O	2:B:1054:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1380:ILE:HA	2:B:1381:PRO:HD2	1.79	0.46
1:A:17:SER:O	1:A:18:TYR:HB2	2.15	0.46
1:A:277:GLY:O	1:A:279:SER:N	2.49	0.46
1:A:438:ARG:HH12	1:A:577:ILE:CB	2.14	0.46
1:A:869:ILE:HG13	1:A:869:ILE:O	2.14	0.46
2:B:1096:ASP:OD1	2:B:1097:SER:N	2.41	0.46
2:B:1148:ASN:CG	2:B:1239:ARG:HH12	2.19	0.46
1:A:539:ILE:HD12	1:A:539:ILE:H	1.78	0.46
1:A:888:ARG:NH1	1:A:890:ASP:OD1	2.48	0.46
1:A:920:LEU:O	1:A:948:THR:HA	2.16	0.46
1:A:239:PHE:CE1	1:A:258:GLY:HA2	2.51	0.46
1:A:280:VAL:HA	1:A:294:PHE:O	2.16	0.46
2:B:1529:VAL:HG21	2:B:1556:TYR:HE1	1.79	0.46
2:B:1648:THR:CA	4:I:1:NAG:H62	2.42	0.45
1:A:77:ASN:OD1	1:A:89:LYS:HG3	2.16	0.45
1:A:585:ASN:OD1	1:A:585:ASN:O	2.34	0.45
1:A:756:PRO:O	1:A:757:ILE:CG2	2.65	0.45
1:A:783:ARG:CB	1:A:894:SER:HB3	2.34	0.45
2:B:1163:PRO:HG2	2:B:1263:ALA:HA	1.98	0.45
2:B:1646:LYS:HB3	2:B:1646:LYS:HZ3	1.78	0.45
1:A:459:LYS:O	1:A:459:LYS:HG3	2.16	0.45
1:A:525:MET:O	1:A:526:THR:CB	2.63	0.45
1:A:621:ASP:OD1	1:A:621:ASP:C	2.55	0.45
2:B:1181:LYS:O	2:B:1183:THR:N	2.49	0.45
2:B:1588:CYS:C	2:B:1590:GLN:N	2.69	0.45
2:B:1608:CYS:O	2:B:1609:THR:C	2.55	0.45
1:A:416:LYS:HD3	1:A:571:THR:CG2	2.46	0.45
1:A:445:ALA:HB2	1:A:561:TYR:CE2	2.52	0.45
1:A:657:VAL:HG12	1:A:698:ARG:NE	2.32	0.45
1:A:804:ASN:C	1:A:806:ASN:H	2.18	0.45
2:B:1072:LYS:HE2	2:B:1075:GLY:CA	2.22	0.45
2:B:1127:ASP:O	2:B:1129:TRP:N	2.49	0.45
2:B:1331:GLY:HA3	2:B:1343:LEU:HD11	1.98	0.45
2:B:1354:LYS:CB	2:B:1386:CYS:O	2.64	0.45
1:A:294:PHE:CD2	1:A:358:ILE:HD13	2.51	0.45
1:A:429:VAL:HG23	1:A:431:ARG:HG2	1.98	0.45
1:A:577:ILE:HG13	1:A:578:LEU:H	1.82	0.45
1:A:775:VAL:HA	1:A:902:LEU:HD12	1.99	0.45
2:B:1082:GLN:HG2	2:B:1105:ARG:O	2.17	0.45
1:A:243:VAL:HB	1:A:246:ALA:HB2	1.98	0.45
1:A:384:ASN:ND2	1:A:386:VAL:HG23	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASN:HD22	1:A:456:GLN:N	2.14	0.45
1:A:501:LYS:C	1:A:503:LYS:N	2.70	0.45
2:B:1012:SER:O	2:B:1013:CYS:C	2.54	0.45
2:B:1233:ASP:O	2:B:1234:GLU:C	2.54	0.45
2:B:1599:GLU:OE2	2:B:1599:GLU:N	2.41	0.45
2:B:1670:TYR:CE1	2:B:1672:ASP:OD1	2.69	0.45
1:A:116:THR:HG21	1:A:147:ILE:CG2	2.45	0.45
1:A:417:ASN:HA	1:A:486:VAL:HB	1.97	0.45
2:B:1028:ASP:H	2:B:1031:LEU:HD21	1.81	0.45
2:B:1148:ASN:HD22	2:B:1149:LEU:N	2.15	0.45
2:B:1523:CYS:O	2:B:1524:ASP:HB3	2.16	0.45
1:A:190:GLU:HG3	1:A:194:LYS:HG2	1.99	0.45
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.52	0.45
1:A:750:PRO:C	1:A:752:HIS:N	2.67	0.45
2:B:1134:LEU:HD22	2:B:1340:VAL:CG1	2.46	0.45
2:B:1341:LEU:H	2:B:1341:LEU:HG	1.48	0.45
2:B:1531:TYR:HB2	2:B:1537:SER:OG	2.17	0.45
1:A:367:GLU:N	1:A:367:GLU:CD	2.70	0.45
2:B:1084:SER:HB3	2:B:1085:PRO:CD	2.40	0.45
1:A:101:LYS:HB2	1:A:163:PHE:CG	2.52	0.45
1:A:331:LEU:HD23	1:A:340:PHE:HE2	1.81	0.45
1:A:647:ILE:HG13	1:A:677:ARG:O	2.17	0.45
1:A:660:ASN:OD1	1:A:662:ALA:N	2.31	0.45
1:A:672:THR:HG23	1:A:674:ASN:O	2.17	0.45
1:A:797:LEU:HD12	1:A:923:SER:O	2.17	0.45
2:B:1135:GLY:HA3	2:B:1203:PHE:CD2	2.52	0.45
2:B:1618:LYS:NZ	2:B:1639:ILE:HD11	2.31	0.45
1:A:11:TYR:CE1	1:A:36:LEU:HD21	2.52	0.44
1:A:303:ARG:NH1	1:A:307:GLY:O	2.49	0.44
1:A:377:ASN:ND2	1:A:388:SER:CB	2.81	0.44
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.26	0.44
1:A:626:THR:HG22	1:A:698:ARG:CB	2.47	0.44
1:A:657:VAL:HG22	1:A:696:GLY:HA3	1.98	0.44
2:B:1169:PRO:O	2:B:1170:PRO:C	2.48	0.44
1:A:495:VAL:HG12	1:A:496:GLU:N	2.21	0.44
1:A:599:ASP:O	1:A:600:ASN:HB2	2.17	0.44
2:B:1086:GLN:NE2	2:B:1086:GLN:CA	2.80	0.44
2:B:1280:HIS:O	2:B:1282:SER:N	2.51	0.44
2:B:1306:LEU:HB3	2:B:1328:THR:HG23	1.99	0.44
2:B:1681:VAL:O	2:B:1682:VAL:C	2.55	0.44
3:C:1:NAG:C6	3:C:2:NAG:C1	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:N	1:A:88:PHE:CD1	2.86	0.44
1:A:285:ILE:HG12	1:A:383:LEU:HB2	2.00	0.44
2:B:1151:ILE:C	2:B:1196:LEU:HD23	2.37	0.44
2:B:1175:ASN:HB2	2:B:1176:PRO:HD3	1.99	0.44
2:B:1679:LEU:HD23	2:B:1679:LEU:N	2.33	0.44
1:A:23:VAL:O	1:A:24:ASP:HB2	2.17	0.44
1:A:386:VAL:O	1:A:387:PRO:C	2.56	0.44
2:B:1182:THR:O	2:B:1183:THR:HB	2.18	0.44
1:A:749:SER:CB	1:A:750:PRO:CD	2.81	0.44
2:B:1013:CYS:O	2:B:1014:GLN:C	2.56	0.44
2:B:1238:TRP:CE2	2:B:1304:ILE:HD12	2.52	0.44
2:B:1274:HIS:HB2	2:B:1281:TYR:HE1	1.83	0.44
2:B:1364:GLU:HG3	2:B:1365:GLU:H	1.83	0.44
1:A:490:LYS:HB3	1:A:491:LEU:H	1.50	0.44
2:B:1057:PRO:O	2:B:1093:ARG:NH2	2.51	0.44
2:B:1067:ARG:HB2	2:B:1086:GLN:OE1	2.18	0.44
2:B:1341:LEU:O	2:B:1343:LEU:N	2.51	0.44
2:B:1529:VAL:CG1	2:B:1557:TYR:CE2	3.00	0.44
1:A:425:GLY:HA2	1:A:432:ALA:HA	1.99	0.44
2:B:1084:SER:CB	2:B:1085:PRO:HD3	2.39	0.44
2:B:1174:GLU:HA	2:B:1174:GLU:OE2	2.18	0.44
2:B:1678:ILE:HD11	2:B:1680:TYR:CE2	2.52	0.44
1:A:451:PRO:HD3	1:A:474:ASN:H	1.82	0.44
1:A:627:LEU:HD11	1:A:699:PHE:HZ	1.82	0.44
1:A:751:ASP:O	3:G:1:NAG:H82	2.18	0.44
1:A:775:VAL:HG22	1:A:902:LEU:CD1	2.47	0.44
2:B:1105:ARG:HG3	2:B:1105:ARG:NH1	2.32	0.44
2:B:1240:ASN:C	2:B:1240:ASN:ND2	2.71	0.44
2:B:1296:THR:O	2:B:1298:LYS:N	2.51	0.44
1:A:302:ASP:OD2	1:A:310:GLN:HG3	2.18	0.44
1:A:336:VAL:HG12	1:A:337:PHE:CD2	2.53	0.44
2:B:1324:LEU:HD22	2:B:1324:LEU:N	2.33	0.44
1:A:645:VAL:HG12	1:A:679:VAL:O	2.18	0.43
2:B:1086:GLN:C	2:B:1425:LEU:HD12	2.38	0.43
2:B:1115:TYR:CD1	2:B:1236:ILE:HG23	2.53	0.43
2:B:1180:MET:HG3	2:B:1214:ARG:NH1	2.33	0.43
1:A:633:ASN:O	1:A:690:GLY:N	2.51	0.43
1:A:640:GLU:HG3	1:A:685:ASN:ND2	2.31	0.43
1:A:755:LEU:HA	1:A:755:LEU:HD23	1.66	0.43
1:A:831:LEU:CD1	1:A:831:LEU:N	2.81	0.43
2:B:1009:GLY:O	2:B:1010:VAL:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HB3	1:A:243:VAL:CG1	2.48	0.43
1:A:762:HIS:C	1:A:762:HIS:CD2	2.91	0.43
1:A:31:SER:OG	1:A:32:SER:N	2.51	0.43
1:A:277:GLY:C	1:A:279:SER:N	2.72	0.43
1:A:463:LEU:CB	1:A:464:PRO:CD	2.84	0.43
1:A:366:GLY:O	1:A:367:GLU:C	2.56	0.43
1:A:377:ASN:ND2	1:A:388:SER:HB3	2.34	0.43
1:A:457:ASP:HB3	1:A:458:ASN:H	1.68	0.43
1:A:523:LYS:HD3	1:A:536:GLU:HG2	2.00	0.43
1:A:569:ALA:C	1:A:571:THR:H	2.21	0.43
1:A:580:GLN:CG	1:A:581:PHE:H	2.18	0.43
1:A:797:LEU:HD23	1:A:882:ILE:HD12	2.01	0.43
1:A:816:ILE:HA	1:A:896:ILE:O	2.18	0.43
2:B:1086:GLN:HE21	2:B:1086:GLN:N	2.15	0.43
2:B:1129:TRP:O	2:B:1131:ILE:N	2.50	0.43
1:A:88:PHE:CE1	1:A:122:ARG:HG2	2.53	0.43
1:A:106:LEU:CD2	1:A:128:CYS:HB3	2.48	0.43
1:A:334:PHE:CD1	1:A:334:PHE:N	2.86	0.43
1:A:364:TYR:CD1	1:A:364:TYR:N	2.86	0.43
2:B:1108:GLU:CG	2:B:1109:ASP:N	2.82	0.43
2:B:1650:LYS:O	2:B:1651:ASP:CB	2.67	0.43
1:A:347:LEU:CD2	1:A:422:LEU:HD13	2.49	0.43
1:A:638:ALA:O	1:A:687:MET:HB3	2.18	0.43
1:A:640:GLU:N	1:A:685:ASN:ND2	2.60	0.43
1:A:653:PHE:CZ	1:A:655:GLY:HA2	2.53	0.43
1:A:799:TRP:CD2	1:A:800:PRO:HD2	2.53	0.43
1:A:885:GLN:HE21	1:A:885:GLN:HB2	1.65	0.43
2:B:1137:LYS:HZ1	2:B:1341:LEU:HD22	1.83	0.43
2:B:1657:TYR:CE2	2:B:1665:VAL:HB	2.53	0.43
1:A:55:GLN:NE2	1:A:69:PRO:HB3	2.34	0.43
1:A:57:LEU:HA	1:A:69:PRO:HA	2.01	0.43
1:A:62:SER:C	1:A:64:THR:H	2.18	0.43
2:B:1534:GLU:HB3	2:B:1538:GLY:N	2.34	0.43
2:B:1554:THR:O	2:B:1558:CYS:HA	2.19	0.43
2:B:1590:GLN:CA	2:B:1590:GLN:NE2	2.81	0.43
2:B:1630:THR:C	2:B:1632:ASN:N	2.72	0.43
1:A:556:THR:CG2	1:A:589:GLN:HE21	2.28	0.43
1:A:768:THR:HG22	1:A:835:ILE:O	2.19	0.43
1:A:812:LEU:O	1:A:813:HIS:HB3	2.19	0.43
2:B:1061:ALA:HA	2:B:1089:ALA:O	2.19	0.43
2:B:1099:ASN:HD22	2:B:1099:ASN:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1167:ILE:O	2:B:1168:SER:CB	2.67	0.43
2:B:1530:ARG:HG3	2:B:1530:ARG:HH11	1.83	0.43
2:B:1650:LYS:HE2	4:I:2:NDG:O6	2.18	0.43
1:A:232:ASN:O	1:A:234:ASP:N	2.52	0.43
1:A:417:ASN:O	1:A:419:TYR:N	2.45	0.43
1:A:450:TYR:HB2	1:A:474:ASN:N	2.33	0.43
1:A:704:GLN:HE21	1:A:707:MET:CG	2.30	0.43
1:A:816:ILE:HG21	1:A:820:MET:HB3	2.01	0.43
2:B:1278:ASP:O	2:B:1279:ASN:HB2	2.19	0.43
2:B:1630:THR:C	2:B:1632:ASN:H	2.23	0.43
1:A:102:GLN:HB3	1:A:103:ASP:H	1.47	0.42
1:A:607:GLU:CG	1:A:632:GLN:HG3	2.48	0.42
1:A:670:PHE:HA	1:A:679:VAL:HA	2.00	0.42
1:A:747:VAL:O	1:A:747:VAL:CG1	2.67	0.42
1:A:803:TYR:O	1:A:803:TYR:CD2	2.72	0.42
1:A:832:ARG:O	1:A:834:LYS:N	2.52	0.42
1:A:913:ASN:OD1	1:A:914:GLN:N	2.52	0.42
1:A:955:ILE:N	1:A:955:ILE:CD1	2.79	0.42
2:B:1342:GLN:HA	2:B:1345:VAL:HG22	2.01	0.42
2:B:1553:TRP:HZ3	2:B:1559:ASN:O	2.02	0.42
1:A:248:ARG:HG2	5:B:3320:NAG:H81	2.00	0.42
1:A:379:ARG:O	1:A:382:GLY:O	2.36	0.42
2:B:1138:LEU:HD21	2:B:1151:ILE:HG21	2.01	0.42
2:B:1630:THR:HG22	2:B:1631:CYS:N	2.34	0.42
1:A:753:VAL:HB	1:A:951:VAL:HG22	2.00	0.42
1:A:835:ILE:CG1	1:A:836:SER:H	2.28	0.42
2:B:1670:TYR:HB3	2:B:1678:ILE:CD1	2.49	0.42
1:A:277:GLY:O	1:A:278:PHE:C	2.58	0.42
1:A:434:LEU:HD23	1:A:435:TYR:N	2.34	0.42
1:A:464:PRO:CG	1:A:465:GLY:N	2.77	0.42
1:A:533:MET:HG3	1:A:533:MET:O	2.19	0.42
1:A:831:LEU:N	1:A:831:LEU:HD12	2.33	0.42
1:A:5:VAL:HG13	1:A:435:TYR:HE2	1.85	0.42
1:A:164:THR:OG1	1:A:168:ARG:HB3	2.19	0.42
1:A:455:ASN:ND2	1:A:457:ASP:H	2.17	0.42
2:B:1345:VAL:CG2	2:B:1346:ASP:H	2.15	0.42
2:B:1529:VAL:CG2	2:B:1556:TYR:HE1	2.33	0.42
1:A:57:LEU:N	1:A:57:LEU:CD1	2.78	0.42
1:A:802:LYS:HG2	1:A:807:THR:HA	2.02	0.42
1:A:19:PHE:CD1	1:A:431:ARG:HA	2.55	0.42
1:A:301:MET:HE3	2:B:1324:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:H	1:A:416:LYS:CD	2.14	0.42
1:A:489:ARG:O	1:A:490:LYS:O	2.37	0.42
1:A:804:ASN:O	1:A:805:ASN:HB2	2.20	0.42
2:B:1336:ASP:C	2:B:1338:SER:N	2.72	0.42
2:B:1568:MET:O	2:B:1569:SER:CB	2.67	0.42
2:B:1642:VAL:HG12	2:B:1680:TYR:HD1	1.85	0.42
1:A:305:SER:HB3	2:B:1552:ASP:HB2	2.02	0.42
1:A:657:VAL:CG2	1:A:696:GLY:HA3	2.50	0.42
1:A:688:LYS:HA	1:A:688:LYS:CE	2.50	0.42
5:A:2458:NAG:HO4	5:A:2458:NAG:C7	2.33	0.42
2:B:1646:LYS:HE3	2:B:1654:ASN:ND2	2.35	0.42
3:E:1:NAG:H62	3:E:2:NAG:O5	2.20	0.42
1:A:376:PHE:CB	1:A:383:LEU:HD11	2.50	0.42
1:A:702:HIS:CE1	2:B:1532:LYS:NZ	2.87	0.42
1:A:791:SER:O	1:A:792:LYS:HG3	2.19	0.42
2:B:1196:LEU:HD12	2:B:1237:GLY:O	2.20	0.42
1:A:115:ARG:O	1:A:115:ARG:HD3	2.19	0.42
1:A:455:ASN:ND2	1:A:457:ASP:N	2.68	0.42
1:A:459:LYS:HB2	1:A:470:VAL:CA	2.50	0.42
1:A:513:PHE:HB2	1:A:516:SER:HB3	2.02	0.42
1:A:556:THR:HG22	1:A:589:GLN:NE2	2.32	0.42
1:A:801:TYR:CD2	1:A:802:LYS:HG3	2.55	0.42
2:B:1044:LEU:HD23	2:B:1044:LEU:C	2.40	0.42
2:B:1115:TYR:CZ	2:B:1236:ILE:HG13	2.54	0.42
2:B:1121:SER:O	2:B:1122:TYR:C	2.58	0.42
2:B:1612:LYS:HD2	2:B:1657:TYR:CD1	2.55	0.42
1:A:821:ASN:O	1:A:884:CYS:HA	2.21	0.41
5:B:3371:NAG:H5	5:B:3371:NAG:HN2	1.84	0.41
1:A:431:ARG:HG2	1:A:431:ARG:NH1	2.35	0.41
1:A:514:LEU:HB3	1:A:515:TYR:H	1.74	0.41
1:A:598:GLU:CD	1:A:598:GLU:N	2.74	0.41
1:A:668:CYS:HA	1:A:680:VAL:O	2.19	0.41
1:A:787:PRO:HG2	1:A:788:SER:H	1.84	0.41
2:B:1169:PRO:CG	2:B:1170:PRO:CD	2.98	0.41
2:B:1345:VAL:O	2:B:1347:ALA:N	2.53	0.41
2:B:1670:TYR:HB3	2:B:1678:ILE:HD13	2.02	0.41
1:A:24:ASP:CG	1:A:99:ARG:HH21	2.23	0.41
1:A:218:ASP:O	1:A:219:ASP:HB2	2.20	0.41
1:A:498:LEU:CD2	1:A:520:SER:HB3	2.50	0.41
1:A:760:TRP:CE3	1:A:908:PHE:HE2	2.39	0.41
2:B:1056:PHE:O	2:B:1056:PHE:CG	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1108:GLU:HG2	2:B:1109:ASP:N	2.35	0.41
1:A:101:LYS:HE2	1:A:167:ASP:HB2	2.03	0.41
1:A:190:GLU:OE1	1:A:205:ASN:HB2	2.21	0.41
1:A:568:ALA:HB1	1:A:574:LEU:H	1.85	0.41
1:A:697:LEU:N	1:A:697:LEU:HD22	2.35	0.41
1:A:702:HIS:CE1	2:B:1532:LYS:HZ1	2.39	0.41
2:B:1168:SER:O	2:B:1169:PRO:O	2.39	0.41
2:B:1355:VAL:O	2:B:1385:SER:HA	2.21	0.41
2:B:1590:GLN:O	2:B:1592:GLY:N	2.53	0.41
1:A:167:ASP:CG	1:A:188:VAL:HG21	2.40	0.41
1:A:247:ALA:CB	1:A:250:LEU:HB2	2.51	0.41
1:A:508:ILE:HD13	1:A:508:ILE:N	2.36	0.41
1:A:653:PHE:HB2	1:A:679:VAL:HG21	2.01	0.41
2:B:1525:ASP:O	2:B:1528:CYS:SG	2.79	0.41
3:C:1:NAG:H61	3:C:2:NAG:C1	2.48	0.41
1:A:72:PHE:CZ	1:A:105:ILE:HD11	2.55	0.41
1:A:498:LEU:HD23	1:A:520:SER:HB3	2.03	0.41
1:A:750:PRO:O	1:A:752:HIS:N	2.51	0.41
1:A:760:TRP:CH2	1:A:905:THR:HB	2.55	0.41
1:A:765:ASN:H	1:A:766:PRO:HD3	1.83	0.41
1:A:814:TYR:HA	1:A:898:TYR:O	2.20	0.41
1:A:185:SER:HB3	1:A:208:LEU:HB2	2.02	0.41
1:A:657:VAL:HG22	1:A:696:GLY:CA	2.50	0.41
1:A:658:ARG:O	1:A:660:ASN:N	2.47	0.41
2:B:1298:LYS:HA	2:B:1298:LYS:HD3	1.87	0.41
2:B:1671:GLU:HG2	2:B:1677:SER:HB3	2.01	0.41
1:A:139:TYR:CD1	1:A:141:PRO:HD3	2.56	0.41
1:A:173:GLY:HA2	1:A:174:PRO:HD2	1.91	0.41
1:A:514:LEU:HD22	1:A:539:ILE:HG21	2.03	0.41
1:A:615:LYS:O	1:A:616:LYS:HB3	2.21	0.41
1:A:703:GLN:O	1:A:704:GLN:CB	2.69	0.41
2:B:1625:TYR:OH	2:B:1634:TYR:HD1	2.04	0.41
1:A:275:TYR:HD2	1:A:278:PHE:HB2	1.86	0.41
1:A:359:ALA:HB3	1:A:408:MET:HE3	2.03	0.41
1:A:460:THR:O	1:A:461:CYS:O	2.38	0.41
1:A:516:SER:O	1:A:517:ARG:HB2	2.21	0.41
1:A:599:ASP:OD1	1:A:601:VAL:HG12	2.21	0.41
1:A:776:VAL:CG1	1:A:777:GLN:N	2.84	0.41
1:A:870:HIS:O	1:A:918:TYR:HA	2.20	0.41
1:A:916:HIS:HA	1:A:953:TRP:NE1	2.36	0.41
2:B:1129:TRP:C	2:B:1131:ILE:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1157:VAL:HG23	2:B:1158:ASP:N	2.29	0.41
2:B:1310:VAL:O	2:B:1333:LEU:N	2.54	0.41
2:B:1534:GLU:OE1	2:B:1534:GLU:HA	2.20	0.41
2:B:1550:ASP:O	2:B:1551:SER:C	2.58	0.41
1:A:43:ALA:O	1:A:52:GLU:HA	2.21	0.41
1:A:268:THR:HG22	1:A:269:GLY:N	2.35	0.41
1:A:438:ARG:HB3	1:A:576:PRO:HA	2.03	0.41
1:A:796:HIS:O	1:A:924:ALA:HA	2.20	0.41
2:B:1033:LEU:HD12	2:B:1035:SER:H	1.86	0.41
2:B:1041:LYS:CD	2:B:1044:LEU:HD22	2.26	0.41
2:B:1142:MET:O	2:B:1143:ARG:C	2.59	0.41
2:B:1165:MET:HG2	2:B:1166:TYR:N	2.36	0.41
2:B:1550:ASP:O	2:B:1553:TRP:HB2	2.21	0.41
2:B:1622:ARG:NH1	2:B:1661:ASP:CG	2.74	0.41
1:A:578:LEU:HD12	1:A:578:LEU:H	1.86	0.40
1:A:614:GLN:O	1:A:615:LYS:C	2.59	0.40
1:A:704:GLN:HG3	1:A:707:MET:CG	2.51	0.40
2:B:1167:ILE:N	2:B:1167:ILE:CD1	2.69	0.40
2:B:1530:ARG:HD3	2:B:1534:GLU:O	2.21	0.40
1:A:384:ASN:ND2	1:A:386:VAL:N	2.69	0.40
1:A:502:LEU:HD23	1:A:553:THR:CG2	2.51	0.40
1:A:537:GLU:O	1:A:538:LEU:HD22	2.21	0.40
2:B:1306:LEU:HD13	2:B:1328:THR:HG21	2.04	0.40
2:B:1384:LYS:O	2:B:1384:LYS:HG3	2.21	0.40
2:B:1611:LYS:HE3	2:B:1669:TYR:OH	2.21	0.40
2:B:1630:THR:HG21	2:B:1634:TYR:CG	2.57	0.40
1:A:159:PHE:CZ	2:B:1261:ARG:HD2	2.57	0.40
1:A:577:ILE:CG1	1:A:578:LEU:N	2.84	0.40
1:A:757:ILE:HG21	1:A:908:PHE:HZ	1.86	0.40
1:A:833:ILE:O	1:A:833:ILE:HG22	2.21	0.40
2:B:1087:ARG:HH22	2:B:1428:GLN:NE2	1.97	0.40
1:A:340:PHE:CE2	1:A:360:ILE:HG21	2.56	0.40
1:A:499:LEU:O	1:A:500:ASP:HB2	2.21	0.40
1:A:625:LEU:HD21	1:A:734:VAL:HG21	2.03	0.40
2:B:1122:TYR:O	2:B:1124:MET:N	2.54	0.40
2:B:1166:TYR:HE2	2:B:1216:ARG:CB	2.30	0.40
2:B:1229:ALA:HA	2:B:1236:ILE:HD11	2.02	0.40
2:B:1370:PHE:CD2	2:B:1399:ILE:HG12	2.57	0.40
2:B:1670:TYR:O	2:B:1677:SER:HA	2.22	0.40
3:C:1:NAG:C6	3:C:2:NAG:C7	2.94	0.40
2:B:1082:GLN:O	2:B:1104:VAL:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1408:GLN:NE2	2:B:1408:GLN:CA	2.77	0.40
2:B:1530:ARG:HA	2:B:1534:GLU:O	2.22	0.40
2:B:1539:HIS:O	2:B:1550:ASP:OD1	2.39	0.40
2:B:1627:THR:C	2:B:1629:ASN:H	2.24	0.40
2:B:1639:ILE:HD12	2:B:1639:ILE:N	2.36	0.40
4:H:1:NAG:O7	4:H:2:NDG:H8C1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	923/957 (96%)	700 (76%)	161 (17%)	62 (7%)	1	6
2	B	593/692 (86%)	403 (68%)	120 (20%)	70 (12%)	0	1
All	All	1516/1649 (92%)	1103 (73%)	281 (18%)	132 (9%)	0	4

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	102	GLN
1	A	233	GLY
1	A	414	ILE
1	A	416	LYS
1	A	420	PRO
1	A	463	LEU
1	A	464	PRO
1	A	467	ALA
1	A	487	LEU
1	A	488	PRO
1	A	490	LYS

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Mol	Chain	Res	Type
1	A	514	LEU
1	A	527	ILE
1	A	528	SER
1	A	616	LYS
1	A	675	GLN
1	A	703	GLN
1	A	749	SER
1	A	833	ILE
1	A	917	SER
2	B	1011	SER
2	B	1027	SER
2	B	1029	GLU
2	B	1041	LYS
2	B	1070	SER
2	B	1074	SER
2	B	1145	LEU
2	B	1167	ILE
2	B	1168	SER
2	B	1169	PRO
2	B	1176	PRO
2	B	1200	VAL
2	B	1233	ASP
2	B	1376	ASN
2	B	1526	PHE
2	B	1568	MET
2	B	1631	CYS
2	B	1672	ASP
2	B	1685	PRO
1	A	41	PRO
1	A	167	ASP
1	A	205	ASN
1	A	313	GLY
1	A	398	ARG
1	A	457	ASP
1	A	613	ASP
1	A	615	LYS
1	A	666	LEU
1	A	677	ARG
1	A	704	GLN
1	A	705	SER
1	A	706	GLU
1	A	759	ASN

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Mol	Chain	Res	Type
1	A	760	TRP
1	A	913	ASN
2	B	1010	VAL
2	B	1080	VAL
2	B	1123	SER
2	B	1139	ALA
2	B	1182	THR
2	B	1260	GLY
2	B	1342	GLN
2	B	1410	LYS
2	B	1411	GLU
2	B	1527	SER
2	B	1535	MET
2	B	1545	GLY
2	B	1571	ASN
2	B	1589	ILE
2	B	1609	THR
2	B	1637	ASP
2	B	1644	GLU
1	A	399	SER
1	A	491	LEU
1	A	507	ALA
1	A	526	THR
1	A	687	MET
2	B	1128	LEU
2	B	1341	LEU
2	B	1407	PRO
2	B	1412	LYS
2	B	1558	CYS
2	B	1570	SER
2	B	1622	ARG
2	B	1674	SER
1	A	63	SER
1	A	118	MET
1	A	166	ALA
1	A	221	TYR
1	A	367	GLU
1	A	461	CYS
1	A	580	GLN
1	A	707	MET
2	B	1067	ARG
2	B	1077	SER

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Mol	Chain	Res	Type
2	B	1130	SER
2	B	1157	VAL
2	B	1281	TYR
2	B	1297	GLU
2	B	1333	LEU
2	B	1409	GLU
2	B	1569	SER
2	B	1606	ASP
2	B	1673	SER
1	A	278	PHE
1	A	417	ASN
1	A	458	ASN
1	A	482	ASP
1	A	758	PRO
1	A	910	ASN
2	B	1076	ASP
2	B	1230	THR
2	B	1384	LYS
2	B	1641	SER
1	A	48	PRO
1	A	289	ASP
1	A	418	GLY
2	B	1036	PRO
2	B	1049	CYS
2	B	1084	SER
2	B	1524	ASP
2	B	1643	LYS
1	A	450	TYR
1	A	757	ILE
2	B	1107	VAL
2	B	1162	SER
2	B	1345	VAL
2	B	1623	GLU
2	B	1639	ILE
1	A	786	GLY
2	B	1193	VAL

5.3.2 Protein sidechains [i](#)

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	787/812 (97%)	698 (89%)	89 (11%)	4	20
2	B	537/616 (87%)	475 (88%)	62 (12%)	4	19
All	All	1324/1428 (93%)	1173 (89%)	151 (11%)	4	19

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	8	PRO
1	A	10	GLU
1	A	34	MET
1	A	35	PHE
1	A	46	THR
1	A	64	THR
1	A	68	GLN
1	A	71	GLU
1	A	99	ARG
1	A	102	GLN
1	A	106	LEU
1	A	115	ARG
1	A	134	THR
1	A	170	LEU
1	A	176	SER
1	A	190	GLU
1	A	205	ASN
1	A	206	ASN
1	A	216	ILE
1	A	232	ASN
1	A	237	ASP
1	A	248	ARG
1	A	275	TYR
1	A	299	LEU
1	A	318	SER
1	A	319	LEU
1	A	321	ARG
1	A	347	LEU
1	A	352	GLN
1	A	375	ILE
1	A	384	ASN
1	A	392	GLU

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Mol	Chain	Res	Type
1	A	394	GLN
1	A	420	PRO
1	A	431	ARG
1	A	434	LEU
1	A	448	GLU
1	A	450	TYR
1	A	455	ASN
1	A	460	THR
1	A	462	SER
1	A	478	CYS
1	A	488	PRO
1	A	499	LEU
1	A	505	LYS
1	A	521	HIS
1	A	532	LEU
1	A	538	LEU
1	A	539	ILE
1	A	551	LYS
1	A	562	ARG
1	A	563	LEU
1	A	566	ARG
1	A	598	GLU
1	A	610	VAL
1	A	627	LEU
1	A	633	ASN
1	A	649	LEU
1	A	650	GLN
1	A	661	GLU
1	A	685	ASN
1	A	688	LYS
1	A	698	ARG
1	A	699	PHE
1	A	701	VAL
1	A	703	GLN
1	A	724	ASP
1	A	745	ARG
1	A	752	HIS
1	A	764	GLU
1	A	768	THR
1	A	770	GLU
1	A	777	GLN
1	A	791	SER

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Mol	Chain	Res	Type
1	A	813	HIS
1	A	832	ARG
1	A	879	CYS
1	A	885	GLN
1	A	888	ARG
1	A	891	ARG
1	A	897	LEU
1	A	900	LYS
1	A	906	GLU
1	A	911	LYS
1	A	912	GLU
1	A	942	THR
1	A	946	LEU
1	A	947	VAL
2	B	1029	GLU
2	B	1033	LEU
2	B	1039	ASP
2	B	1040	LEU
2	B	1047	ASP
2	B	1055	GLU
2	B	1072	LYS
2	B	1086	GLN
2	B	1088	ILE
2	B	1090	LEU
2	B	1093	ARG
2	B	1099	ASN
2	B	1119	ASP
2	B	1125	LYS
2	B	1128	LEU
2	B	1133	ASN
2	B	1148	ASN
2	B	1157	VAL
2	B	1167	ILE
2	B	1178	TYR
2	B	1195	THR
2	B	1198	ASP
2	B	1220	GLU
2	B	1224	ASP
2	B	1233	ASP
2	B	1240	ASN
2	B	1241	ASP
2	B	1243	SER

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Mol	Chain	Res	Type
2	B	1246	LEU
2	B	1261	ARG
2	B	1278	ASP
2	B	1286	THR
2	B	1306	LEU
2	B	1316	ASN
2	B	1323	GLU
2	B	1336	ASP
2	B	1341	LEU
2	B	1351	ILE
2	B	1352	ARG
2	B	1357	LEU
2	B	1408	GLN
2	B	1415	THR
2	B	1417	LYS
2	B	1526	PHE
2	B	1535	MET
2	B	1550	ASP
2	B	1559	ASN
2	B	1561	THR
2	B	1571	ASN
2	B	1590	GLN
2	B	1611	LYS
2	B	1614	CYS
2	B	1617	CYS
2	B	1621	ASP
2	B	1624	PRO
2	B	1625	TYR
2	B	1639	ILE
2	B	1647	ASP
2	B	1656	THR
2	B	1660	GLU
2	B	1678	ILE
2	B	1679	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	68	GLN
1	A	92	GLN
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	205	ASN
1	A	271	GLN
1	A	314	GLN
1	A	320	GLN
1	A	352	GLN
1	A	377	ASN
1	A	384	ASN
1	A	394	GLN
1	A	455	ASN
1	A	504	GLN
1	A	575	GLN
1	A	580	GLN
1	A	633	ASN
1	A	650	GLN
1	A	675	GLN
1	A	685	ASN
1	A	692	GLN
1	A	703	GLN
1	A	704	GLN
1	A	718	GLN
1	A	762	HIS
1	A	777	GLN
1	A	784	ASN
1	A	785	ASN
1	A	798	GLN
1	A	813	HIS
1	A	885	GLN
1	A	914	GLN
1	A	915	ASN
2	B	1015	GLN
2	B	1043	ASN
2	B	1099	ASN
2	B	1148	ASN
2	B	1199	GLN
2	B	1240	ASN
2	B	1255	HIS
2	B	1279	ASN
2	B	1301	GLN
2	B	1303	ASN
2	B	1316	ASN
2	B	1319	GLN

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Mol	Chain	Res	Type
2	B	1376	ASN
2	B	1408	GLN
2	B	1428	GLN
2	B	1571	ASN
2	B	1590	GLN
2	B	1632	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 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	1,3	14,14,15	0.54	0	17,19,21	0.95	0
3	NAG	C	2	3	14,14,15	0.62	0	17,19,21	0.79	0
3	NAG	D	1	1,3	14,14,15	0.53	0	17,19,21	0.82	1 (5%)
3	NAG	D	2	3	14,14,15	0.44	0	17,19,21	0.81	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.77	0	17,19,21	1.09	1 (5%)
3	NAG	E	2	3	14,14,15	0.52	0	17,19,21	0.67	0
4	NAG	F	1	4,1	14,14,15	0.64	0	17,19,21	1.06	1 (5%)
4	NDG	F	2	4	14,14,15	0.67	0	17,19,21	0.79	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.68	0	17,19,21	1.08	2 (11%)
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	0.57	0
4	NAG	H	1	4,2	14,14,15	0.77	1 (7%)	17,19,21	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDG	H	2	4	14,14,15	0.78	1 (7%)	17,19,21	0.66	0
4	NAG	I	1	4,2	14,14,15	0.78	0	17,19,21	1.28	1 (5%)
4	NDG	I	2	4	14,14,15	0.68	0	17,19,21	0.80	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	NAG	E	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	1/6/23/26	0/1/1/1
4	NDG	F	2	4	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	1/6/23/26	0/1/1/1
4	NDG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NDG	I	2	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	NDG	C1-C2	2.26	1.55	1.52
4	H	1	NAG	C1-C2	2.05	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	NAG	C4-C3-C2	4.30	117.32	111.02
3	G	1	NAG	C2-N2-C7	-2.92	118.99	122.90
4	H	1	NAG	C4-C3-C2	2.70	114.97	111.02
3	E	1	NAG	C4-C3-C2	2.66	114.91	111.02
4	F	1	NAG	C2-N2-C7	-2.61	119.40	122.90
3	D	1	NAG	C2-N2-C7	-2.57	119.46	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NDG	C2-N2-C7	-2.36	119.73	122.90
3	D	2	NAG	C2-N2-C7	-2.24	119.90	122.90
4	H	1	NAG	C2-N2-C7	-2.17	120.00	122.90
3	G	1	NAG	O5-C1-C2	-2.12	108.01	111.29
4	F	2	NDG	C2-N2-C7	-2.08	120.11	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	2	NDG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
4	I	2	NDG	C4-C5-C6-O6

There are no ring outliers.

10 monomers are involved in 21 short contacts:

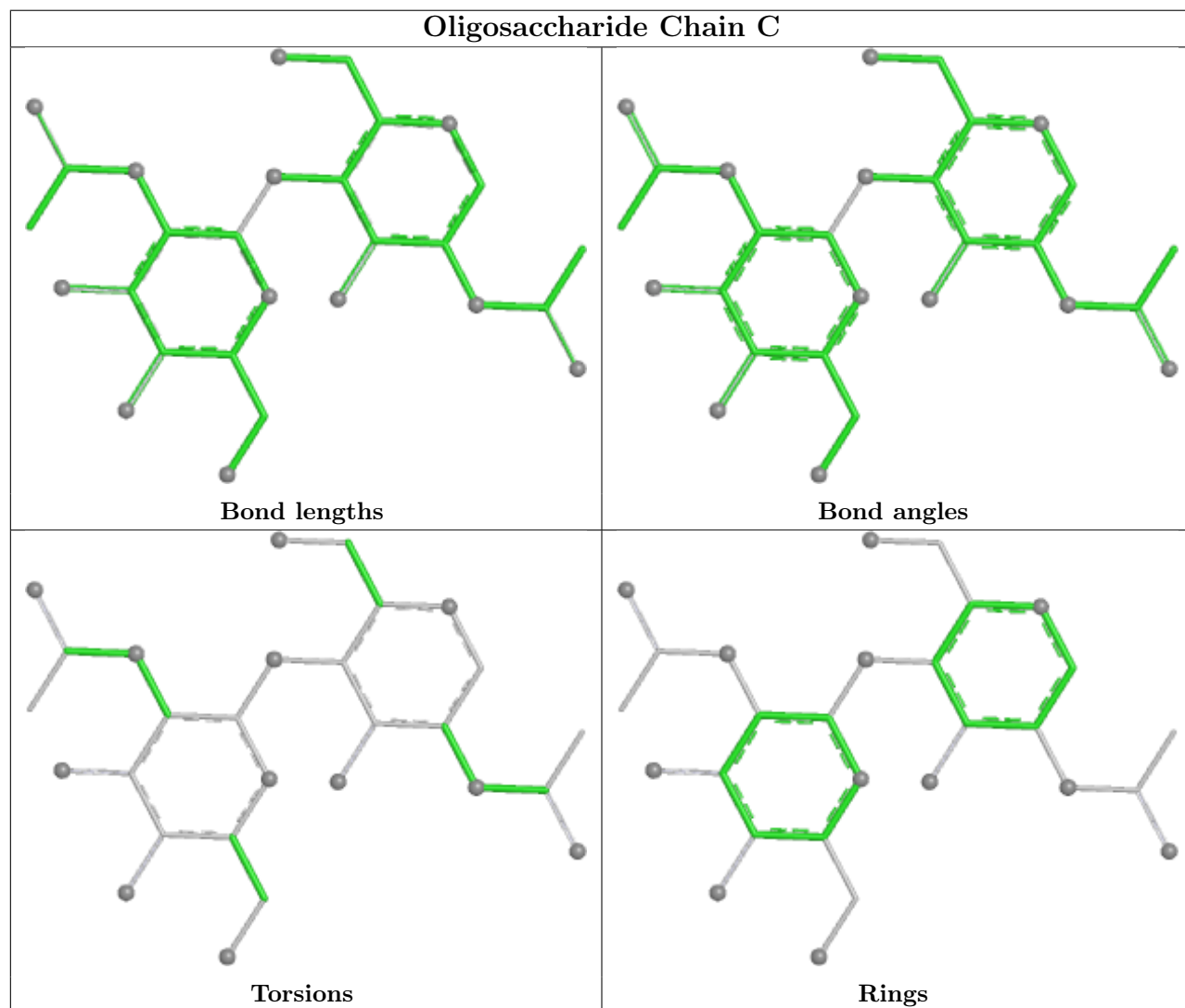
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	4	0
3	C	1	NAG	8	0
4	H	2	NDG	4	0
3	C	2	NAG	8	0
4	I	1	NAG	3	0
3	E	1	NAG	2	0

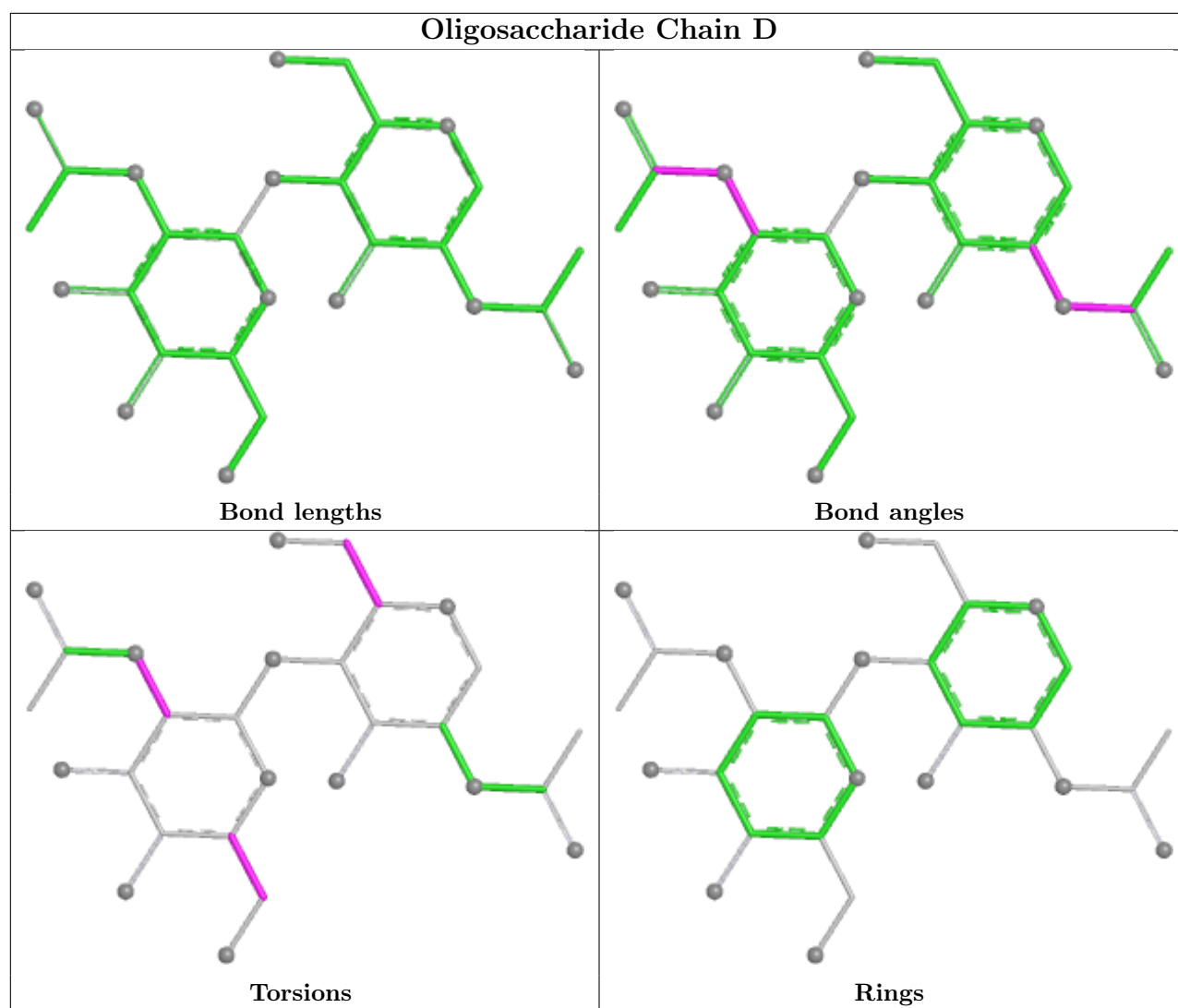
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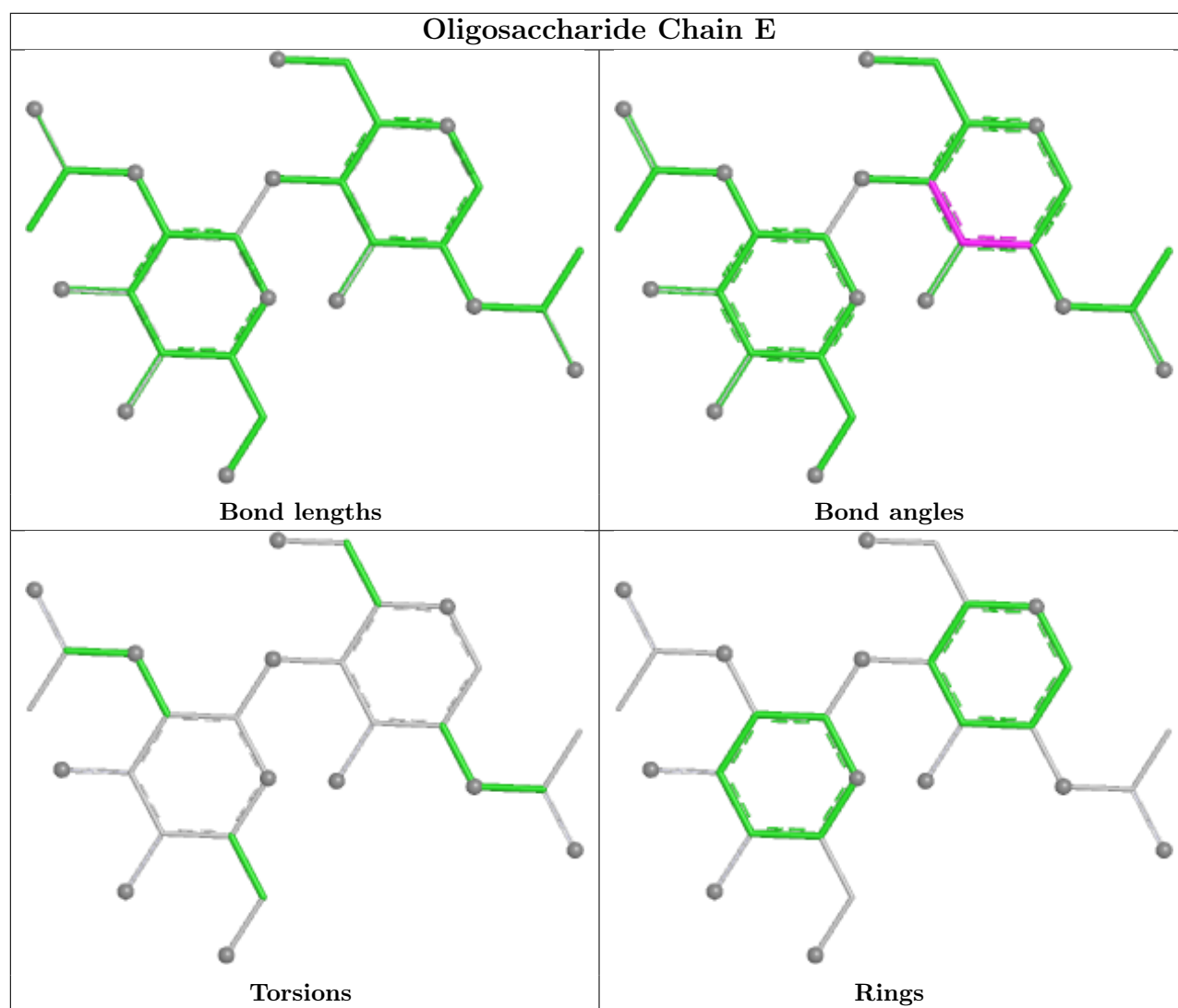
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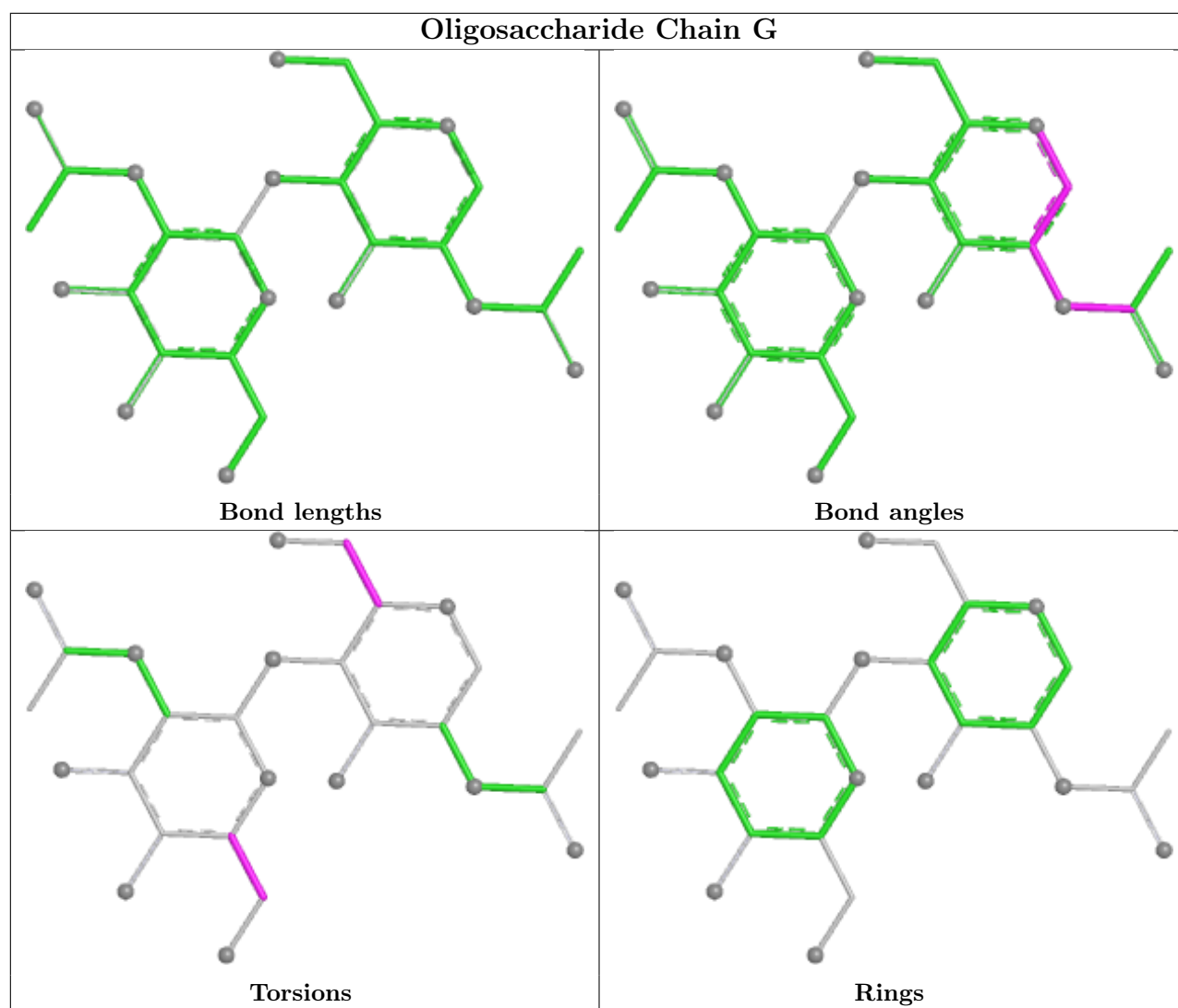
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
3	G	2	NAG	1	0
3	E	2	NAG	1	0
4	I	2	NDG	2	0

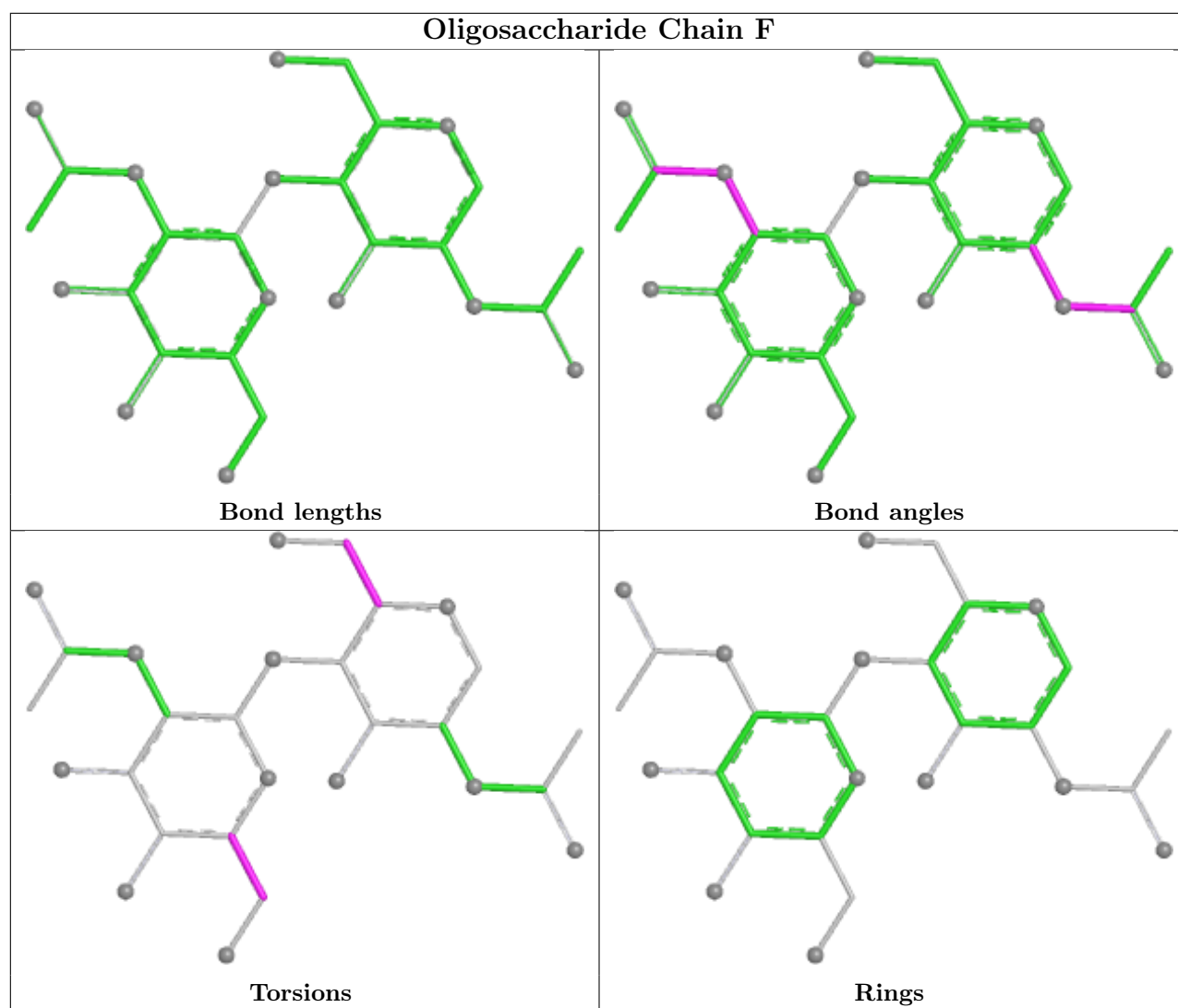
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

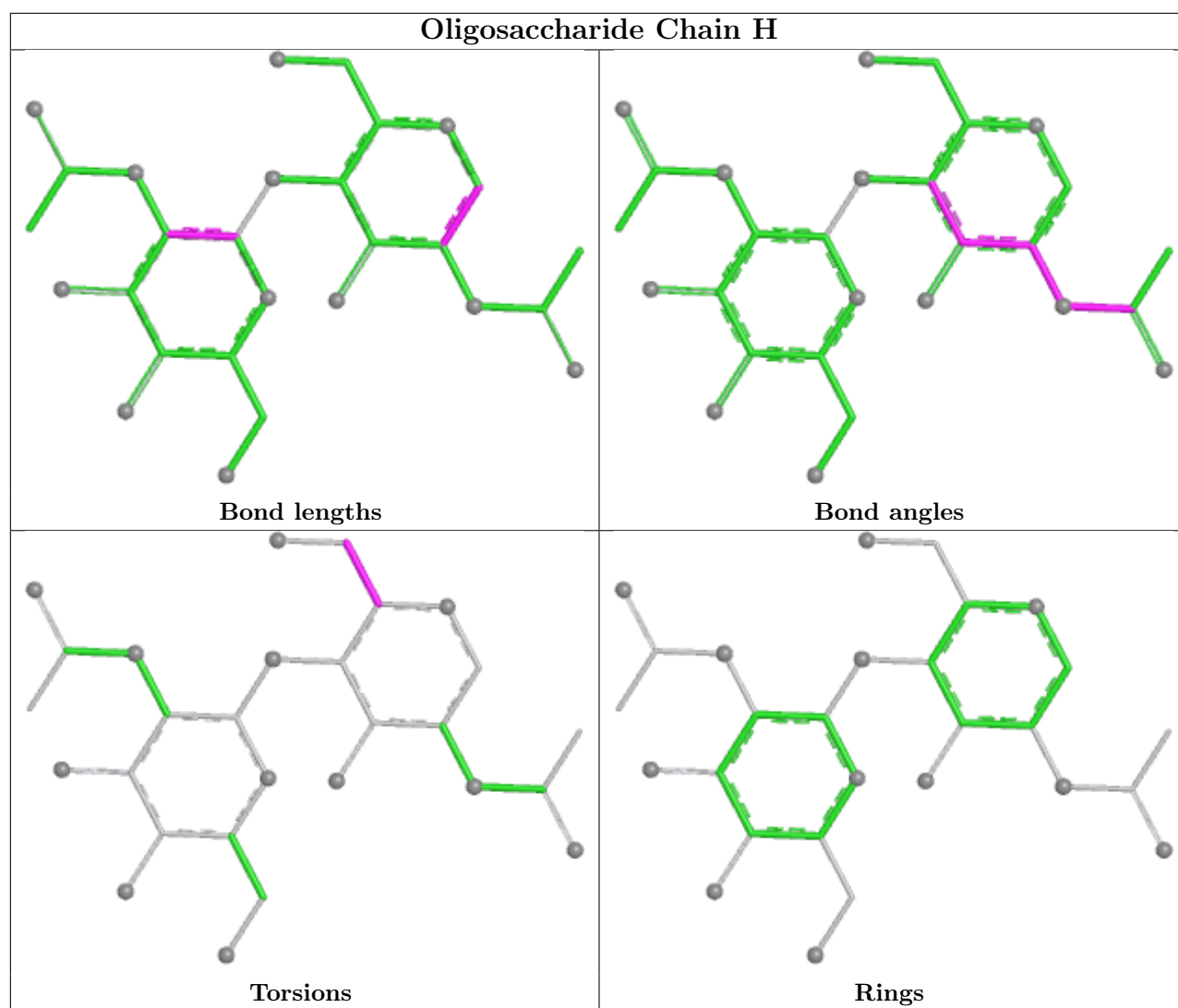


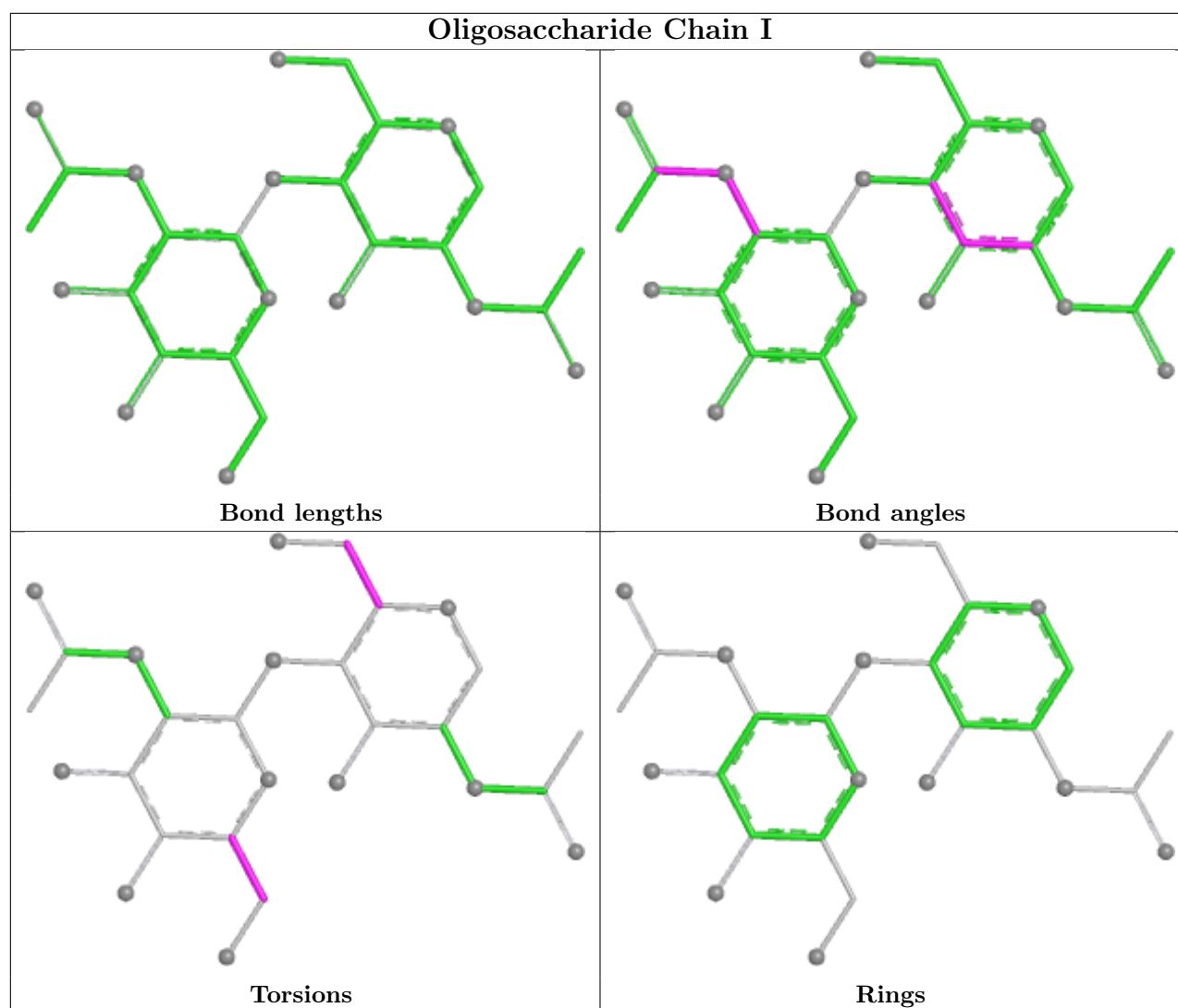












5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	2821	1	14,14,15	0.71	0	17,19,21	0.70	0
5	NAG	A	2458	1	14,14,15	0.71	0	17,19,21	0.64	0
5	NAG	B	3371	2	14,14,15	0.75	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	2260	1	14,14,15	0.64	0	17,19,21	0.84	0
5	NAG	B	3320	2	14,14,15	0.87	0	17,19,21	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2821	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	1/6/23/26	0/1/1/1
5	NAG	B	3371	2	-	2/6/23/26	0/1/1/1
5	NAG	B	3320	2	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	A	2260	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3371	NAG	C2-N2-C7	-2.37	119.72	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2821	NAG	C1
5	B	3320	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2260	NAG	C3-C2-N2-C7
5	A	2458	NAG	C3-C2-N2-C7
5	A	2260	NAG	C4-C5-C6-O6
5	A	2821	NAG	O5-C5-C6-O6
5	B	3371	NAG	O5-C5-C6-O6
5	A	2260	NAG	O5-C5-C6-O6
5	B	3371	NAG	C4-C5-C6-O6
5	A	2821	NAG	C4-C5-C6-O6
5	B	3320	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2458	NAG	5	0
5	B	3371	NAG	2	0
5	A	2260	NAG	4	0
5	B	3320	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.