Full wwPDB X-ray Structure Validation Report (i)

Sep 29, 2024 – 02:16 AM EDT

PDB ID	:	1JV2
Title	:	CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN ALPHAVBETA3
Authors	:	Xiong, J.P.; Stehle, T.; Diefenbach, B.; Zhang, R.; Dunker, R.; Scott, D.; Joachimiak, A.; Goodman, S.L.; Arnaout, M.A.
Deposited on	:	2001-08-28
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 (i) 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 (i)) were used in the production of this report:

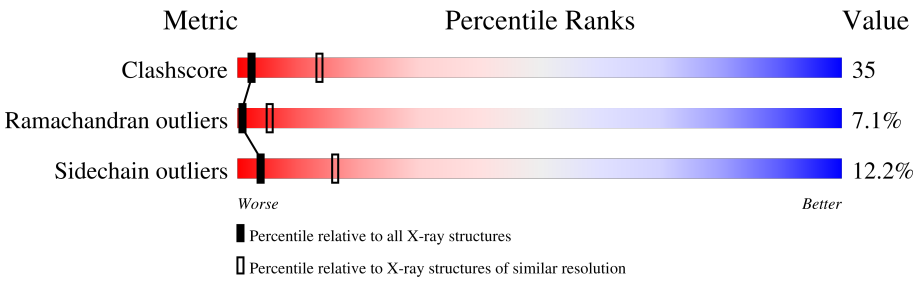
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	44% 44% 8% • •
2	B	692	32% 36% 10% • 22%
3	C	2	100%
3	D	2	100%
3	E	2	50% 50%
3	G	2	100%
4	F	2	50% 50%
4	H	2	50% 50%

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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
4	NDG	I	2	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11656 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
			Total	C	N	O	S			
1	A	927	7216	4568	1224	1389	35	0	0	0

- Molecule 2 is a protein called PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	539	4182	2594	700	842	46	0	0	0

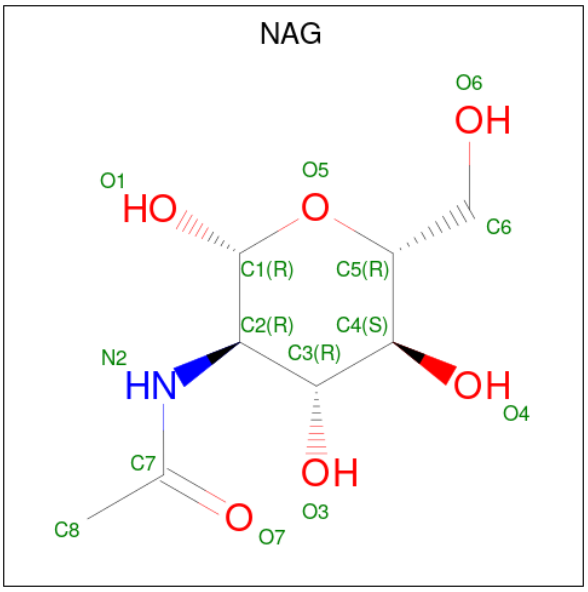
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- 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
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	H	2	28	16	2	10	0	0	0
			Total	C	N	O			
4	I	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0

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

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

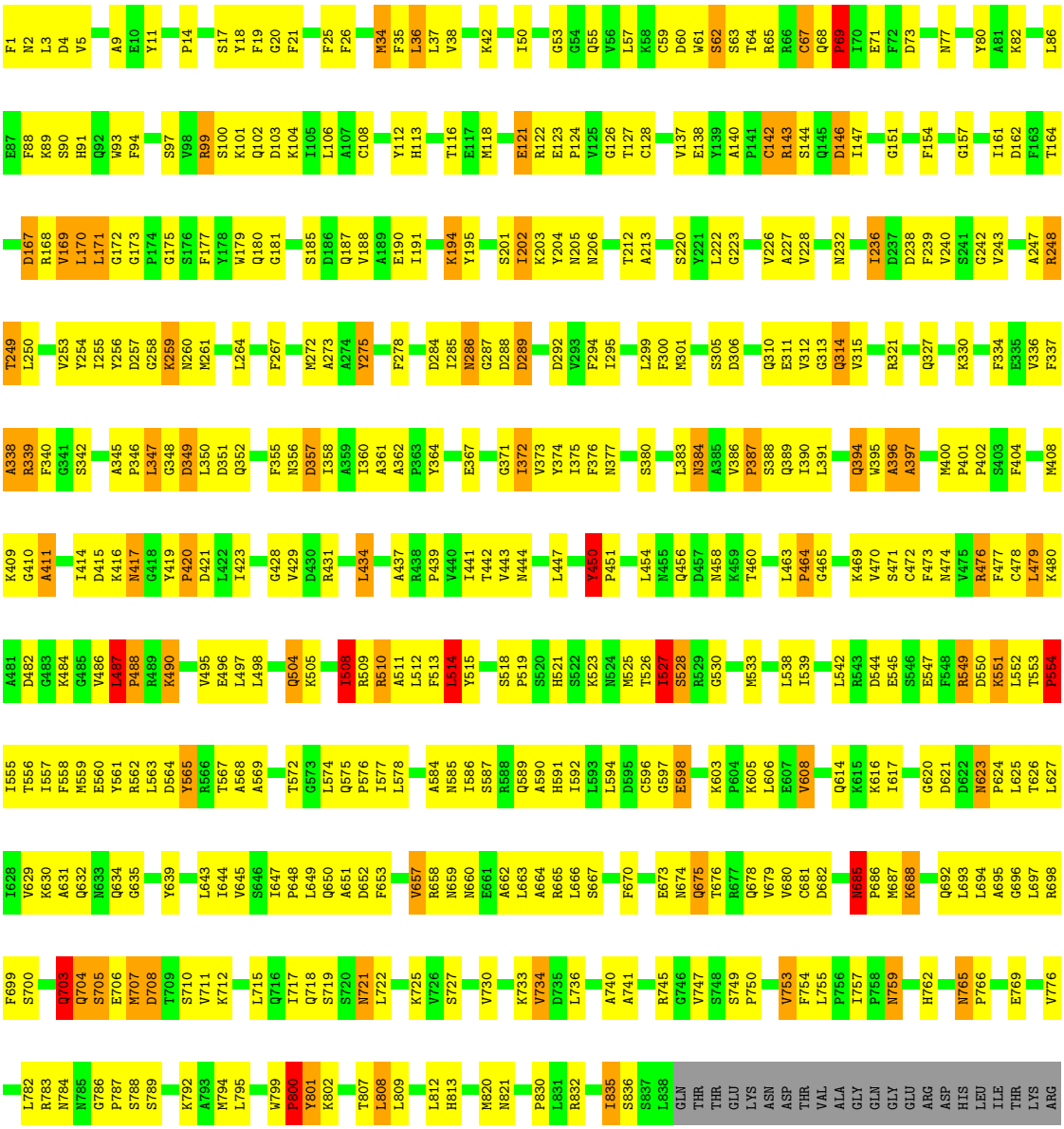
3 Residue-property plots (i)

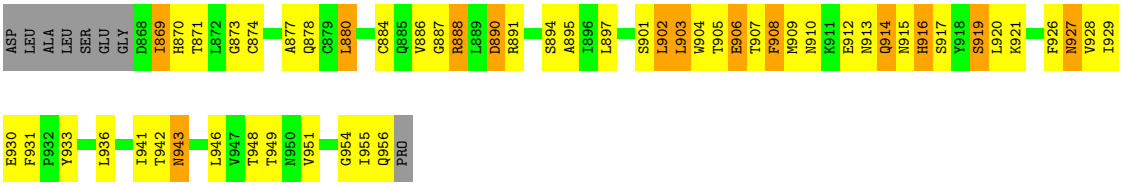
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

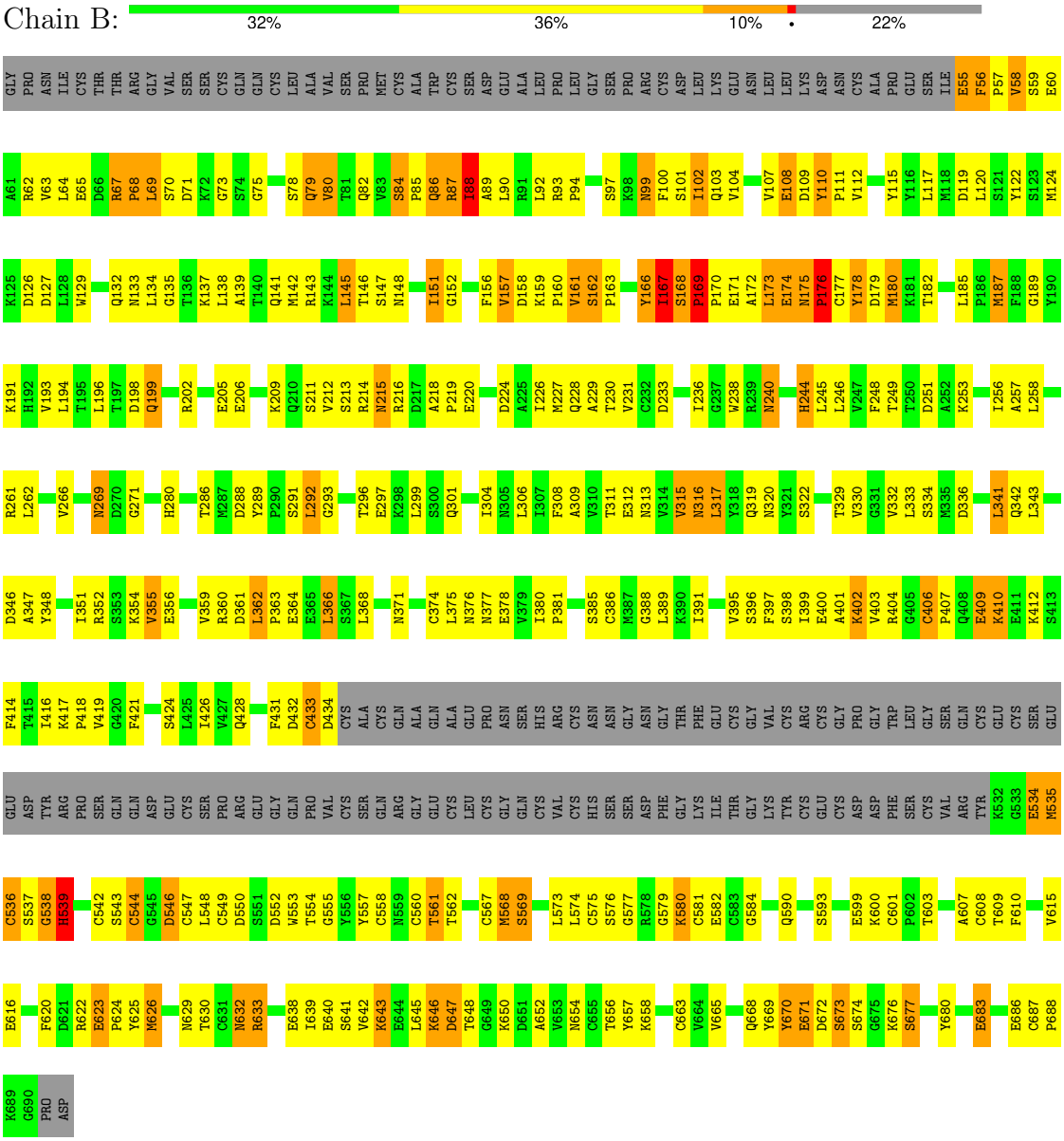
Chain A: 44% 44% 8% • •





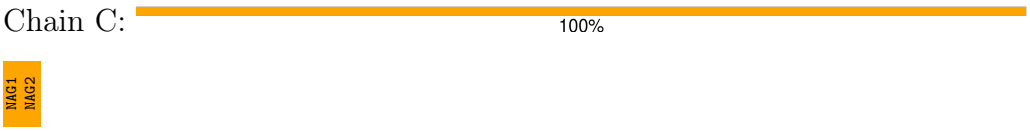
• Molecule 2: PLATELET MEMBRANE GLYCOPROTEIN IIIA BETA SUBUNIT

Chain B:



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

Chain C:



• 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: 100%

NAG1 NAG2

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

Chain F: 50% 50%

NAG1 NDG2

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

Chain H: 50% 50%

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 (i)

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	X-PLOR 3.851	Depositor
R, R_{free}	0.255 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11656	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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	0.48	0/7372	0.80	12/9994 (0.1%)
2	B	0.48	0/4256	0.79	6/5754 (0.1%)
All	All	0.48	0/11628	0.79	18/15748 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	912	GLU	N-CA-C	8.62	134.26	111.00
1	A	703	GLN	N-CA-C	7.21	130.47	111.00
2	B	378	GLU	N-CA-C	-6.11	94.52	111.00
2	B	169	PRO	C-N-CD	5.90	140.79	128.40
1	A	687	MET	N-CA-C	-5.89	95.10	111.00
1	A	685	ASN	C-N-CD	5.81	140.60	128.40
1	A	954	GLY	N-CA-C	5.59	127.08	113.10
1	A	808	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	800	PRO	N-CA-C	-5.53	97.72	112.10
2	B	538	GLY	N-CA-C	-5.47	99.44	113.10
2	B	64	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	880	LEU	N-CA-C	-5.44	96.31	111.00
1	A	338	ALA	N-CA-C	-5.37	96.50	111.00
1	A	450	TYR	C-N-CD	5.35	139.64	128.40
1	A	755	LEU	N-CA-C	5.28	125.26	111.00
2	B	180	MET	N-CA-C	-5.27	96.77	111.00
2	B	590	GLN	N-CA-C	5.11	124.81	111.00
1	A	67	CYS	CA-CB-SG	5.08	123.14	114.00

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	7036	492	0
2	B	4182	0	4030	308	0
3	C	28	0	25	3	0
3	D	28	0	25	3	0
3	E	28	0	25	3	0
3	G	28	0	25	1	0
4	F	28	0	24	7	0
4	H	28	0	24	3	0
4	I	28	0	24	10	0
5	A	28	0	26	8	0
5	B	28	0	26	5	0
6	A	5	0	0	0	0
6	B	1	0	0	0	0
All	All	11656	0	11290	800	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 35.

All (800) 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)
4:F:2:NDG:H2	4:F:2:NDG:H6C2	1.19	1.12
1:A:585:ASN:HD22	3:E:1:NAG:H62	1.13	1.10
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.34	1.08
1:A:127:THR:HG22	1:A:140:ALA:HB2	1.39	1.03
2:B:648:THR:HA	4:I:2:NDG:C1	1.89	1.02
2:B:646:LYS:O	4:I:2:NDG:H8C3	1.63	0.98
1:A:808:LEU:HD13	1:A:920:LEU:HD22	1.46	0.98
2:B:94:PRO:HD3	2:B:433:CYS:HB3	1.44	0.98
1:A:749:SER:HB3	1:A:750:PRO:HD3	1.47	0.97
2:B:167:ILE:HD11	2:B:216:ARG:HE	1.29	0.97
2:B:371:ASN:ND2	5:B:3371:NAG:H62	1.78	0.96
4:F:1:NAG:H61	4:F:1:NAG:H2	1.47	0.96
1:A:458:ASN:HD22	5:A:2458:NAG:H4	1.31	0.95
1:A:585:ASN:ND2	3:E:1:NAG:H62	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HG22	1:A:951:VAL:HG12	1.44	0.95
1:A:463:LEU:HG	1:A:464:PRO:HD2	1.46	0.94
1:A:59:CYS:HA	1:A:67:CYS:HB2	1.49	0.94
2:B:138:LEU:HD23	2:B:151:ILE:HD11	1.49	0.94
2:B:648:THR:HG22	4:I:2:NDG:H2	1.48	0.93
2:B:371:ASN:HD22	5:B:3371:NAG:H62	1.35	0.92
2:B:672:ASP:H	2:B:676:LYS:HB3	1.35	0.91
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.51	0.91
2:B:403:VAL:HG11	2:B:431:PHE:HE2	1.36	0.91
1:A:286:ASN:H	1:A:286:ASN:HD22	1.18	0.90
2:B:639:ILE:H	2:B:639:ILE:HD12	1.34	0.90
1:A:259:LYS:HE3	1:A:259:LYS:HA	1.50	0.90
1:A:585:ASN:HD22	3:E:1:NAG:C6	1.82	0.90
1:A:835:ILE:HG12	1:A:836:SER:H	1.35	0.89
1:A:439:PRO:HB3	1:A:487:LEU:HD22	1.55	0.88
2:B:169:PRO:HB2	2:B:170:PRO:CD	2.04	0.88
2:B:110:TYR:HD1	2:B:111:PRO:HD2	1.36	0.87
2:B:403:VAL:HG11	2:B:431:PHE:CE2	2.09	0.87
1:A:869:ILE:HG23	1:A:870:HIS:H	1.38	0.87
4:F:2:NDG:H6C2	4:F:2:NDG:C2	2.02	0.86
1:A:556:THR:HG22	1:A:589:GLN:HG2	1.58	0.86
1:A:260:ASN:HD22	5:A:2260:NAG:H61	1.40	0.86
1:A:339:ARG:O	1:A:362:ALA:HA	1.76	0.85
2:B:84:SER:OG	2:B:85:PRO:HD3	1.75	0.85
2:B:57:PRO:HA	2:B:93:ARG:NH2	1.91	0.85
1:A:236:ILE:HD12	1:A:236:ILE:H	1.42	0.84
2:B:642:VAL:HG11	2:B:646:LYS:HA	1.59	0.84
1:A:745:ARG:HB3	2:B:603:THR:HG21	1.58	0.83
1:A:921:LYS:HD2	1:A:946:LEU:HD12	1.59	0.83
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.14	0.83
2:B:366:LEU:HB3	2:B:403:VAL:HG12	1.61	0.82
2:B:212:VAL:HG12	2:B:213:SER:H	1.44	0.81
1:A:667:SER:HA	2:B:535:MET:SD	2.20	0.81
1:A:508:ILE:HD12	1:A:508:ILE:H	1.47	0.80
1:A:106:LEU:HD11	1:A:128:CYS:HB3	1.62	0.80
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.62	0.80
1:A:515:TYR:HE1	1:A:539:ILE:HD13	1.46	0.80
2:B:88:ILE:HD13	2:B:89:ALA:N	1.97	0.80
1:A:487:LEU:HG	1:A:488:PRO:HD3	1.62	0.79
1:A:620:GLY:H	1:A:703:GLN:HB2	1.45	0.79
2:B:168:SER:H	2:B:169:PRO:HD3	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD21	1:A:350:LEU:HD13	1.65	0.78
2:B:169:PRO:HB2	2:B:170:PRO:HD2	1.65	0.78
1:A:59:CYS:HA	1:A:67:CYS:CB	2.14	0.78
1:A:550:ASP:H	1:A:551:LYS:NZ	1.81	0.78
1:A:605:LYS:HD2	1:A:634:GLN:HB3	1.66	0.78
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.63	0.78
1:A:474:ASN:HD21	1:A:539:ILE:HG13	1.46	0.78
1:A:711:VAL:HG23	1:A:736:LEU:HD11	1.65	0.78
2:B:173:LEU:HA	2:B:176:PRO:HD2	1.63	0.78
2:B:652:ALA:HB1	2:B:669:TYR:O	1.84	0.77
1:A:168:ARG:HG2	1:A:168:ARG:HH11	1.49	0.77
1:A:469:LYS:H	1:A:469:LYS:HD3	1.49	0.77
1:A:80:TYR:HB2	1:A:86:LEU:HD23	1.66	0.77
1:A:710:SER:HA	1:A:736:LEU:HD13	1.65	0.77
2:B:391:ILE:HD12	2:B:391:ILE:H	1.48	0.77
1:A:2:ASN:HD22	1:A:577:ILE:HD13	1.49	0.76
1:A:608:VAL:HG13	1:A:717:ILE:HD11	1.66	0.76
1:A:77:ASN:HD21	1:A:89:LYS:N	1.83	0.76
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.68	0.76
4:F:1:NAG:H2	4:F:1:NAG:C6	2.15	0.76
1:A:338:ALA:HA	1:A:364:TYR:HB2	1.66	0.76
1:A:657:VAL:HG13	1:A:698:ARG:HE	1.51	0.76
1:A:712:LYS:HA	1:A:733:LYS:HA	1.66	0.75
1:A:112:TYR:HB3	1:A:126:GLY:HA2	1.66	0.75
1:A:300:PHE:HB3	1:A:313:GLY:HA2	1.68	0.75
1:A:789:SER:HB3	1:A:890:ASP:HA	1.68	0.75
2:B:71:ASP:HB3	2:B:108:GLU:HB2	1.67	0.75
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.69	0.74
1:A:248:ARG:NH1	1:A:248:ARG:HB2	2.03	0.74
1:A:820:MET:HG3	1:A:886:VAL:HG22	1.68	0.74
1:A:286:ASN:HD22	1:A:286:ASN:N	1.82	0.74
2:B:639:ILE:HG22	2:B:640:GLU:H	1.51	0.74
1:A:334:PHE:HE1	1:A:387:PRO:HG2	1.52	0.73
2:B:643:LYS:HD3	2:B:643:LYS:H	1.53	0.73
1:A:450:TYR:HD1	1:A:474:ASN:HB2	1.53	0.73
2:B:167:ILE:HD11	2:B:216:ARG:NE	2.04	0.73
1:A:946:LEU:H	1:A:946:LEU:HD23	1.54	0.72
2:B:194:LEU:HB2	2:B:206:GLU:HG3	1.70	0.72
2:B:160:PRO:HA	2:B:187:MET:HG2	1.71	0.72
2:B:567:CYS:SG	2:B:584:GLY:O	2.48	0.72
1:A:349:ASP:H	1:A:420:PRO:HG2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.26	0.71
1:A:260:ASN:HD22	5:A:2260:NAG:C6	2.02	0.71
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.19	0.71
2:B:93:ARG:HA	2:B:432:ASP:O	1.89	0.71
2:B:399:ILE:HD13	2:B:416:ILE:HD13	1.71	0.71
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.72	0.71
2:B:119:ASP:O	2:B:124:MET:HG3	1.90	0.71
2:B:230:THR:HG23	2:B:304:ILE:HG13	1.71	0.71
2:B:359:VAL:HG12	2:B:360:ARG:H	1.55	0.71
2:B:73:GLY:HA3	2:B:109:ASP:O	1.91	0.71
2:B:166:TYR:CZ	2:B:216:ARG:HG3	2.26	0.71
1:A:77:ASN:HD21	1:A:89:LYS:H	1.39	0.70
1:A:550:ASP:H	1:A:551:LYS:HZ1	1.37	0.70
1:A:927:ASN:HD22	1:A:928:VAL:N	1.89	0.70
2:B:56:PHE:CD2	2:B:56:PHE:N	2.58	0.70
1:A:180:GLN:HE22	1:A:213:ALA:HB3	1.56	0.70
1:A:740:ALA:HA	1:A:786:GLY:HA3	1.74	0.69
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.73	0.69
2:B:56:PHE:N	2:B:56:PHE:HD2	1.90	0.69
1:A:620:GLY:C	1:A:891:ARG:HH12	1.96	0.69
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.75	0.69
2:B:212:VAL:HG12	2:B:213:SER:N	2.06	0.69
1:A:59:CYS:CA	1:A:67:CYS:HB2	2.23	0.69
2:B:361:ASP:O	2:B:362:LEU:HB3	1.91	0.69
2:B:639:ILE:HD12	2:B:639:ILE:N	2.08	0.69
2:B:309:ALA:HB1	2:B:333:LEU:HD13	1.73	0.68
2:B:187:MET:HE2	2:B:187:MET:HA	1.76	0.68
1:A:458:ASN:HD22	5:A:2458:NAG:C4	2.06	0.68
2:B:157:VAL:HG13	2:B:158:ASP:H	1.59	0.68
2:B:58:VAL:CG1	2:B:93:ARG:H	2.07	0.67
2:B:58:VAL:HG12	2:B:93:ARG:H	1.59	0.67
2:B:650:LYS:HG2	4:I:1:NAG:H62	1.76	0.67
1:A:260:ASN:ND2	5:A:2260:NAG:C6	2.57	0.67
2:B:99:ASN:HD22	2:B:99:ASN:H	1.42	0.67
2:B:88:ILE:HD13	2:B:89:ALA:H	1.60	0.67
2:B:87:ARG:HH12	2:B:428:GLN:CD	1.98	0.67
2:B:371:ASN:HD22	5:B:3371:NAG:C6	2.05	0.67
1:A:417:ASN:HA	1:A:486:VAL:HG23	1.77	0.66
1:A:706:GLU:C	1:A:708:ASP:H	1.98	0.66
2:B:122:TYR:HA	2:B:212:VAL:HG11	1.76	0.66
2:B:185:LEU:CD1	2:B:211:SER:HB3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.77	0.66
2:B:168:SER:N	2:B:169:PRO:HD3	2.09	0.66
2:B:187:MET:HA	2:B:187:MET:CE	2.25	0.66
4:H:1:NAG:O6	4:H:2:NDG:C1	2.44	0.66
1:A:423:ILE:HG12	1:A:434:LEU:CD2	2.25	0.66
2:B:111:PRO:HA	2:B:146:THR:HG21	1.77	0.66
2:B:375:LEU:HD13	2:B:630:THR:HG22	1.76	0.66
1:A:377:ASN:O	1:A:383:LEU:HD12	1.96	0.66
1:A:552:LEU:HD11	1:A:592:ILE:H	1.59	0.66
1:A:487:LEU:HG	1:A:488:PRO:CD	2.26	0.66
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.77	0.66
2:B:399:ILE:HG22	2:B:400:GLU:H	1.59	0.66
1:A:375:ILE:HG12	1:A:389:GLN:HB3	1.78	0.66
1:A:624:PRO:HG2	4:H:2:NDG:H3	1.77	0.65
1:A:68:GLN:HB3	1:A:69:PRO:HD2	1.77	0.65
2:B:354:LYS:HA	2:B:386:CYS:O	1.95	0.65
1:A:605:LYS:H	1:A:635:GLY:H	1.44	0.65
1:A:25:PHE:HE1	1:A:410:GLY:HA2	1.61	0.65
1:A:474:ASN:ND2	1:A:539:ILE:HG13	2.10	0.65
2:B:347:ALA:O	2:B:351:ILE:HG12	1.96	0.65
1:A:164:THR:HG22	1:A:228:VAL:HG21	1.78	0.65
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.77	0.65
3:G:1:NAG:H61	3:G:2:NAG:O5	1.97	0.65
1:A:515:TYR:CE1	1:A:539:ILE:HD13	2.30	0.65
1:A:835:ILE:HG12	1:A:836:SER:N	2.11	0.65
2:B:657:TYR:CE2	2:B:665:VAL:HB	2.31	0.65
4:F:1:NAG:C6	4:F:1:NAG:C2	2.72	0.65
1:A:510:ARG:NH1	1:A:555:ILE:HG12	2.11	0.64
1:A:544:ASP:O	1:A:547:GLU:HG2	1.97	0.64
2:B:639:ILE:H	2:B:639:ILE:CD1	2.09	0.64
2:B:670:TYR:HD1	2:B:671:GLU:H	1.43	0.64
1:A:458:ASN:ND2	5:A:2458:NAG:C4	2.61	0.64
2:B:58:VAL:HG22	2:B:93:ARG:HH21	1.63	0.64
1:A:539:ILE:N	1:A:539:ILE:HD12	2.11	0.64
2:B:417:LYS:HB3	2:B:424:SER:CB	2.27	0.64
1:A:906:GLU:C	1:A:908:PHE:H	2.01	0.64
1:A:1:PHE:HB2	1:A:388:SER:HB3	1.79	0.64
1:A:562:ARG:HB3	1:A:562:ARG:NH1	2.12	0.64
1:A:450:TYR:CD1	1:A:474:ASN:HB2	2.32	0.63
1:A:914:GLN:HB3	1:A:916:HIS:ND1	2.12	0.63
2:B:623:GLU:HB3	2:B:624:PRO:HD2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:TYR:HD1	1:A:390:ILE:HG22	1.63	0.63
1:A:463:LEU:CG	1:A:464:PRO:HD2	2.25	0.63
1:A:783:ARG:HB2	1:A:894:SER:HB3	1.80	0.63
1:A:248:ARG:HB2	1:A:248:ARG:HH11	1.63	0.63
4:F:2:NDG:H2	4:F:2:NDG:C6	2.03	0.63
1:A:707:MET:HG3	1:A:707:MET:O	1.98	0.62
2:B:168:SER:H	2:B:169:PRO:CD	2.10	0.62
2:B:534:GLU:HG2	2:B:544:CYS:SG	2.38	0.62
1:A:42:LYS:NZ	1:A:93:TRP:HE1	1.98	0.62
2:B:672:ASP:N	2:B:676:LYS:HB3	2.12	0.62
1:A:549:ARG:HG3	1:A:551:LYS:HZ1	1.64	0.62
1:A:802:LYS:O	1:A:877:ALA:HB1	2.00	0.62
1:A:222:LEU:HD12	1:A:223:GLY:N	2.14	0.62
1:A:254:TYR:OH	3:D:1:NAG:H62	2.00	0.62
1:A:539:ILE:HD12	1:A:539:ILE:H	1.64	0.61
1:A:741:ALA:H	1:A:786:GLY:HA3	1.63	0.61
2:B:308:PHE:HB2	2:B:330:VAL:HG12	1.81	0.61
2:B:312:GLU:HA	2:B:315:VAL:CG2	2.30	0.61
2:B:537:SER:HB2	2:B:539:HIS:H	1.64	0.61
1:A:645:VAL:HB	1:A:679:VAL:HB	1.82	0.61
1:A:820:MET:HE2	1:A:895:ALA:HB1	1.81	0.61
2:B:639:ILE:HG22	2:B:640:GLU:N	2.14	0.61
2:B:111:PRO:HA	2:B:146:THR:CG2	2.31	0.61
2:B:97:SER:HB3	2:B:402:LYS:HG3	1.82	0.61
2:B:167:ILE:CD1	2:B:216:ARG:HE	2.10	0.61
2:B:151:ILE:O	2:B:196:LEU:HA	2.00	0.61
1:A:704:GLN:HG2	1:A:707:MET:SD	2.41	0.61
2:B:129:TRP:O	2:B:132:GLN:HG2	2.00	0.61
2:B:87:ARG:HH12	2:B:428:GLN:NE2	1.99	0.60
1:A:647:ILE:HD11	1:A:670:PHE:HE2	1.66	0.60
1:A:753:VAL:CG2	1:A:951:VAL:HG12	2.25	0.60
2:B:375:LEU:HD11	2:B:633:ARG:HB3	1.83	0.60
2:B:214:ARG:HG3	2:B:214:ARG:HH11	1.65	0.60
1:A:626:THR:HG22	1:A:698:ARG:HB3	1.84	0.60
2:B:134:LEU:HG	2:B:135:GLY:H	1.66	0.60
2:B:170:PRO:HD2	2:B:173:LEU:HD12	1.83	0.60
1:A:232:ASN:HB2	1:A:264:LEU:HD21	1.83	0.60
2:B:249:THR:HA	2:B:309:ALA:O	2.01	0.60
1:A:549:ARG:HG3	1:A:551:LYS:NZ	2.16	0.60
1:A:562:ARG:HB3	1:A:562:ARG:HH11	1.66	0.60
1:A:314:GLN:NE2	1:A:330:LYS:HG2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HB3	1:A:250:LEU:HB2	1.84	0.59
1:A:787:PRO:HA	1:A:891:ARG:HH11	1.67	0.59
2:B:87:ARG:O	2:B:88:ILE:HB	2.01	0.59
1:A:625:LEU:HD21	1:A:734:VAL:HG21	1.83	0.59
2:B:399:ILE:HG22	2:B:400:GLU:N	2.17	0.59
1:A:222:LEU:HD12	1:A:223:GLY:H	1.66	0.59
2:B:269:ASN:HD22	2:B:271:GLY:H	1.49	0.59
2:B:668:GLN:HE21	2:B:670:TYR:HD2	1.50	0.59
1:A:203:LYS:HD2	1:A:203:LYS:H	1.66	0.59
1:A:168:ARG:HH11	1:A:168:ARG:CG	2.15	0.59
1:A:458:ASN:ND2	5:A:2458:NAG:H4	2.06	0.59
1:A:608:VAL:O	1:A:730:VAL:HG21	2.03	0.59
1:A:563:LEU:HG	1:A:564:ASP:H	1.68	0.59
1:A:809:LEU:HG	1:A:920:LEU:HD13	1.85	0.59
2:B:406:CYS:HB2	2:B:431:PHE:HB3	1.85	0.59
1:A:629:VAL:O	1:A:694:LEU:HD12	2.03	0.59
1:A:869:ILE:HG23	1:A:870:HIS:N	2.15	0.59
1:A:902:LEU:HD23	1:A:902:LEU:O	2.02	0.59
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.32	0.58
1:A:170:LEU:HG	1:A:239:PHE:CD2	2.38	0.58
1:A:239:PHE:CZ	1:A:258:GLY:HA2	2.38	0.58
1:A:903:LEU:HD22	1:A:905:THR:H	1.68	0.58
1:A:127:THR:HG22	1:A:140:ALA:CB	2.24	0.58
2:B:670:TYR:HB3	2:B:676:LYS:HE2	1.85	0.58
1:A:248:ARG:HD3	1:A:248:ARG:N	2.17	0.58
1:A:608:VAL:HA	1:A:630:LYS:O	2.03	0.58
1:A:749:SER:HB3	1:A:750:PRO:CD	2.29	0.58
2:B:104:VAL:HG21	2:B:418:PRO:HG2	1.84	0.58
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.85	0.58
1:A:349:ASP:HB3	1:A:352:GLN:H	1.67	0.58
1:A:621:ASP:N	1:A:891:ARG:HH12	2.02	0.58
1:A:629:VAL:O	1:A:694:LEU:HA	2.03	0.58
1:A:644:ILE:HD13	1:A:680:VAL:HG22	1.85	0.58
1:A:97:SER:HB2	1:A:161:ILE:HG12	1.84	0.58
2:B:616:GLU:HG2	2:B:657:TYR:OH	2.04	0.58
1:A:456:GLN:NE2	1:A:545:GLU:HG3	2.19	0.58
1:A:789:SER:CB	1:A:890:ASP:HA	2.32	0.58
1:A:951:VAL:O	1:A:951:VAL:HG23	2.04	0.58
2:B:426:ILE:HD12	2:B:426:ILE:N	2.19	0.57
2:B:668:GLN:NE2	2:B:670:TYR:HD2	2.02	0.57
1:A:180:GLN:NE2	1:A:213:ALA:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:O	1:A:191:ILE:HG13	2.04	0.57
1:A:478:CYS:SG	1:A:533:MET:HB2	2.45	0.57
1:A:549:ARG:HE	1:A:549:ARG:HA	1.68	0.57
1:A:653:PHE:HA	1:A:699:PHE:HD1	1.68	0.57
2:B:359:VAL:HG12	2:B:360:ARG:N	2.19	0.57
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.87	0.57
1:A:666:LEU:O	2:B:535:MET:SD	2.63	0.57
1:A:349:ASP:C	1:A:351:ASP:H	2.06	0.57
1:A:443:VAL:HG23	1:A:480:LYS:O	2.05	0.57
1:A:177:PHE:CD1	1:A:212:THR:HA	2.40	0.57
2:B:397:PHE:O	2:B:398:SER:HB3	2.03	0.57
1:A:2:ASN:HD22	1:A:577:ILE:CD1	2.16	0.57
2:B:231:VAL:HG11	2:B:271:GLY:O	2.05	0.57
1:A:334:PHE:CE1	1:A:387:PRO:HG2	2.38	0.57
1:A:873:GLY:HA3	1:A:921:LYS:HB3	1.86	0.57
2:B:97:SER:HB3	2:B:402:LYS:CG	2.34	0.57
1:A:88:PHE:CE1	1:A:122:ARG:HG2	2.40	0.56
1:A:621:ASP:OD1	1:A:787:PRO:HB3	2.05	0.56
1:A:657:VAL:CG1	1:A:698:ARG:HE	2.18	0.56
2:B:228:GLN:C	2:B:230:THR:H	2.09	0.56
2:B:539:HIS:O	2:B:542:CYS:HB3	2.06	0.56
1:A:53:GLY:O	1:A:94:PHE:HB3	2.05	0.56
1:A:914:GLN:HB3	1:A:916:HIS:CE1	2.40	0.56
2:B:171:GLU:C	2:B:173:LEU:H	2.09	0.56
2:B:205:GLU:HG3	2:B:209:LYS:NZ	2.21	0.56
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.87	0.56
1:A:703:GLN:O	1:A:705:SER:N	2.37	0.56
1:A:955:ILE:HD11	2:B:686:GLU:O	2.06	0.56
1:A:605:LYS:HD2	1:A:634:GLN:CB	2.33	0.56
1:A:617:ILE:HG13	1:A:617:ILE:O	2.06	0.56
1:A:942:THR:O	1:A:943:ASN:HB2	2.06	0.56
2:B:159:LYS:NZ	2:B:288:ASP:HA	2.21	0.56
2:B:168:SER:HA	2:B:174:GLU:OE2	2.05	0.56
1:A:464:PRO:HG2	1:A:465:GLY:H	1.70	0.55
2:B:647:ASP:HB3	2:B:668:GLN:HE22	1.71	0.55
2:B:84:SER:CB	2:B:85:PRO:HD3	2.35	0.55
2:B:93:ARG:HB2	2:B:94:PRO:HD2	1.87	0.55
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.88	0.55
1:A:286:ASN:N	1:A:286:ASN:ND2	2.52	0.55
1:A:350:LEU:HG	1:A:357:ASP:OD1	2.06	0.55
1:A:707:MET:HA	1:A:707:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:LEU:HD11	1:A:926:PHE:CD1	2.41	0.55
2:B:355:VAL:HG21	2:B:395:VAL:HG21	1.88	0.55
1:A:9:ALA:HB3	1:A:434:LEU:CB	2.36	0.55
1:A:57:LEU:N	1:A:57:LEU:HD12	2.22	0.55
1:A:417:ASN:HA	1:A:486:VAL:CG2	2.36	0.55
2:B:341:LEU:HD23	2:B:342:GLN:H	1.72	0.55
1:A:62:SER:O	1:A:64:THR:N	2.40	0.55
1:A:175:GLY:HA2	1:A:179:TRP:HA	1.89	0.55
2:B:244:HIS:O	2:B:245:LEU:HD12	2.06	0.55
1:A:137:VAL:HG12	1:A:195:TYR:CD1	2.42	0.55
1:A:498:LEU:HD12	1:A:558:PHE:CD2	2.42	0.55
1:A:514:LEU:HB2	1:A:539:ILE:HB	1.88	0.55
1:A:299:LEU:HD11	1:A:339:ARG:NH1	2.21	0.54
2:B:341:LEU:HD23	2:B:342:GLN:N	2.22	0.54
1:A:180:GLN:HE22	1:A:213:ALA:H	1.53	0.54
1:A:736:LEU:O	1:A:936:LEU:HD23	2.07	0.54
2:B:156:PHE:HB2	2:B:189:GLY:O	2.07	0.54
1:A:213:ALA:CB	3:D:2:NAG:H83	2.36	0.54
1:A:605:LYS:HB3	1:A:634:GLN:HB3	1.88	0.54
2:B:319:GLN:HG2	2:B:330:VAL:HG21	1.90	0.54
2:B:623:GLU:CB	2:B:624:PRO:HD2	2.37	0.54
1:A:557:ILE:N	1:A:557:ILE:HD12	2.23	0.54
1:A:450:TYR:CB	1:A:451:PRO:HD3	2.38	0.54
1:A:674:ASN:C	1:A:676:THR:H	2.11	0.54
1:A:511:ALA:HB2	1:A:555:ILE:HG21	1.89	0.54
1:A:345:ALA:HB2	1:A:408:MET:HG3	1.89	0.54
1:A:871:THR:HA	1:A:919:SER:HB2	1.89	0.54
2:B:141:GLN:HG3	2:B:341:LEU:HD11	1.89	0.54
1:A:124:PRO:HD2	1:A:154:PHE:CD2	2.42	0.54
2:B:568:MET:O	2:B:569:SER:HB3	2.06	0.54
1:A:647:ILE:HD12	1:A:651:ALA:HB3	1.90	0.54
1:A:61:TRP:HB2	1:A:414:ILE:HD11	1.90	0.54
2:B:348:TYR:CZ	2:B:352:ARG:HD2	2.42	0.53
2:B:388:GLY:O	2:B:633:ARG:HD3	2.06	0.53
1:A:157:GLY:HA2	1:A:172:GLY:O	2.08	0.53
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.91	0.53
1:A:660:ASN:HB3	1:A:663:LEU:HD12	1.90	0.53
2:B:62:ARG:HD2	2:B:85:PRO:HB3	1.90	0.53
1:A:627:LEU:HD12	1:A:699:PHE:HE2	1.74	0.53
1:A:451:PRO:HD2	1:A:473:PHE:HA	1.90	0.53
1:A:42:LYS:NZ	1:A:93:TRP:NE1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:HA	1:A:292:ASP:OD1	2.09	0.53
1:A:800:PRO:HB3	1:A:808:LEU:HD11	1.90	0.53
2:B:624:PRO:C	2:B:626:MET:H	2.12	0.53
5:B:3371:NAG:O7	5:B:3371:NAG:H3	2.08	0.53
1:A:239:PHE:N	1:A:256:TYR:O	2.40	0.53
1:A:477:PHE:CD2	1:A:477:PHE:N	2.77	0.53
2:B:624:PRO:O	2:B:625:TYR:HB2	2.09	0.53
2:B:645:LEU:HD23	2:B:645:LEU:H	1.74	0.53
1:A:255:ILE:O	1:A:264:LEU:HB2	2.09	0.53
1:A:375:ILE:O	1:A:375:ILE:HG13	2.09	0.53
1:A:3:LEU:CD2	1:A:350:LEU:HD22	2.39	0.52
1:A:169:VAL:O	1:A:185:SER:HA	2.08	0.52
2:B:152:GLY:N	2:B:196:LEU:HD23	2.25	0.52
1:A:220:SER:O	1:A:243:VAL:HG12	2.08	0.52
1:A:373:VAL:HG23	1:A:404:PHE:HE2	1.74	0.52
1:A:384:ASN:ND2	1:A:386:VAL:HG22	2.24	0.52
1:A:34:MET:HG3	1:A:414:ILE:HA	1.92	0.52
2:B:368:LEU:HG	2:B:399:ILE:CG2	2.39	0.52
1:A:19:PHE:CD1	1:A:431:ARG:HA	2.44	0.52
1:A:657:VAL:HG12	1:A:659:ASN:HD21	1.73	0.52
2:B:185:LEU:HD11	2:B:211:SER:HB3	1.91	0.52
2:B:557:TYR:O	2:B:558:CYS:HB2	2.10	0.52
1:A:99:ARG:HG3	1:A:162:ASP:HA	1.91	0.52
2:B:59:SER:O	2:B:90:LEU:HA	2.10	0.52
2:B:599:GLU:HG2	2:B:600:LYS:N	2.23	0.52
2:B:670:TYR:O	2:B:677:SER:HA	2.09	0.52
2:B:226:ILE:HD11	2:B:248:PHE:CD1	2.45	0.52
1:A:238:ASP:HB3	1:A:256:TYR:O	2.09	0.52
1:A:542:LEU:HD11	1:A:555:ILE:CD1	2.40	0.52
2:B:157:VAL:HG13	2:B:158:ASP:N	2.24	0.52
2:B:561:THR:HG22	2:B:562:THR:H	1.75	0.52
1:A:77:ASN:ND2	1:A:89:LYS:H	2.07	0.51
1:A:487:LEU:CG	1:A:488:PRO:HD3	2.35	0.51
1:A:542:LEU:HD11	1:A:555:ILE:HD13	1.91	0.51
1:A:511:ALA:O	1:A:512:LEU:HD23	2.10	0.51
1:A:915:ASN:ND2	1:A:915:ASN:H	2.08	0.51
2:B:341:LEU:C	2:B:343:LEU:H	2.12	0.51
1:A:312:VAL:HG12	1:A:336:VAL:HA	1.92	0.51
1:A:347:LEU:HD12	1:A:358:ILE:N	2.25	0.51
2:B:90:LEU:HD11	2:B:401:ALA:HB3	1.91	0.51
2:B:134:LEU:HG	2:B:135:GLY:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ARG:HD3	1:A:519:PRO:HG3	1.91	0.51
1:A:794:MET:O	1:A:926:PHE:HA	2.10	0.51
1:A:21:PHE:HE1	2:B:266:VAL:HG11	1.76	0.51
1:A:526:THR:HG22	1:A:527:ILE:N	2.26	0.51
2:B:269:ASN:ND2	2:B:271:GLY:H	2.09	0.51
2:B:159:LYS:HD2	2:B:289:TYR:CZ	2.45	0.51
1:A:561:TYR:CZ	1:A:584:ALA:HA	2.45	0.51
1:A:928:VAL:CG2	1:A:941:ILE:HB	2.41	0.51
2:B:642:VAL:CG2	2:B:680:TYR:HB3	2.40	0.51
1:A:643:LEU:HB3	1:A:681:CYS:HB2	1.93	0.51
1:A:799:TRP:C	1:A:800:PRO:O	2.45	0.51
1:A:375:ILE:CG1	1:A:389:GLN:HB3	2.41	0.50
2:B:656:THR:HA	2:B:665:VAL:O	2.11	0.50
1:A:558:PHE:CZ	1:A:585:ASN:OD1	2.64	0.50
1:A:558:PHE:CE2	1:A:560:GLU:HG3	2.46	0.50
1:A:794:MET:HG2	1:A:929:ILE:HD13	1.93	0.50
1:A:394:GLN:N	1:A:394:GLN:HE21	2.09	0.50
2:B:257:ALA:O	2:B:258:LEU:HB2	2.11	0.50
1:A:142:CYS:C	1:A:144:SER:H	2.14	0.50
2:B:319:GLN:O	2:B:322:SER:HB3	2.12	0.50
1:A:498:LEU:O	1:A:558:PHE:N	2.44	0.50
1:A:597:GLY:O	1:A:598:GLU:HB3	2.12	0.50
1:A:873:GLY:CA	1:A:921:LYS:HB3	2.41	0.50
1:A:914:GLN:OE1	1:A:914:GLN:HA	2.11	0.50
2:B:62:ARG:HA	2:B:88:ILE:HG12	1.94	0.50
1:A:61:TRP:CZ2	1:A:415:ASP:HB3	2.46	0.50
1:A:146:ASP:OD1	1:A:151:GLY:HA3	2.11	0.49
1:A:301:MET:HA	1:A:310:GLN:O	2.12	0.49
1:A:340:PHE:CZ	1:A:360:ILE:HG21	2.47	0.49
1:A:305:SER:HB3	2:B:552:ASP:HB2	1.93	0.49
1:A:808:LEU:O	1:A:809:LEU:HB2	2.11	0.49
1:A:927:ASN:HD22	1:A:927:ASN:C	2.14	0.49
2:B:623:GLU:HB3	2:B:624:PRO:CD	2.42	0.49
1:A:477:PHE:CE1	1:A:495:VAL:HG11	2.47	0.49
1:A:624:PRO:CG	4:H:2:NDG:H3	2.41	0.49
2:B:157:VAL:HG12	2:B:189:GLY:H	1.76	0.49
2:B:297:GLU:O	2:B:301:GLN:HG3	2.12	0.49
1:A:5:VAL:HG12	1:A:5:VAL:O	2.12	0.49
1:A:11:TYR:CD1	1:A:36:LEU:HD22	2.47	0.49
2:B:104:VAL:CG2	2:B:421:PHE:HE2	2.25	0.49
1:A:236:ILE:H	1:A:236:ILE:CD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:THR:HG22	1:A:527:ILE:H	1.76	0.49
1:A:887:GLY:O	1:A:888:ARG:HB3	2.12	0.49
2:B:366:LEU:HB3	2:B:403:VAL:CG1	2.37	0.49
2:B:647:ASP:HB3	2:B:668:GLN:NE2	2.27	0.49
1:A:482:ASP:HB2	1:A:530:GLY:HA2	1.93	0.49
1:A:18:TYR:CE1	1:A:42:LYS:HD2	2.48	0.49
1:A:273:ALA:HB3	2:B:292:LEU:HD22	1.95	0.49
1:A:300:PHE:HB3	1:A:313:GLY:CA	2.41	0.49
1:A:914:GLN:C	1:A:916:HIS:H	2.16	0.49
2:B:534:GLU:C	2:B:536:CYS:H	2.16	0.49
2:B:535:MET:C	2:B:537:SER:H	2.16	0.49
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.94	0.49
2:B:262:LEU:N	2:B:262:LEU:HD23	2.28	0.49
1:A:121:GLU:HG2	1:A:123:GLU:HG3	1.95	0.48
1:A:248:ARG:HH11	1:A:248:ARG:CB	2.26	0.48
1:A:632:GLN:HG2	1:A:692:GLN:HG3	1.95	0.48
1:A:747:VAL:HG13	1:A:747:VAL:O	2.12	0.48
2:B:173:LEU:C	2:B:175:ASN:H	2.16	0.48
2:B:646:LYS:HD2	2:B:646:LYS:H	1.77	0.48
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.94	0.48
1:A:242:GLY:HA2	1:A:253:VAL:HG22	1.95	0.48
1:A:248:ARG:HH11	1:A:248:ARG:H	1.60	0.48
1:A:300:PHE:CB	1:A:313:GLY:HA2	2.41	0.48
1:A:9:ALA:HB3	1:A:434:LEU:HB2	1.94	0.48
1:A:232:ASN:HB2	1:A:264:LEU:CD2	2.44	0.48
1:A:554:PRO:HG3	1:A:591:HIS:CD2	2.48	0.48
2:B:151:ILE:C	2:B:196:LEU:HD23	2.33	0.48
2:B:233:ASP:HA	2:B:238:TRP:HD1	1.78	0.48
4:F:1:NAG:H61	4:F:1:NAG:C2	2.20	0.48
1:A:674:ASN:HB3	1:A:676:THR:HG22	1.96	0.48
2:B:69:LEU:HD21	2:B:78:SER:HB2	1.95	0.48
2:B:161:VAL:HG22	2:B:162:SER:H	1.78	0.48
2:B:360:ARG:O	2:B:361:ASP:HB2	2.13	0.48
2:B:687:CYS:HB3	2:B:688:PRO:HD2	1.95	0.48
1:A:168:ARG:CG	1:A:168:ARG:NH1	2.74	0.48
1:A:249:THR:CG2	2:B:256:ILE:HD13	2.43	0.48
2:B:341:LEU:C	2:B:343:LEU:N	2.67	0.48
2:B:356:GLU:HA	2:B:385:SER:HB3	1.95	0.48
2:B:641:SER:OG	2:B:683:GLU:HB3	2.13	0.48
1:A:394:GLN:HE21	1:A:394:GLN:H	1.60	0.48
2:B:56:PHE:CZ	2:B:93:ARG:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ASN:HD22	2:B:137:LYS:HD3	1.78	0.48
1:A:285:ILE:HB	1:A:294:PHE:HZ	1.78	0.48
2:B:58:VAL:HG12	2:B:93:ARG:N	2.28	0.48
2:B:101:SER:HA	2:B:398:SER:HA	1.95	0.48
2:B:535:MET:O	2:B:537:SER:N	2.45	0.48
1:A:177:PHE:HB2	1:A:180:GLN:HG3	1.96	0.48
1:A:88:PHE:CZ	1:A:122:ARG:HG2	2.49	0.48
1:A:138:GLU:CD	1:A:143:ARG:HH22	2.17	0.48
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.48	0.48
1:A:340:PHE:C	1:A:342:SER:H	2.17	0.48
1:A:518:SER:OG	1:A:519:PRO:HD2	2.14	0.47
1:A:639:TYR:O	1:A:719:SER:HB2	2.14	0.47
1:A:657:VAL:CG1	1:A:698:ARG:HH21	2.27	0.47
1:A:801:TYR:HB3	1:A:878:GLN:O	2.13	0.47
2:B:193:VAL:O	2:B:194:LEU:HB3	2.14	0.47
2:B:212:VAL:CG1	2:B:213:SER:H	2.22	0.47
1:A:239:PHE:O	1:A:255:ILE:HA	2.13	0.47
1:A:249:THR:HG22	1:A:273:ALA:HA	1.96	0.47
1:A:441:ILE:HD11	1:A:576:PRO:HB2	1.95	0.47
1:A:936:LEU:N	1:A:936:LEU:HD12	2.28	0.47
2:B:82:GLN:HG2	2:B:107:VAL:HG12	1.96	0.47
2:B:215:ASN:H	2:B:215:ASN:HD22	1.63	0.47
1:A:170:LEU:HD13	1:A:226:VAL:HG21	1.97	0.47
1:A:227:ALA:O	1:A:240:VAL:HB	2.13	0.47
1:A:470:VAL:HG22	1:A:471:SER:N	2.29	0.47
1:A:606:LEU:CB	1:A:727:SER:HB3	2.45	0.47
1:A:3:LEU:HA	1:A:437:ALA:HA	1.96	0.47
1:A:441:ILE:O	1:A:578:LEU:HA	2.14	0.47
1:A:754:PHE:HE2	2:B:658:LYS:HE2	1.79	0.47
2:B:90:LEU:HD11	2:B:401:ALA:CB	2.45	0.47
1:A:201:SER:OG	1:A:202:ILE:N	2.48	0.47
1:A:753:VAL:O	1:A:951:VAL:HA	2.14	0.47
2:B:58:VAL:HG12	2:B:92:LEU:HA	1.96	0.47
2:B:159:LYS:HZ1	2:B:288:ASP:HA	1.79	0.47
1:A:228:VAL:HG23	1:A:238:ASP:O	2.14	0.47
1:A:510:ARG:O	1:A:542:LEU:HD12	2.14	0.47
2:B:57:PRO:HA	2:B:93:ARG:HH22	1.74	0.47
2:B:115:TYR:HB3	2:B:246:LEU:HD12	1.96	0.47
2:B:100:PHE:CZ	2:B:399:ILE:HB	2.49	0.47
2:B:648:THR:CA	4:I:2:NDG:C1	2.79	0.47
1:A:14:PRO:HG2	1:A:17:SER:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:LEU:H	1:A:488:PRO:CD	2.28	0.47
1:A:523:LYS:HA	1:A:523:LYS:HD2	1.78	0.47
2:B:102:ILE:CG2	2:B:397:PHE:HB2	2.44	0.47
2:B:119:ASP:O	2:B:124:MET:HE3	2.14	0.47
2:B:124:MET:HA	2:B:127:ASP:OD1	2.15	0.47
2:B:333:LEU:HG	2:B:334:SER:H	1.79	0.47
1:A:36:LEU:HG	1:A:423:ILE:HD13	1.96	0.46
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.96	0.46
1:A:497:LEU:HA	1:A:558:PHE:O	2.14	0.46
1:A:608:VAL:HG13	1:A:717:ILE:CD1	2.42	0.46
2:B:158:ASP:OD1	2:B:159:LYS:N	2.47	0.46
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.95	0.46
1:A:17:SER:HA	1:A:42:LYS:O	2.15	0.46
1:A:416:LYS:H	1:A:416:LYS:HD2	1.80	0.46
1:A:510:ARG:H	1:A:510:ARG:HD3	1.79	0.46
1:A:260:ASN:O	1:A:261:MET:HB3	2.15	0.46
1:A:349:ASP:HB3	1:A:352:GLN:HA	1.96	0.46
1:A:620:GLY:CA	1:A:891:ARG:HH12	2.27	0.46
1:A:740:ALA:HB2	1:A:788:SER:O	2.15	0.46
1:A:792:LYS:HB2	1:A:930:GLU:HB3	1.95	0.46
1:A:36:LEU:HD11	1:A:434:LEU:HD23	1.98	0.46
1:A:61:TRP:CZ2	1:A:415:ASP:CB	2.99	0.46
1:A:705:SER:HB2	1:A:933:TYR:HE2	1.81	0.46
1:A:802:LYS:HG2	1:A:807:THR:HA	1.97	0.46
2:B:366:LEU:HA	2:B:402:LYS:O	2.15	0.46
1:A:495:VAL:HG23	1:A:561:TYR:HB3	1.98	0.46
3:C:1:NAG:C6	3:C:2:NAG:C1	2.94	0.46
1:A:102:GLN:C	1:A:104:LYS:H	2.17	0.46
1:A:765:ASN:HA	1:A:766:PRO:HD2	1.71	0.46
1:A:927:ASN:HA	1:A:942:THR:HG22	1.97	0.46
2:B:168:SER:O	2:B:169:PRO:O	2.33	0.46
1:A:61:TRP:CG	1:A:414:ILE:HG12	2.50	0.46
1:A:253:VAL:HG21	1:A:295:ILE:CG2	2.46	0.46
1:A:498:LEU:HD12	1:A:558:PHE:HD2	1.78	0.46
1:A:594:LEU:C	1:A:596:CYS:H	2.19	0.46
1:A:91:HIS:NE2	3:C:2:NAG:H82	2.31	0.46
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.97	0.46
1:A:527:ILE:O	1:A:528:SER:HB2	2.16	0.46
1:A:657:VAL:CG2	1:A:663:LEU:HD13	2.46	0.46
2:B:104:VAL:HG21	2:B:421:PHE:HE2	1.81	0.46
2:B:426:ILE:HD12	2:B:426:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:ASN:H	2:B:632:ASN:ND2	2.14	0.46
1:A:171:LEU:C	1:A:171:LEU:HD23	2.37	0.46
1:A:349:ASP:HB3	1:A:352:GLN:N	2.31	0.46
1:A:434:LEU:HA	1:A:434:LEU:HD22	1.74	0.46
1:A:578:LEU:N	1:A:578:LEU:HD22	2.31	0.46
1:A:886:VAL:HG12	1:A:887:GLY:N	2.30	0.46
1:A:180:GLN:HE22	1:A:213:ALA:CB	2.25	0.46
1:A:339:ARG:HB3	1:A:342:SER:HB2	1.97	0.46
1:A:514:LEU:HB3	1:A:515:TYR:CD1	2.51	0.46
2:B:115:TYR:CD1	2:B:236:ILE:HG23	2.51	0.46
2:B:199:GLN:HB2	2:B:202:ARG:HB3	1.98	0.46
1:A:301:MET:HG2	1:A:311:GLU:HA	1.97	0.45
1:A:525:MET:HB3	1:A:526:THR:H	1.59	0.45
2:B:92:LEU:O	2:B:431:PHE:HA	2.15	0.45
2:B:404:ARG:HG3	2:B:548:LEU:HD13	1.99	0.45
2:B:549:CYS:SG	2:B:555:GLY:O	2.73	0.45
1:A:299:LEU:HD21	2:B:257:ALA:HB3	1.97	0.45
1:A:658:ARG:HB3	1:A:665:ARG:HH21	1.81	0.45
2:B:315:VAL:HG12	2:B:316:ASN:N	2.30	0.45
2:B:642:VAL:HG21	2:B:680:TYR:HB3	1.97	0.45
2:B:647:ASP:CB	2:B:668:GLN:HE22	2.28	0.45
1:A:239:PHE:CE1	1:A:258:GLY:HA2	2.52	0.45
1:A:497:LEU:O	1:A:498:LEU:HD23	2.17	0.45
1:A:784:ASN:HD21	1:A:789:SER:HA	1.81	0.45
1:A:410:GLY:O	1:A:411:ALA:HB2	2.17	0.45
1:A:469:LYS:HD3	1:A:469:LYS:N	2.23	0.45
2:B:102:ILE:HG23	2:B:397:PHE:HB2	1.99	0.45
1:A:647:ILE:HB	1:A:651:ALA:CB	2.46	0.45
1:A:710:SER:CA	1:A:736:LEU:HD13	2.42	0.45
1:A:278:PHE:HE2	1:A:342:SER:O	1.99	0.45
1:A:526:THR:C	1:A:527:ILE:HG12	2.36	0.45
1:A:820:MET:CE	1:A:895:ALA:HB1	2.46	0.45
1:A:565:TYR:HB3	1:A:575:GLN:HE21	1.81	0.45
1:A:721:ASN:O	1:A:725:LYS:HB3	2.17	0.45
2:B:554:THR:HG23	2:B:560:CYS:HB3	1.99	0.45
1:A:19:PHE:HD1	1:A:431:ARG:HA	1.82	0.45
2:B:622:ARG:HG2	2:B:623:GLU:N	2.31	0.45
1:A:336:VAL:O	1:A:337:PHE:HB2	2.16	0.45
2:B:162:SER:CB	2:B:163:PRO:CD	2.95	0.45
2:B:646:LYS:HD2	4:I:2:NDG:H8C1	1.98	0.45
1:A:55:GLN:OE1	1:A:69:PRO:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PRO:HG3	1:A:711:VAL:CG1	2.47	0.45
2:B:173:LEU:CA	2:B:176:PRO:HD2	2.40	0.45
1:A:550:ASP:N	1:A:551:LYS:HZ1	2.10	0.44
1:A:706:GLU:C	1:A:708:ASP:N	2.67	0.44
2:B:676:LYS:HG2	2:B:677:SER:N	2.32	0.44
1:A:1:PHE:HB3	1:A:377:ASN:OD1	2.17	0.44
1:A:11:TYR:CE1	1:A:36:LEU:HD22	2.51	0.44
1:A:314:GLN:HE22	1:A:330:LYS:HG2	1.81	0.44
1:A:550:ASP:CG	1:A:551:LYS:H	2.20	0.44
1:A:617:ILE:HD11	1:A:736:LEU:HD12	1.99	0.44
1:A:799:TRP:CD1	1:A:800:PRO:O	2.71	0.44
1:A:946:LEU:H	1:A:946:LEU:CD2	2.25	0.44
2:B:332:VAL:HG12	2:B:674:SER:OG	2.17	0.44
2:B:593:SER:HB3	2:B:601:CYS:SG	2.57	0.44
2:B:607:ALA:C	2:B:609:THR:H	2.20	0.44
1:A:64:THR:O	1:A:65:ARG:HB2	2.17	0.44
1:A:188:VAL:C	1:A:190:GLU:H	2.20	0.44
1:A:565:TYR:HB3	1:A:575:GLN:NE2	2.31	0.44
2:B:156:PHE:HA	2:B:189:GLY:O	2.17	0.44
2:B:409:GLU:O	2:B:410:LYS:HB2	2.18	0.44
1:A:68:GLN:CB	1:A:69:PRO:HD2	2.43	0.44
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.99	0.44
1:A:248:ARG:HH11	1:A:248:ARG:N	2.15	0.44
1:A:645:VAL:HG22	1:A:715:LEU:CD2	2.47	0.44
1:A:784:ASN:ND2	1:A:789:SER:HA	2.32	0.44
1:A:478:CYS:O	1:A:479:LEU:HB3	2.16	0.44
1:A:741:ALA:N	1:A:786:GLY:HA3	2.30	0.44
1:A:800:PRO:O	1:A:801:TYR:HB2	2.17	0.44
1:A:869:ILE:HG13	1:A:870:HIS:ND1	2.33	0.44
1:A:21:PHE:CE1	2:B:266:VAL:HG11	2.53	0.44
1:A:108:CYS:SG	1:A:161:ILE:HD13	2.58	0.44
1:A:469:LYS:H	1:A:469:LYS:CD	2.26	0.44
1:A:812:LEU:O	1:A:813:HIS:HB3	2.18	0.44
2:B:79:GLN:O	2:B:80:VAL:O	2.36	0.44
2:B:652:ALA:HB2	2:B:670:TYR:HA	1.99	0.44
1:A:36:LEU:HD11	1:A:434:LEU:CD2	2.47	0.44
2:B:115:TYR:CE1	2:B:236:ILE:HG23	2.52	0.44
1:A:549:ARG:HA	1:A:549:ARG:NE	2.33	0.44
1:A:555:ILE:N	1:A:590:ALA:O	2.46	0.44
1:A:821:ASN:HD22	1:A:821:ASN:HA	1.70	0.44
2:B:112:VAL:HG21	2:B:142:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:SER:N	2:B:169:PRO:CD	2.74	0.44
2:B:227:MET:O	2:B:231:VAL:HG22	2.18	0.44
2:B:333:LEU:HG	2:B:334:SER:N	2.32	0.44
2:B:355:VAL:O	2:B:385:SER:HA	2.18	0.44
2:B:646:LYS:H	2:B:646:LYS:CD	2.31	0.44
1:A:259:LYS:HA	1:A:259:LYS:CE	2.33	0.44
1:A:97:SER:OG	1:A:108:CYS:HB2	2.18	0.43
1:A:170:LEU:HD11	1:A:239:PHE:HB3	2.00	0.43
1:A:264:LEU:O	3:D:1:NAG:H81	2.18	0.43
1:A:348:GLY:O	1:A:356:ASN:HA	2.18	0.43
1:A:450:TYR:CB	1:A:451:PRO:CD	2.96	0.43
1:A:513:PHE:CD1	1:A:521:HIS:HB2	2.53	0.43
1:A:946:LEU:HD23	1:A:946:LEU:N	2.29	0.43
2:B:356:GLU:HA	2:B:385:SER:CB	2.47	0.43
2:B:363:PRO:HB2	2:B:366:LEU:CD2	2.48	0.43
2:B:652:ALA:CB	2:B:670:TYR:HA	2.47	0.43
1:A:25:PHE:CE1	1:A:410:GLY:HA2	2.49	0.43
1:A:390:ILE:O	1:A:390:ILE:HG13	2.18	0.43
2:B:82:GLN:O	2:B:104:VAL:HA	2.18	0.43
1:A:521:HIS:CE1	1:A:538:LEU:HD11	2.52	0.43
2:B:62:ARG:HG3	2:B:63:VAL:N	2.32	0.43
2:B:573:LEU:HD23	2:B:574:LEU:N	2.32	0.43
1:A:340:PHE:O	1:A:361:ALA:O	2.36	0.43
2:B:143:ARG:C	2:B:145:LEU:H	2.20	0.43
2:B:650:LYS:HG2	4:I:1:NAG:C6	2.46	0.43
1:A:275:TYR:CE1	2:B:256:ILE:HD11	2.54	0.43
2:B:240:ASN:HD22	2:B:240:ASN:N	2.17	0.43
2:B:646:LYS:O	4:I:2:NDG:C8	2.51	0.43
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.84	0.43
1:A:187:GLN:NE2	1:A:206:ASN:HB2	2.34	0.43
1:A:429:VAL:HB	1:A:431:ARG:HH11	1.83	0.43
1:A:808:LEU:O	1:A:808:LEU:HD12	2.18	0.43
2:B:62:ARG:NH1	2:B:85:PRO:HB2	2.34	0.43
2:B:65:GLU:HG3	2:B:65:GLU:O	2.19	0.43
2:B:146:THR:HG22	2:B:147:SER:N	2.33	0.43
1:A:787:PRO:HA	1:A:891:ARG:HD3	2.00	0.43
2:B:244:HIS:ND1	2:B:244:HIS:N	2.66	0.43
2:B:366:LEU:HD11	2:B:414:PHE:CE2	2.54	0.43
2:B:418:PRO:HB2	2:B:421:PHE:CD2	2.53	0.43
2:B:580:LYS:HZ3	2:B:580:LYS:HB2	1.83	0.43
2:B:599:GLU:HG2	2:B:600:LYS:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:O	1:A:103:ASP:HB2	2.19	0.43
2:B:139:ALA:O	2:B:143:ARG:N	2.52	0.43
1:A:102:GLN:O	1:A:102:GLN:HG2	2.19	0.43
1:A:372:ILE:HA	1:A:391:LEU:O	2.18	0.43
1:A:339:ARG:HD3	1:A:364:TYR:CD1	2.54	0.42
1:A:376:PHE:CD1	1:A:376:PHE:N	2.84	0.42
1:A:605:LYS:H	1:A:635:GLY:N	2.14	0.42
2:B:71:ASP:CB	2:B:108:GLU:HB2	2.42	0.42
2:B:126:ASP:N	2:B:126:ASP:OD2	2.51	0.42
2:B:173:LEU:HD11	2:B:178:TYR:CE1	2.54	0.42
2:B:356:GLU:HB3	2:B:419:VAL:CG2	2.49	0.42
2:B:363:PRO:HB2	2:B:366:LEU:HD23	2.00	0.42
1:A:26:PHE:HB2	1:A:37:LEU:HD21	2.01	0.42
1:A:800:PRO:HG3	1:A:921:LYS:O	2.19	0.42
2:B:138:LEU:HA	2:B:341:LEU:HD12	2.00	0.42
1:A:113:HIS:NE2	1:A:124:PRO:HB3	2.34	0.42
1:A:173:GLY:O	1:A:181:GLY:HA2	2.19	0.42
2:B:575:CYS:C	2:B:577:GLY:H	2.23	0.42
1:A:272:MET:HE3	5:B:3320:NAG:H2	2.01	0.42
1:A:384:ASN:HD21	1:A:386:VAL:HG22	1.84	0.42
1:A:454:LEU:HA	5:A:2458:NAG:H61	2.00	0.42
1:A:454:LEU:HG	1:A:591:HIS:O	2.19	0.42
1:A:474:ASN:ND2	1:A:539:ILE:HA	2.34	0.42
1:A:476:ARG:HG3	1:A:476:ARG:O	2.18	0.42
1:A:721:ASN:HD22	1:A:722:LEU:H	1.67	0.42
1:A:776:VAL:HG11	1:A:949:THR:HG21	2.00	0.42
2:B:87:ARG:HG3	2:B:88:ILE:H	1.84	0.42
2:B:567:CYS:O	2:B:568:MET:O	2.37	0.42
1:A:253:VAL:HG21	1:A:295:ILE:HG21	2.00	0.42
1:A:416:LYS:HD2	1:A:416:LYS:N	2.34	0.42
1:A:901:SER:O	1:A:902:LEU:HB3	2.19	0.42
1:A:2:ASN:HA	1:A:389:GLN:OE1	2.19	0.42
1:A:113:HIS:HD2	1:A:122:ARG:O	2.02	0.42
1:A:409:LYS:HD2	1:A:410:GLY:H	1.84	0.42
1:A:717:ILE:HG22	1:A:718:GLN:N	2.34	0.42
1:A:769:GLU:OE1	1:A:835:ILE:HA	2.20	0.42
1:A:20:GLY:HA2	1:A:38:VAL:HG13	2.02	0.42
1:A:116:THR:HG22	1:A:147:ILE:HG21	2.00	0.42
1:A:180:GLN:NE2	1:A:213:ALA:H	2.17	0.42
1:A:557:ILE:O	1:A:587:SER:HB2	2.20	0.42
1:A:741:ALA:H	1:A:786:GLY:CA	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:PRO:HD3	2:B:84:SER:HA	2.02	0.42
2:B:226:ILE:HD11	2:B:248:PHE:CG	2.54	0.42
2:B:374:CYS:SG	2:B:395:VAL:HB	2.60	0.42
2:B:553:TRP:HE3	2:B:560:CYS:O	2.01	0.42
1:A:420:PRO:O	1:A:421:ASP:CG	2.57	0.42
2:B:246:LEU:HD23	2:B:306:LEU:HD13	2.02	0.42
1:A:441:ILE:HB	1:A:578:LEU:HD13	2.02	0.42
1:A:762:HIS:ND1	1:A:762:HIS:C	2.73	0.42
1:A:792:LYS:HA	1:A:887:GLY:HA2	2.01	0.42
1:A:871:THR:HG23	1:A:871:THR:O	2.20	0.42
2:B:191:LYS:HG3	2:B:280:HIS:CD2	2.55	0.42
2:B:406:CYS:O	2:B:406:CYS:SG	2.77	0.42
1:A:487:LEU:N	1:A:488:PRO:CD	2.82	0.42
1:A:603:LYS:HB2	1:A:603:LYS:HE3	1.79	0.42
1:A:749:SER:CB	1:A:750:PRO:HD3	2.34	0.42
2:B:647:ASP:CG	2:B:648:THR:N	2.73	0.42
1:A:578:LEU:HD22	1:A:578:LEU:H	1.85	0.41
1:A:586:ILE:HD12	1:A:586:ILE:HA	1.78	0.41
1:A:809:LEU:HD22	1:A:901:SER:OG	2.20	0.41
2:B:111:PRO:HB2	2:B:148:ASN:HD22	1.85	0.41
1:A:674:ASN:ND2	1:A:675:GLN:H	2.18	0.41
1:A:194:LYS:HE2	1:A:194:LYS:HB2	1.82	0.41
1:A:712:LYS:CA	1:A:733:LYS:HA	2.42	0.41
2:B:575:CYS:HB2	2:B:579:GLY:O	2.19	0.41
1:A:395:TRP:CB	1:A:429:VAL:HG21	2.50	0.41
1:A:504:GLN:HB3	1:A:505:LYS:H	1.55	0.41
1:A:647:ILE:HD12	1:A:651:ALA:CB	2.51	0.41
2:B:215:ASN:HD22	2:B:215:ASN:N	2.18	0.41
2:B:622:ARG:CG	2:B:623:GLU:H	2.34	0.41
2:B:622:ARG:CG	2:B:623:GLU:N	2.83	0.41
2:B:658:LYS:HA	2:B:663:CYS:O	2.19	0.41
1:A:568:ALA:HB1	1:A:574:LEU:H	1.85	0.41
2:B:214:ARG:HG3	2:B:214:ARG:NH1	2.31	0.41
3:C:1:NAG:H61	3:C:2:NAG:O5	2.20	0.41
1:A:404:PHE:CD2	1:A:404:PHE:C	2.92	0.41
2:B:58:VAL:H	2:B:93:ARG:HH21	1.68	0.41
2:B:650:LYS:HA	4:I:1:NAG:O6	2.21	0.41
1:A:1:PHE:O	1:A:2:ASN:OD1	2.38	0.41
1:A:396:ALA:O	1:A:397:ALA:HB2	2.21	0.41
1:A:487:LEU:O	1:A:488:PRO:O	2.39	0.41
1:A:627:LEU:O	1:A:696:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:THR:HG22	1:A:808:LEU:N	2.36	0.41
2:B:103:GLN:HG3	2:B:396:SER:HB2	2.01	0.41
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.91	0.41
1:A:50:ILE:HD12	1:A:89:LYS:HB2	2.02	0.41
2:B:173:LEU:C	2:B:175:ASN:N	2.73	0.41
2:B:568:MET:O	2:B:569:SER:CB	2.68	0.41
2:B:580:LYS:NZ	2:B:582:GLU:HB2	2.36	0.41
2:B:615:VAL:O	2:B:620:PHE:HD1	2.03	0.41
1:A:347:LEU:CD1	1:A:357:ASP:HB2	2.51	0.41
1:A:355:PHE:CZ	1:A:380:SER:HB3	2.56	0.41
1:A:375:ILE:CD1	1:A:389:GLN:HB3	2.51	0.41
1:A:614:GLN:NE2	1:A:616:LYS:HD2	2.36	0.41
1:A:830:PRO:C	1:A:832:ARG:H	2.24	0.41
1:A:906:GLU:C	1:A:908:PHE:N	2.71	0.41
2:B:251:ASP:HA	2:B:311:THR:OG1	2.21	0.41
2:B:293:GLY:O	2:B:296:THR:HB	2.21	0.41
2:B:375:LEU:HA	2:B:375:LEU:HD23	1.74	0.41
2:B:646:LYS:HD2	4:I:2:NDG:C8	2.51	0.41
1:A:623:ASN:O	1:A:700:SER:HA	2.21	0.41
1:A:784:ASN:O	1:A:891:ARG:O	2.39	0.41
2:B:534:GLU:CG	2:B:544:CYS:SG	3.06	0.41
1:A:429:VAL:HG23	1:A:431:ARG:HG3	2.03	0.40
1:A:631:ALA:HA	1:A:717:ILE:HD11	2.03	0.40
2:B:120:LEU:HA	2:B:120:LEU:HD12	1.83	0.40
2:B:380:ILE:HA	2:B:381:PRO:HD2	1.88	0.40
1:A:674:ASN:O	1:A:676:THR:N	2.47	0.40
1:A:693:LEU:HA	1:A:693:LEU:HD13	1.81	0.40
2:B:55:GLU:C	2:B:56:PHE:HD2	2.25	0.40
2:B:67:ARG:O	2:B:68:PRO:C	2.59	0.40
2:B:111:PRO:HB3	2:B:148:ASN:HB3	2.02	0.40
2:B:177:CYS:SG	2:B:214:ARG:HB3	2.62	0.40
2:B:638:GLU:O	2:B:638:GLU:HG3	2.21	0.40
1:A:55:GLN:HG3	1:A:57:LEU:HD11	2.04	0.40
1:A:496:GLU:O	1:A:559:MET:HA	2.21	0.40
1:A:653:PHE:HA	1:A:699:PHE:CD1	2.52	0.40
2:B:315:VAL:O	2:B:317:LEU:N	2.55	0.40
2:B:421:PHE:N	2:B:421:PHE:CD1	2.86	0.40
2:B:575:CYS:O	2:B:577:GLY:N	2.55	0.40
2:B:625:TYR:HD1	2:B:625:TYR:HA	1.76	0.40
1:A:104:LYS:HE3	1:A:167:ASP:OD1	2.22	0.40
1:A:349:ASP:C	1:A:351:ASP:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:LYS:HG3	1:A:567:THR:HG23	2.04	0.40
1:A:645:VAL:HG21	1:A:697:LEU:CD1	2.51	0.40
1:A:651:ALA:O	1:A:652:ASP:HB2	2.22	0.40
1:A:908:PHE:HB3	1:A:909:MET:H	1.51	0.40
2:B:178:TYR:CG	2:B:179:ASP:N	2.89	0.40
2:B:185:LEU:HD12	2:B:211:SER:HB3	2.01	0.40
2:B:534:GLU:OE1	2:B:544:CYS:SG	2.80	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%)	708 (77%)	157 (17%)	58 (6%)	1 7
2	B	535/692 (77%)	388 (72%)	102 (19%)	45 (8%)	0 4
All	All	1458/1649 (88%)	1096 (75%)	259 (18%)	103 (7%)	1 5

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	69	PRO
1	A	118	MET
1	A	169	VAL
1	A	205	ASN
1	A	396	ALA
1	A	411	ALA
1	A	417	ASN
1	A	420	PRO
1	A	450	TYR
1	A	484	LYS

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Mol	Chain	Res	Type
1	A	487	LEU
1	A	488	PRO
1	A	504	GLN
1	A	514	LEU
1	A	527	ILE
1	A	572	THR
1	A	685	ASN
1	A	688	LYS
1	A	703	GLN
1	A	704	GLN
1	A	705	SER
1	A	757	ILE
1	A	869	ILE
1	A	874	CYS
1	A	888	ARG
2	B	70	SER
2	B	80	VAL
2	B	88	ILE
2	B	162	SER
2	B	167	ILE
2	B	168	SER
2	B	169	PRO
2	B	176	PRO
2	B	199	GLN
2	B	377	ASN
2	B	536	CYS
2	B	546	ASP
2	B	568	MET
2	B	569	SER
1	A	71	GLU
1	A	82	LYS
1	A	101	LYS
1	A	167	ASP
1	A	287	GLY
1	A	289	ASP
1	A	397	ALA
1	A	464	PRO
1	A	528	SER
1	A	554	PRO
1	A	707	MET
1	A	708	ASP
1	A	759	ASN

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Mol	Chain	Res	Type
1	A	801	TYR
1	A	835	ILE
1	A	917	SER
2	B	75	GLY
2	B	84	SER
2	B	86	GLN
2	B	157	VAL
2	B	182	THR
2	B	253	LYS
2	B	316	ASN
2	B	346	ASP
2	B	433	CYS
2	B	576	SER
2	B	673	SER
2	B	677	SER
1	A	569	ALA
1	A	675	GLN
1	A	908	PHE
1	A	943	ASN
2	B	172	ALA
2	B	407	PRO
2	B	410	LYS
2	B	412	LYS
2	B	547	CYS
2	B	608	CYS
1	A	62	SER
1	A	194	LYS
1	A	598	GLU
1	A	662	ALA
2	B	362	LEU
2	B	535	MET
2	B	538	GLY
2	B	539	HIS
2	B	671	GLU
1	A	288	ASP
1	A	371	GLY
1	A	800	PRO
1	A	890	ASP
1	A	910	ASN
2	B	315	VAL
2	B	402	LYS
2	B	623	GLU

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Mol	Chain	Res	Type
2	B	643	LYS
2	B	647	ASP
1	A	202	ILE
1	A	387	PRO
2	B	175	ASN
2	B	229	ALA
2	B	543	SER
1	A	508	ILE

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%)	702 (89%)	85 (11%)	5 21
2	B	484/616 (79%)	414 (86%)	70 (14%)	2 11
All	All	1271/1428 (89%)	1116 (88%)	155 (12%)	4 16

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	34	MET
1	A	36	LEU
1	A	60	ASP
1	A	69	PRO
1	A	73	ASP
1	A	90	SER
1	A	99	ARG
1	A	100	SER
1	A	121	GLU
1	A	142	CYS
1	A	143	ARG
1	A	146	ASP
1	A	170	LEU
1	A	171	LEU

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Mol	Chain	Res	Type
1	A	236	ILE
1	A	248	ARG
1	A	249	THR
1	A	257	ASP
1	A	259	LYS
1	A	275	TYR
1	A	286	ASN
1	A	289	ASP
1	A	306	ASP
1	A	314	GLN
1	A	321	ARG
1	A	327	GLN
1	A	339	ARG
1	A	347	LEU
1	A	349	ASP
1	A	357	ASP
1	A	367	GLU
1	A	372	ILE
1	A	384	ASN
1	A	394	GLN
1	A	434	LEU
1	A	442	THR
1	A	444	ASN
1	A	447	LEU
1	A	460	THR
1	A	472	CYS
1	A	476	ARG
1	A	479	LEU
1	A	487	LEU
1	A	490	LYS
1	A	508	ILE
1	A	510	ARG
1	A	514	LEU
1	A	527	ILE
1	A	549	ARG
1	A	551	LYS
1	A	553	THR
1	A	554	PRO
1	A	565	TYR
1	A	608	VAL
1	A	623	ASN
1	A	649	LEU

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Mol	Chain	Res	Type
1	A	650	GLN
1	A	657	VAL
1	A	673	GLU
1	A	678	GLN
1	A	682	ASP
1	A	685	ASN
1	A	688	LYS
1	A	703	GLN
1	A	721	ASN
1	A	734	VAL
1	A	753	VAL
1	A	759	ASN
1	A	765	ASN
1	A	880	LEU
1	A	897	LEU
1	A	902	LEU
1	A	903	LEU
1	A	904	TRP
1	A	906	GLU
1	A	907	THR
1	A	913	ASN
1	A	914	GLN
1	A	916	HIS
1	A	919	SER
1	A	927	ASN
1	A	931	PHE
1	A	948	THR
1	A	956	GLN
2	B	55	GLU
2	B	56	PHE
2	B	58	VAL
2	B	60	GLU
2	B	67	ARG
2	B	68	PRO
2	B	69	LEU
2	B	79	GLN
2	B	86	GLN
2	B	87	ARG
2	B	88	ILE
2	B	99	ASN
2	B	102	ILE
2	B	108	GLU

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Mol	Chain	Res	Type
2	B	110	TYR
2	B	117	LEU
2	B	145	LEU
2	B	151	ILE
2	B	161	VAL
2	B	166	TYR
2	B	167	ILE
2	B	173	LEU
2	B	174	GLU
2	B	176	PRO
2	B	178	TYR
2	B	180	MET
2	B	187	MET
2	B	198	ASP
2	B	215	ASN
2	B	220	GLU
2	B	224	ASP
2	B	240	ASN
2	B	244	HIS
2	B	261	ARG
2	B	269	ASN
2	B	286	THR
2	B	291	SER
2	B	292	LEU
2	B	299	LEU
2	B	313	ASN
2	B	317	LEU
2	B	320	ASN
2	B	329	THR
2	B	336	ASP
2	B	341	LEU
2	B	355	VAL
2	B	364	GLU
2	B	366	LEU
2	B	376	ASN
2	B	389	LEU
2	B	406	CYS
2	B	409	GLU
2	B	434	ASP
2	B	534	GLU
2	B	539	HIS
2	B	544	CYS

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Mol	Chain	Res	Type
2	B	546	ASP
2	B	550	ASP
2	B	561	THR
2	B	580	LYS
2	B	610	PHE
2	B	626	MET
2	B	629	ASN
2	B	632	ASN
2	B	633	ARG
2	B	646	LYS
2	B	654	ASN
2	B	670	TYR
2	B	673	SER
2	B	683	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	47	GLN
1	A	77	ASN
1	A	92	GLN
1	A	113	HIS
1	A	152	GLN
1	A	180	GLN
1	A	182	GLN
1	A	205	ASN
1	A	271	GLN
1	A	314	GLN
1	A	384	ASN
1	A	394	GLN
1	A	455	ASN
1	A	456	GLN
1	A	474	ASN
1	A	494	GLN
1	A	524	ASN
1	A	575	GLN
1	A	580	GLN
1	A	614	GLN
1	A	659	ASN
1	A	674	ASN
1	A	678	GLN

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Mol	Chain	Res	Type
1	A	685	ASN
1	A	759	ASN
1	A	778	HIS
1	A	821	ASN
1	A	913	ASN
1	A	915	ASN
1	A	927	ASN
2	B	99	ASN
2	B	133	ASN
2	B	148	ASN
2	B	215	ASN
2	B	240	ASN
2	B	269	ASN
2	B	279	ASN
2	B	319	GLN
2	B	428	GLN
2	B	629	ASN
2	B	632	ASN
2	B	668	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.53	0	17,19,21	0.83	1 (5%)
3	NAG	C	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.72	0
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	1.35	2 (11%)
3	NAG	D	2	3	14,14,15	0.79	1 (7%)	17,19,21	0.71	0
3	NAG	E	1	1,3	14,14,15	0.73	0	17,19,21	0.92	1 (5%)
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.64	0
4	NAG	F	1	1,4	14,14,15	0.80	1 (7%)	17,19,21	0.92	1 (5%)
4	NDG	F	2	4	14,14,15	0.59	0	17,19,21	0.71	0
3	NAG	G	1	1,3	14,14,15	0.49	0	17,19,21	0.84	0
3	NAG	G	2	3	14,14,15	0.47	0	17,19,21	0.64	0
4	NAG	H	1	4,2	14,14,15	0.44	0	17,19,21	1.15	1 (5%)
4	NDG	H	2	4	14,14,15	0.47	0	17,19,21	0.70	0
4	NAG	I	1	4,2	14,14,15	0.55	0	17,19,21	1.31	2 (11%)
4	NDG	I	2	4	14,14,15	0.79	0	17,19,21	0.82	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	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NDG	F	2	4	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,2	-	0/6/23/26	0/1/1/1
4	NDG	I	2	4	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	C1-C2	2.38	1.55	1.52
4	F	1	NAG	C1-C2	2.31	1.55	1.52
3	D	2	NAG	C1-C2	2.11	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	NAG	C4-C3-C2	-3.92	105.28	111.02
4	H	1	NAG	C2-N2-C7	-3.53	118.17	122.90
3	D	1	NAG	O5-C1-C2	-2.83	106.91	111.29
4	F	1	NAG	C2-N2-C7	-2.81	119.14	122.90
4	I	1	NAG	C1-O5-C5	2.41	115.42	112.19
3	E	1	NAG	C2-N2-C7	-2.22	119.93	122.90
4	I	2	NDG	O5-C1-C2	-2.16	107.96	111.29
4	I	1	NAG	C2-N2-C7	-2.10	120.09	122.90
3	C	1	NAG	C2-N2-C7	-2.02	120.20	122.90

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	I	2	NDG	O5-C5-C6-O6
4	I	2	NDG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
4	F	2	NDG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
4	H	2	NDG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C4-C5-C6-O6
3	D	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C1-C2-N2-C7
4	F	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6

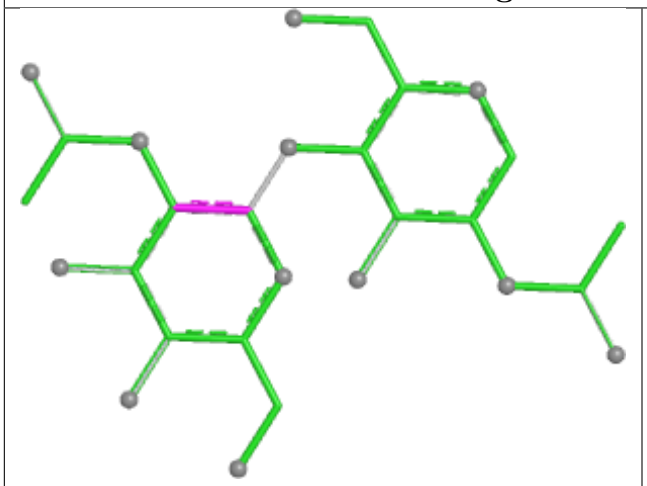
There are no ring outliers.

13 monomers are involved in 30 short contacts:

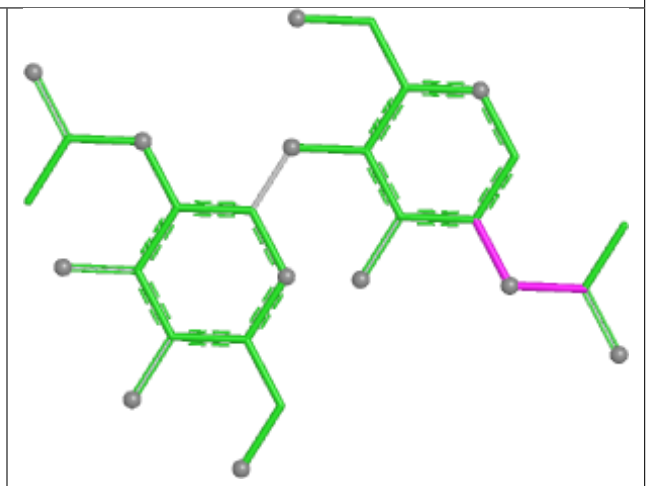
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NDG	3	0
4	I	2	NDG	7	0
4	H	2	NDG	3	0
3	E	1	NAG	3	0
3	G	1	NAG	1	0
4	F	1	NAG	4	0
3	C	1	NAG	2	0
4	I	1	NAG	3	0
3	C	2	NAG	3	0
4	H	1	NAG	1	0
3	D	2	NAG	1	0
3	D	1	NAG	2	0
3	G	2	NAG	1	0

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

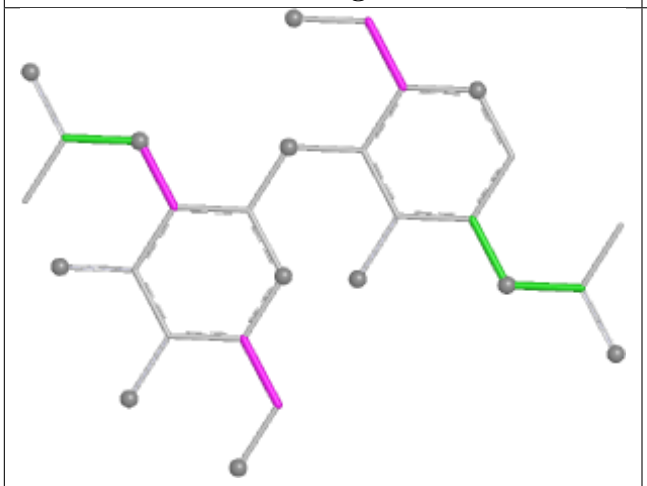
Oligosaccharide Chain C



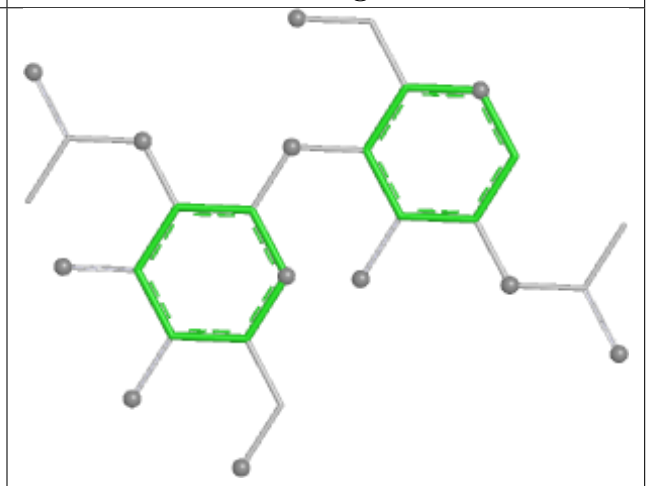
Bond lengths



Bond angles

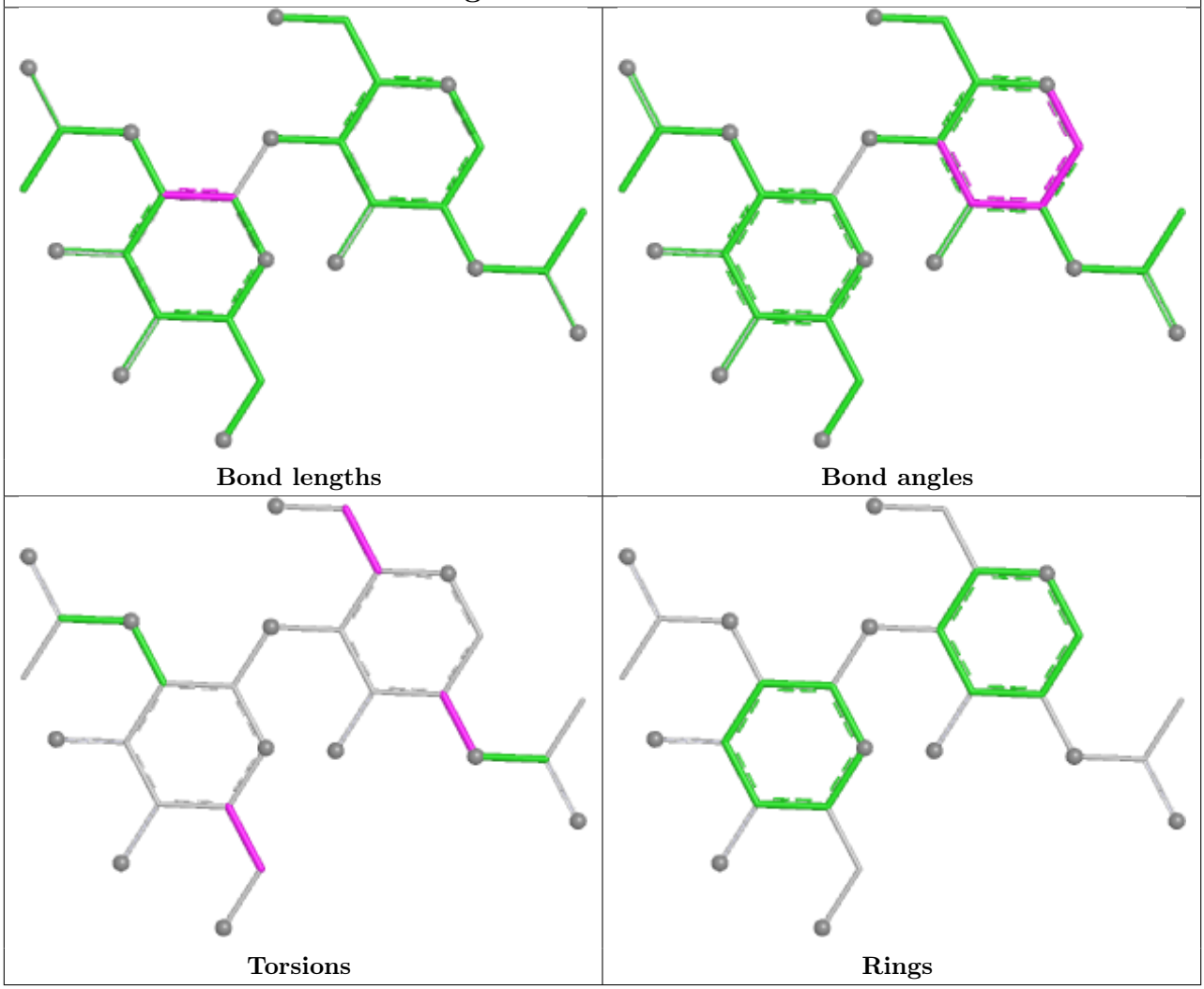


Torsions

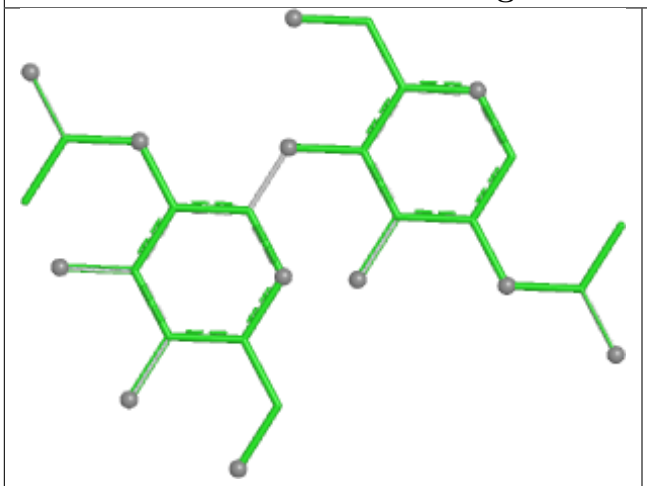


Rings

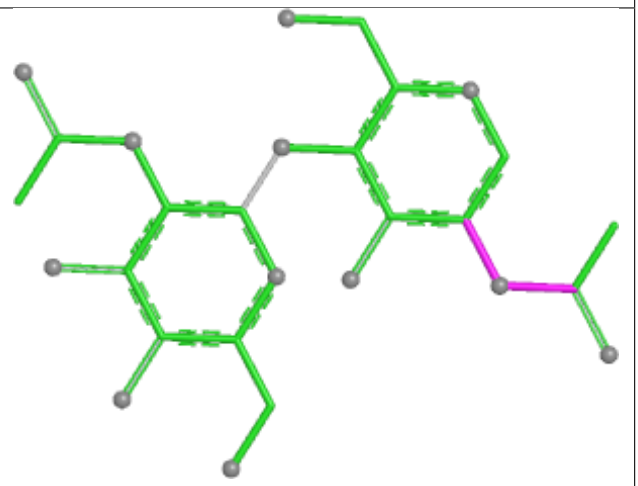
Oligosaccharide Chain D



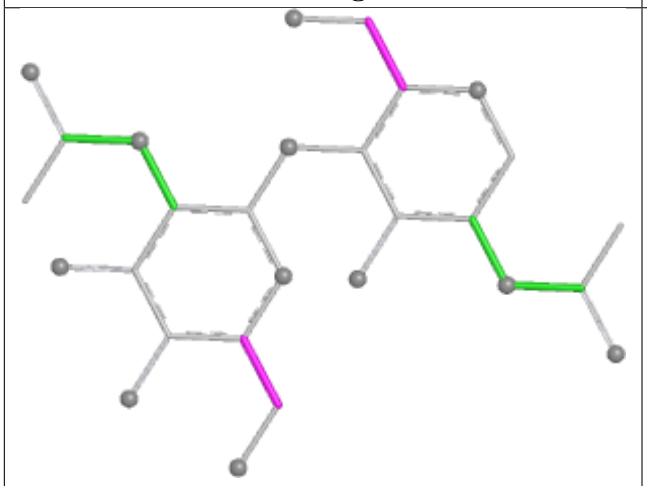
Oligosaccharide Chain E



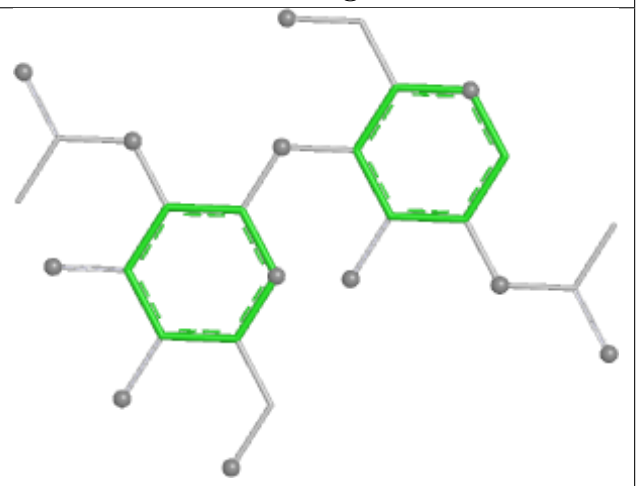
Bond lengths



Bond angles

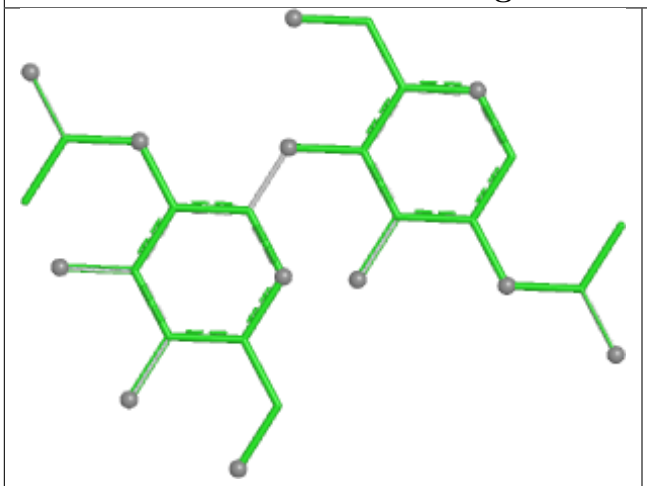


Torsions

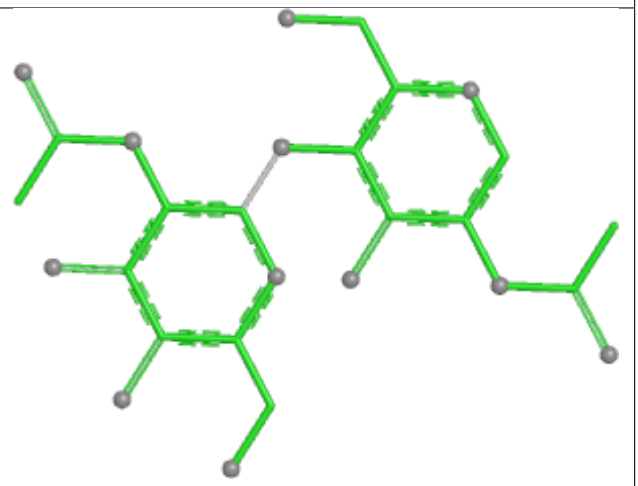


Rings

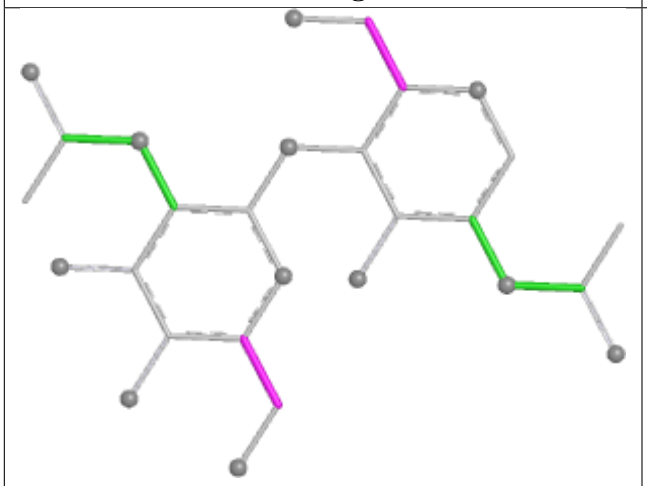
Oligosaccharide Chain G



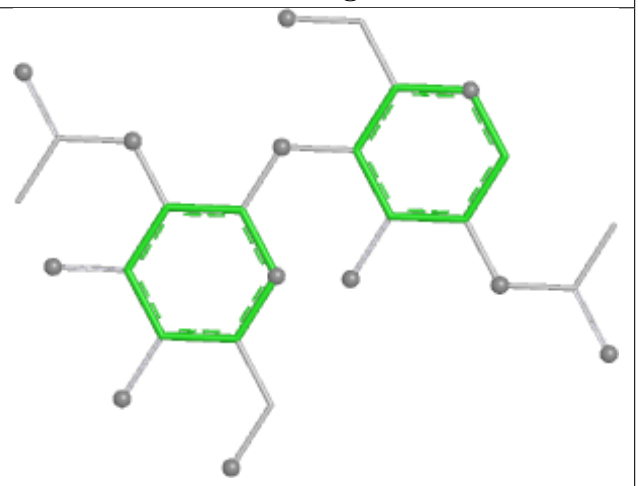
Bond lengths



Bond angles

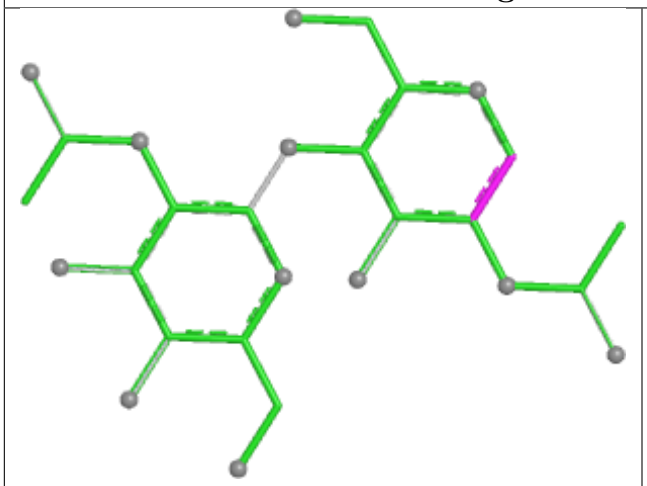


Torsions

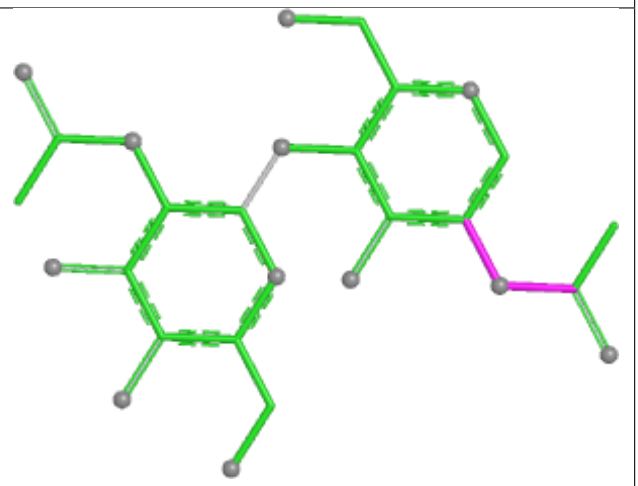


Rings

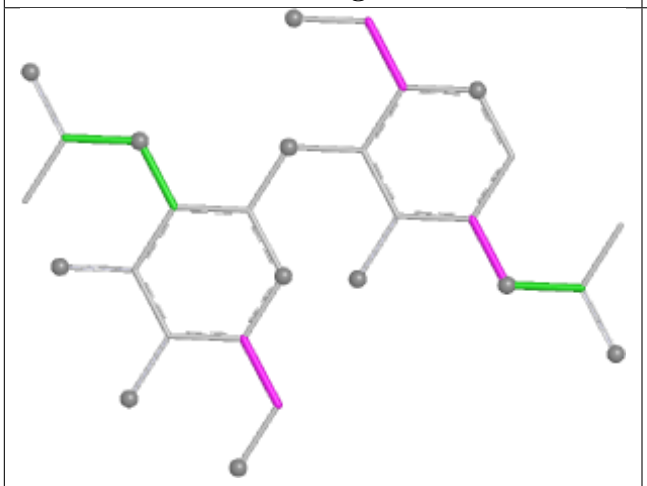
Oligosaccharide Chain F



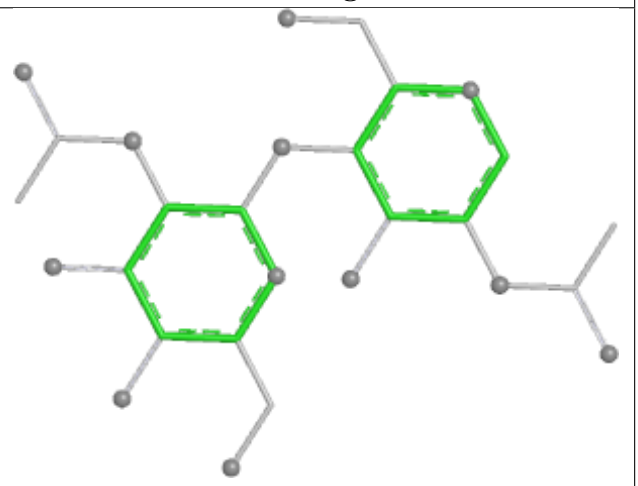
Bond lengths



Bond angles

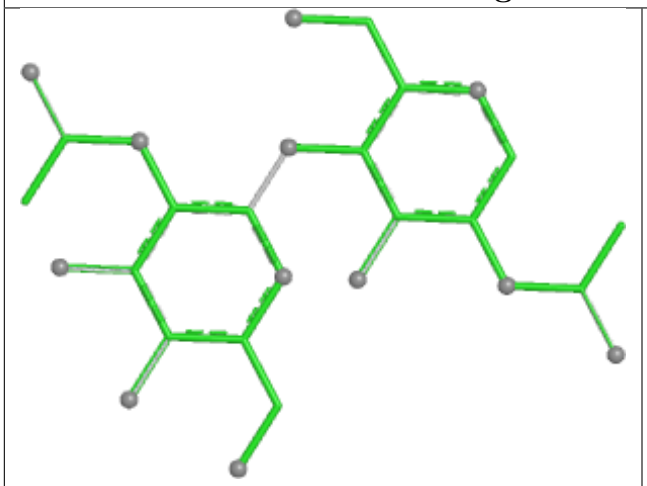


Torsions

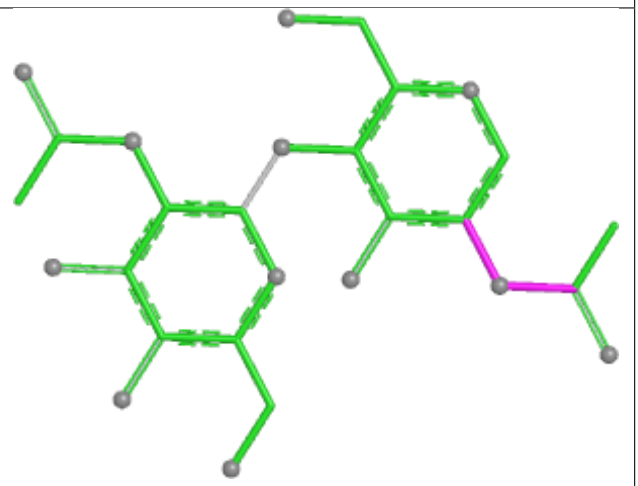


Rings

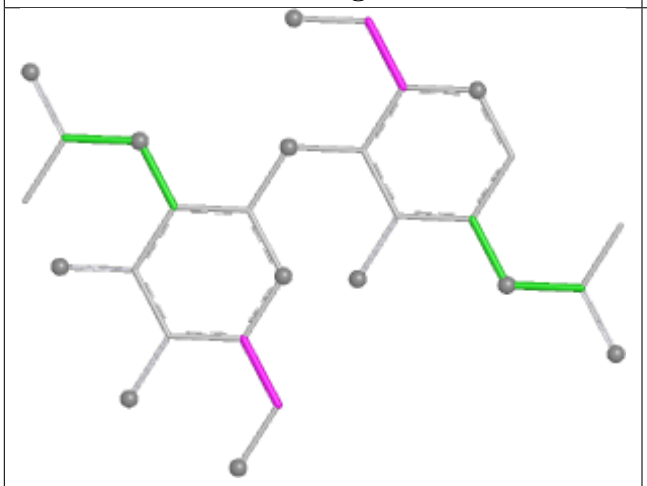
Oligosaccharide Chain H



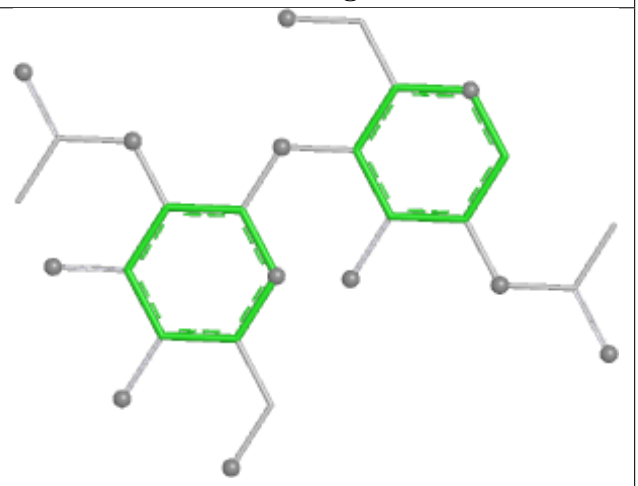
Bond lengths



Bond angles

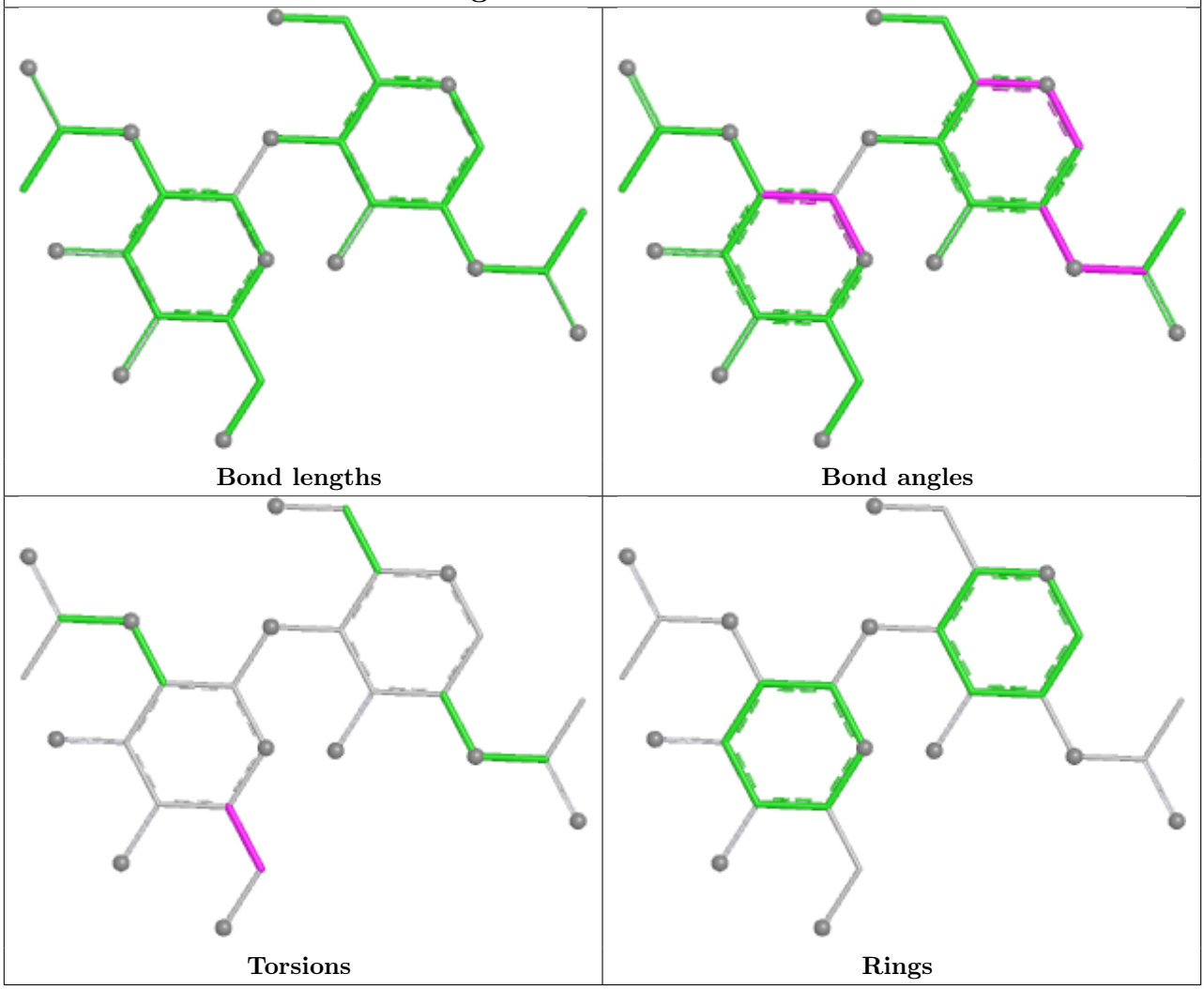


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	B	3320	2	14,14,15	0.45	0	17,19,21	0.86	1 (5%)
5	NAG	A	2458	1	14,14,15	0.74	0	17,19,21	0.85	1 (5%)
5	NAG	A	2260	1	14,14,15	0.50	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	3371	2	14,14,15	0.59	0	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
5	NAG	B	3320	2	-	1/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2260	1	-	3/6/23/26	0/1/1/1
5	NAG	B	3371	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3371	NAG	C2-N2-C7	-3.10	118.75	122.90
5	A	2458	NAG	C2-N2-C7	-2.27	119.86	122.90
5	B	3320	NAG	C2-N2-C7	-2.15	120.02	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3371	NAG	O5-C5-C6-O6
5	B	3371	NAG	C4-C5-C6-O6
5	B	3320	NAG	O5-C5-C6-O6
5	A	2260	NAG	O5-C5-C6-O6
5	A	2260	NAG	C1-C2-N2-C7
5	B	3371	NAG	C1-C2-N2-C7
5	A	2260	NAG	C3-C2-N2-C7
5	A	2458	NAG	C3-C2-N2-C7
5	B	3371	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3320	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2458	NAG	5	0
5	A	2260	NAG	3	0
5	B	3371	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.