



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:57 AM UTC

PDB ID : 4E36 / pdb_00004e36
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 variant N392K
Authors : Birtley, J.R.; Saridakis, E.; Pegias, P.; Stratikos, E.; Mavridis, I.M.
Deposited on : 2012-03-09
Resolution : 3.22 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

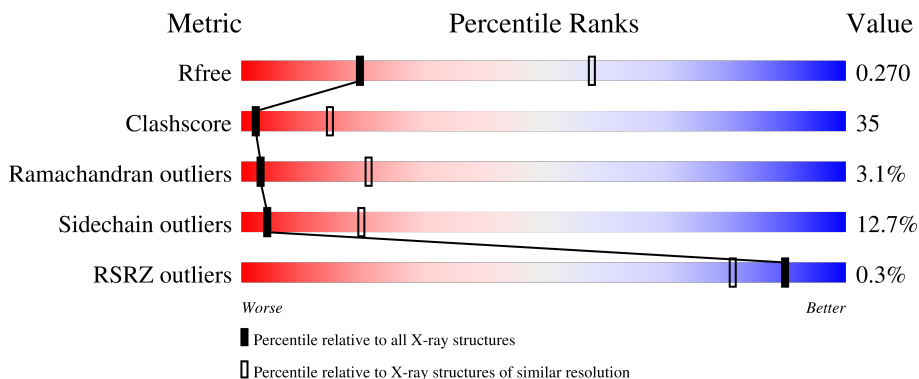
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 Å.

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



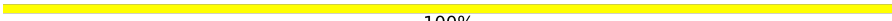
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	967	
1	B	967	
2	C	2	
2	D	2	
2	F	2	

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Mol	Chain	Length	Quality of chain
3	E	4	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14341 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	869	7030	4537	1167	1299	27	2	2	0
1	B	859	6969	4501	1157	1284	27	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	2	VAL	PHE	SEE REMARK 999	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

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



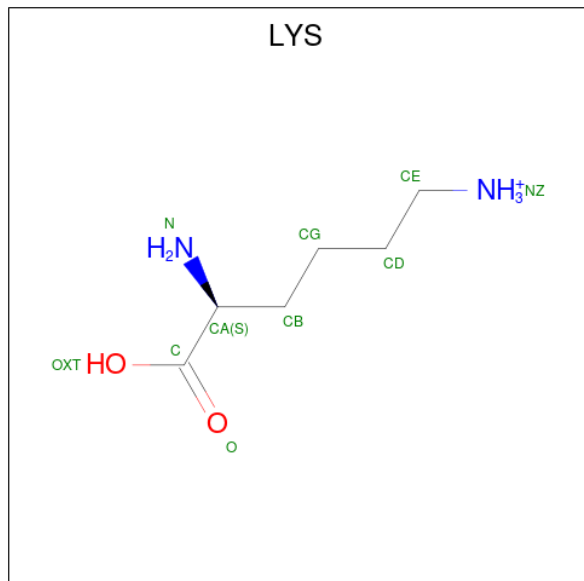
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



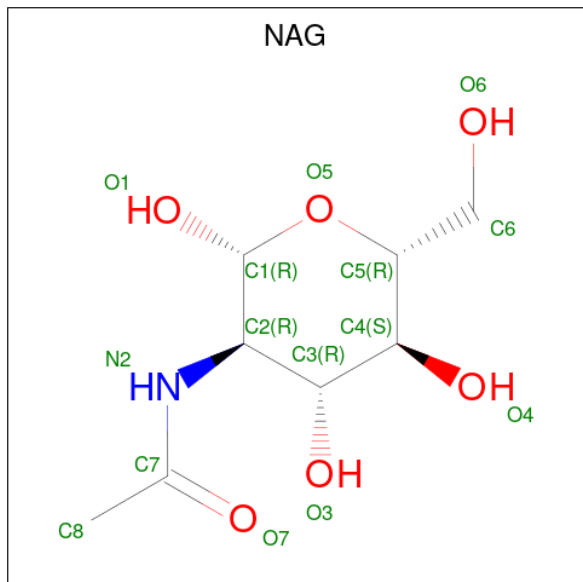
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	B	1	Total	C	N	O	0	0
			10	6	2	2		

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



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

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



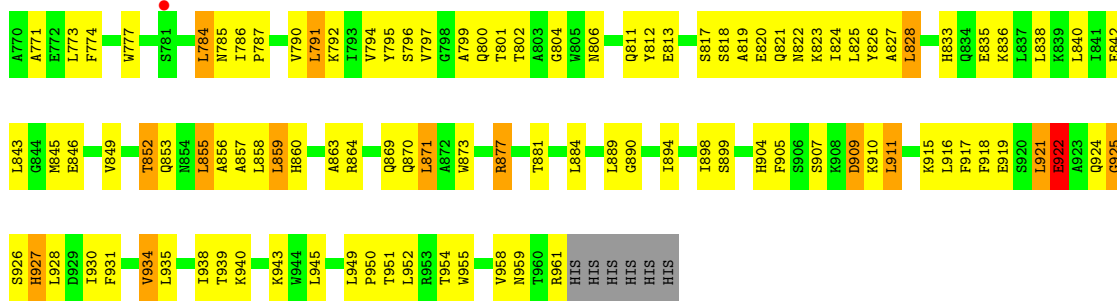
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

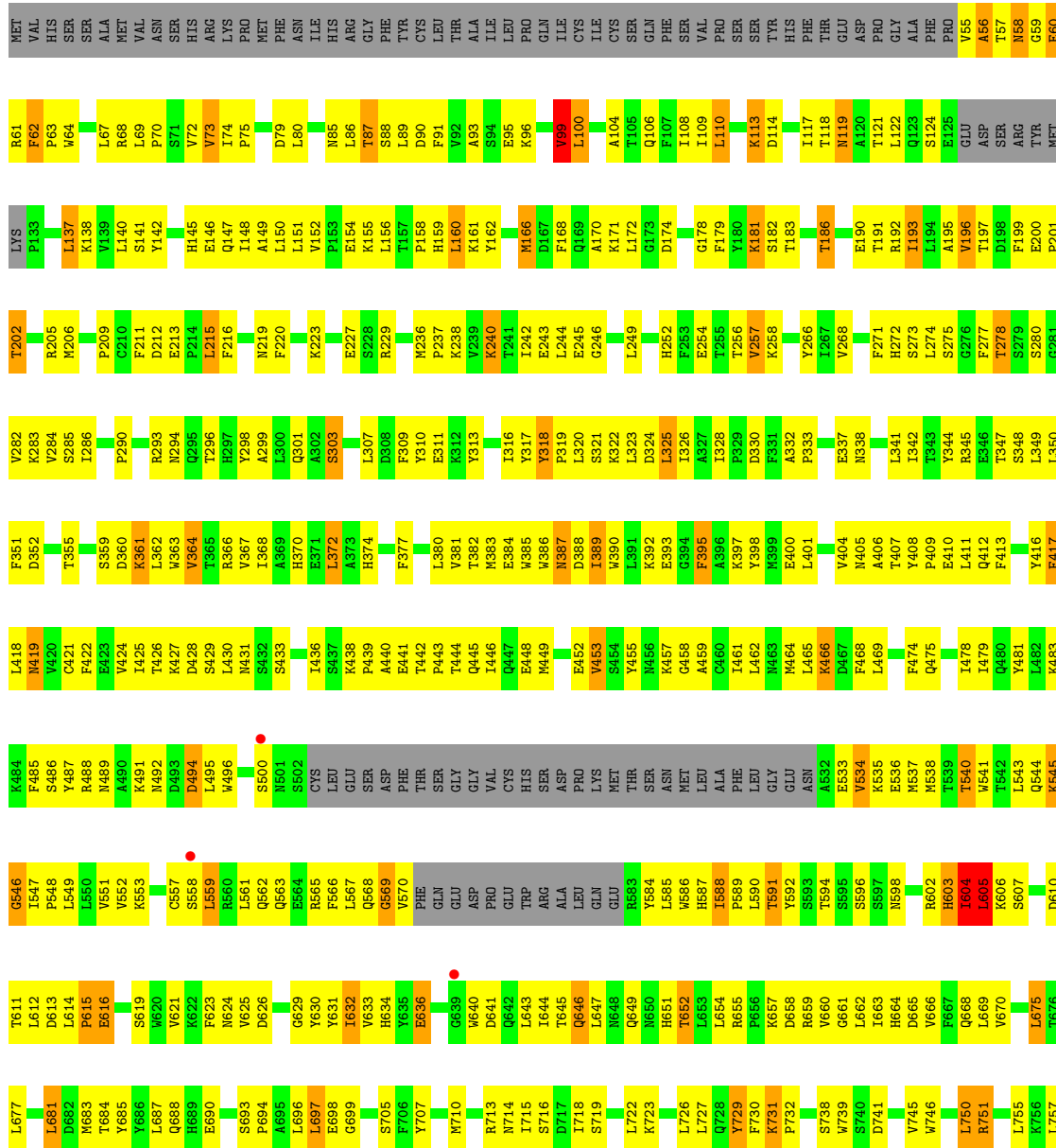
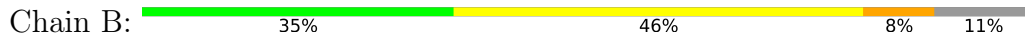
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		

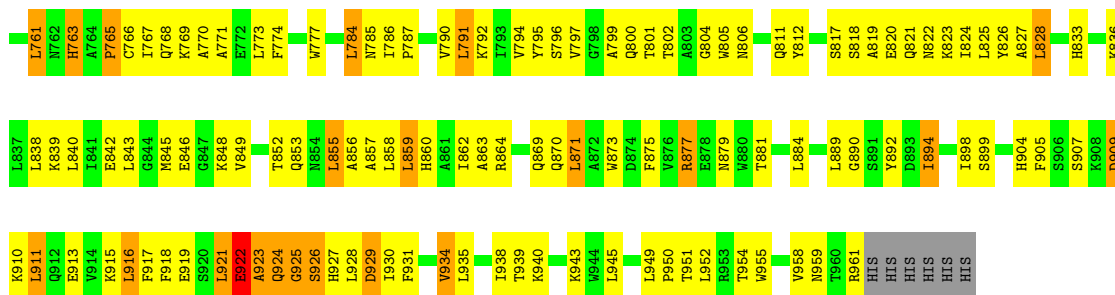
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	66	Total	O	0	0
			66	66		
8	B	40	Total	O	0	0
			40	40		



● Molecule 1: Endoplasmic reticulum aminopeptidase 2





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 100%

MAG1
MAG2

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

Chain F: 50% 50%

MAG1
MAG2

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

Chain E: 100%

MAG1
MAG2
MAN3
MAN4

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.34Å 134.45Å 127.37Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	11.00 – 3.22 11.00 – 3.22	Depositor EDS
% Data completeness (in resolution range)	89.4 (11.00-3.22) 96.5 (11.00-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.209 , 0.261 0.218 , 0.270	Depositor DCC
R_{free} test set	2014 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtrriage
Anisotropy	0.302	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14341	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MES, ZN, MAN, NAG

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	0/7207	0.86	12/9769 (0.1%)
1	B	0.44	0/7139	0.86	10/9674 (0.1%)
All	All	0.46	0/14346	0.86	22/19443 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	62	PHE	CA-C-N	10.56	130.17	119.82
1	B	62	PHE	C-N-CA	10.56	130.17	119.82
1	A	62	PHE	CA-C-N	10.02	129.64	119.82
1	A	62	PHE	C-N-CA	10.02	129.64	119.82
1	A	318	TYR	CA-C-N	7.74	127.64	119.05
1	A	318	TYR	C-N-CA	7.74	127.64	119.05
1	A	531	ASN	N-CA-C	7.47	122.01	109.76
1	B	318	TYR	CA-C-N	6.68	126.93	119.32
1	B	318	TYR	C-N-CA	6.68	126.93	119.32
1	B	87	THR	N-CA-C	-6.28	104.69	112.72
1	A	328	ILE	CA-C-N	6.19	127.58	119.84
1	A	328	ILE	C-N-CA	6.19	127.58	119.84
1	B	328	ILE	CA-C-N	5.81	127.10	119.84
1	B	328	ILE	C-N-CA	5.81	127.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	THR	N-CA-C	-5.62	105.53	112.72
1	A	56	ALA	N-CA-C	-5.53	100.31	107.73
1	A	729	TYR	N-CA-C	-5.46	102.93	110.35
1	B	923	ALA	N-CA-C	-5.25	105.59	112.41
1	B	729	TYR	N-CA-C	-5.21	103.26	110.35
1	A	180	TYR	N-CA-C	5.18	117.74	109.81
1	B	348	SER	N-CA-C	-5.17	107.36	113.97
1	A	348	SER	N-CA-C	-5.05	107.51	113.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	922	GLU	Peptide

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	7030	0	6950	484	1
1	B	6969	0	6937	515	1
2	C	28	0	25	5	0
2	D	28	0	25	2	0
2	F	28	0	25	2	0
3	E	50	0	43	5	0
4	A	10	0	12	0	0
4	B	10	0	12	4	0
5	A	42	0	39	2	0
5	B	14	0	13	0	0
6	A	12	0	12	1	0
6	B	12	0	12	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	66	0	0	5	0
8	B	40	0	0	8	0
All	All	14341	0	14105	1005	2

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 (1005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:HG3	2:C:1:NAG:H82	1.27	1.07
1:A:227:GLU:HG3	2:C:1:NAG:C8	1.84	1.07
1:A:56:ALA:HB1	1:A:57:THR:HA	1.40	1.02
1:B:488:ARG:HG2	1:B:489:ASN:H	1.24	1.00
1:B:741:ASP:OD2	1:B:787:PRO:HB3	1.61	0.99
1:A:741:ASP:OD2	1:A:787:PRO:HB3	1.63	0.97
1:A:205:ARG:HH21	1:A:212:ASP:HB3	1.30	0.97
1:A:488:ARG:HG2	1:A:489:ASN:H	1.26	0.97
1:B:604:ILE:HD12	1:B:604:ILE:H	1.30	0.96
1:B:205:ARG:HH21	1:B:212:ASP:HB3	1.24	0.96
3:E:3:MAN:O3	3:E:4:MAN:H5	1.66	0.94
1:A:355:THR:HG21	1:A:820:GLU:HB2	1.50	0.94
1:B:355:THR:HG21	1:B:820:GLU:HB2	1.47	0.94
1:B:56:ALA:HB2	1:B:62:PHE:H	1.34	0.92
1:B:236:MET:HE3	1:B:256:THR:HA	1.51	0.92
1:A:551:VAL:HG12	1:A:634:HIS:HB3	1.53	0.91
1:A:533:GLU:HA	8:A:1132:HOH:O	1.68	0.90
1:B:551:VAL:HG12	1:B:634:HIS:HB3	1.53	0.90
1:A:122:LEU:HD11	1:A:162:TYR:HB3	1.54	0.90
1:A:604:ILE:H	1:A:604:ILE:HD12	1.37	0.90
1:B:122:LEU:HD11	1:B:162:TYR:HB3	1.53	0.89
1:B:56:ALA:HB1	1:B:61:ARG:HA	1.54	0.88
1:A:236:MET:HE3	1:A:256:THR:HA	1.56	0.88
1:A:528:LEU:HD23	1:A:529:GLY:HA2	1.56	0.88
1:A:73:VAL:HG11	1:A:108:ILE:HG12	1.55	0.87
1:A:666:VAL:HG21	1:A:683:MET:SD	2.15	0.87
3:E:3:MAN:C3	3:E:4:MAN:H5	2.07	0.85
1:B:801:THR:HG23	1:B:804:GLY:H	1.41	0.84
1:B:56:ALA:CB	1:B:61:ARG:HA	2.07	0.84
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.58	0.84
1:B:75:PRO:HG3	1:B:211:PHE:CD1	2.12	0.84
1:A:75:PRO:HG3	1:A:211:PHE:CD1	2.13	0.83
1:B:73:VAL:HG11	1:B:108:ILE:HG12	1.58	0.83
1:B:666:VAL:HG21	1:B:683:MET:SD	2.18	0.83
1:B:57:THR:HB	1:B:58:ASN:CG	2.04	0.82
1:A:191:THR:H	1:B:191:THR:HB	1.42	0.82
1:A:801:THR:HG23	1:A:804:GLY:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:MET:O	1:A:540:THR:HG23	1.79	0.81
1:A:104:ALA:HB2	1:A:158:PRO:HD3	1.61	0.80
1:B:533:GLU:HB3	8:B:1134:HOH:O	1.82	0.80
1:B:278:THR:CG2	1:B:282:VAL:HB	2.12	0.79
1:B:56:ALA:HB2	1:B:62:PHE:N	1.97	0.79
1:A:681:LEU:HB3	1:A:955:TRP:CE2	2.18	0.79
1:B:537:MET:O	1:B:540:THR:HG23	1.82	0.78
1:B:594:THR:HG22	1:B:621:VAL:HG12	1.64	0.78
1:A:278:THR:CG2	1:A:282:VAL:HB	2.13	0.78
1:A:594:THR:HG22	1:A:621:VAL:HG12	1.65	0.78
1:A:152:VAL:HG12	1:A:154:GLU:H	1.50	0.77
1:B:488:ARG:HG2	1:B:489:ASN:N	2.00	0.77
1:B:429:SER:O	1:B:430:LEU:HD23	1.85	0.77
1:B:446:ILE:O	1:B:449:MET:HB2	1.84	0.77
1:B:681:LEU:HB3	1:B:955:TRP:CE2	2.19	0.77
1:B:710:MET:HB3	1:B:719:SER:HB3	1.67	0.77
1:A:429:SER:O	1:A:430:LEU:HD23	1.85	0.76
1:A:56:ALA:CB	1:A:57:THR:HA	2.15	0.76
1:A:125:GLU:OE1	1:A:125:GLU:HA	1.84	0.76
1:A:662:LEU:HB3	1:A:683:MET:HE1	1.67	0.76
1:A:548:PRO:HG3	1:A:586:TRP:CD2	2.21	0.75
1:B:548:PRO:HG3	1:B:586:TRP:CD2	2.22	0.75
1:A:57:THR:HG23	1:A:141:SER:O	1.86	0.75
1:A:138:LYS:HB3	1:A:151:LEU:HB2	1.68	0.75
1:B:662:LEU:HB3	1:B:683:MET:HE1	1.69	0.75
1:A:278:THR:HG21	1:A:282:VAL:HB	1.69	0.75
1:B:278:THR:HG21	1:B:282:VAL:HB	1.67	0.74
1:A:446:ILE:O	1:A:449:MET:HB2	1.88	0.74
1:A:528:LEU:CD2	1:A:529:GLY:HA2	2.18	0.74
1:B:160:LEU:HA	8:B:1127:HOH:O	1.87	0.74
1:A:710:MET:HB3	1:A:719:SER:HB3	1.69	0.74
1:B:338:ASN:HB2	1:B:341:LEU:O	1.86	0.74
1:B:384:GLU:HA	1:B:489:ASN:HD22	1.51	0.73
1:A:227:GLU:CG	2:C:1:NAG:H82	2.12	0.73
1:B:138:LYS:HB3	1:B:151:LEU:HB2	1.68	0.73
1:B:540:THR:O	1:B:544:GLN:HG2	1.88	0.73
1:B:152:VAL:HG12	1:B:154:GLU:H	1.53	0.73
1:B:488:ARG:CG	1:B:489:ASN:H	2.02	0.73
1:B:537:MET:CE	1:B:589:PRO:HG3	2.19	0.73
1:B:56:ALA:CB	1:B:62:PHE:N	2.51	0.73
1:B:677:LEU:HG	1:B:681:LEU:CD2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:SER:O	1:B:821:GLN:HG3	1.89	0.73
1:A:488:ARG:HG2	1:A:489:ASN:N	2.01	0.73
1:A:677:LEU:HG	1:A:681:LEU:CD2	2.18	0.72
1:A:662:LEU:O	1:A:666:VAL:HG23	1.89	0.72
1:B:388:ASP:OD2	1:B:492:ASN:HB2	1.89	0.72
1:B:784:LEU:HD22	1:B:785:ASN:N	2.04	0.72
1:A:118:THR:O	1:A:119:ASN:HB2	1.89	0.71
1:B:688:GLN:HB3	1:B:729:TYR:HE2	1.55	0.71
1:A:540:THR:O	1:A:544:GLN:HG2	1.89	0.71
1:B:408:TYR:HB3	1:B:411:LEU:HG	1.72	0.71
1:B:333:PRO:HG3	4:B:1005:LYS:HE3	1.70	0.71
1:B:954:THR:O	1:B:958:VAL:HG23	1.90	0.71
1:A:528:LEU:CB	1:A:529:GLY:HA2	2.20	0.71
1:B:57:THR:HB	1:B:58:ASN:ND2	2.06	0.71
1:B:602:ARG:O	1:B:603:HIS:HB2	1.91	0.71
1:A:605:LEU:HD12	1:A:606:LYS:N	2.06	0.70
1:B:605:LEU:HD12	1:B:606:LYS:N	2.05	0.70
1:A:954:THR:O	1:A:958:VAL:HG23	1.91	0.70
1:A:433:SER:O	1:A:545:LYS:HD3	1.91	0.70
1:B:311:GLU:HG2	1:B:317:TYR:HA	1.73	0.70
1:A:784:LEU:HD22	1:A:785:ASN:N	2.05	0.70
1:B:662:LEU:O	1:B:666:VAL:HG23	1.91	0.70
1:B:918:PHE:CE2	1:B:931:PHE:HA	2.26	0.70
1:A:537:MET:CE	1:A:589:PRO:HG3	2.21	0.70
1:A:615:PRO:O	1:A:616:GLU:HB2	1.91	0.70
1:A:401:LEU:HD12	1:A:417:PHE:CD2	2.27	0.70
1:B:797:VAL:O	1:B:800:GLN:HG2	1.92	0.70
1:B:385:TRP:HD1	1:B:387:ASN:ND2	1.90	0.69
1:A:488:ARG:CG	1:A:489:ASN:H	2.03	0.69
1:A:688:GLN:HB3	1:A:729:TYR:HE2	1.55	0.69
1:B:828:LEU:HD23	1:B:840:LEU:HD21	1.74	0.69
1:A:465:LEU:HD13	1:A:538:MET:SD	2.32	0.69
1:A:338:ASN:HB2	1:A:341:LEU:O	1.93	0.69
1:B:924:GLN:O	1:B:926:SER:N	2.26	0.68
1:B:545:LYS:CG	1:B:546:GLY:H	2.06	0.68
1:B:452:GLU:H	1:B:452:GLU:CD	2.01	0.68
1:B:615:PRO:O	1:B:616:GLU:HB2	1.91	0.68
1:A:828:LEU:HD23	1:A:840:LEU:HD21	1.76	0.68
1:A:602:ARG:O	1:A:603:HIS:HB2	1.93	0.68
1:A:727:LEU:HD11	1:A:763:HIS:HB2	1.75	0.68
1:A:364:VAL:O	1:A:368:ILE:HG13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:TRP:CZ2	1:B:877:ARG:HD3	2.29	0.68
1:A:382:THR:O	1:A:489:ASN:HA	1.94	0.68
1:A:385:TRP:HD1	1:A:387:ASN:ND2	1.92	0.68
1:A:918:PHE:CE2	1:A:931:PHE:HA	2.28	0.68
1:B:442:THR:HG23	1:B:445:GLN:H	1.59	0.68
1:B:563:GLN:HG3	1:B:563:GLN:O	1.94	0.68
1:A:442:THR:HG23	1:A:445:GLN:H	1.58	0.67
1:A:67:LEU:HA	1:A:145:HIS:HD2	1.60	0.67
1:B:67:LEU:HA	1:B:145:HIS:HD2	1.59	0.67
1:B:468:PHE:CD2	1:B:469:LEU:HG	2.29	0.67
1:A:311:GLU:HG2	1:A:317:TYR:HA	1.77	0.67
1:A:195:ALA:HB3	1:A:268:VAL:HG22	1.76	0.67
1:B:918:PHE:CE2	1:B:934:VAL:HG11	2.30	0.67
1:A:388:ASP:OD2	1:A:492:ASN:HB2	1.95	0.67
1:B:419:ASN:N	1:B:419:ASN:HD22	1.93	0.67
1:B:56:ALA:HB1	1:B:61:ARG:CA	2.23	0.66
1:B:441:GLU:HB2	1:B:445:GLN:OE1	1.96	0.66
1:B:626:ASP:OD1	1:B:655:ARG:HD3	1.95	0.66
1:A:419:ASN:N	1:A:419:ASN:HD22	1.94	0.66
1:B:677:LEU:HB3	1:B:951:THR:HG21	1.75	0.66
1:B:626:ASP:HA	1:B:657:LYS:HB2	1.78	0.66
1:B:727:LEU:HD21	1:B:761:LEU:HB3	1.78	0.66
1:B:118:THR:O	1:B:119:ASN:HB2	1.93	0.66
1:A:452:GLU:CD	1:A:452:GLU:H	2.03	0.65
1:A:533:GLU:HG2	1:A:533:GLU:O	1.95	0.65
1:B:298:TYR:CZ	1:B:361:LYS:HD2	2.31	0.65
1:B:718:ILE:HD12	1:B:949:LEU:HD11	1.77	0.65
1:A:384:GLU:HA	1:A:489:ASN:HD22	1.59	0.65
1:A:408:TYR:HB3	1:A:411:LEU:HG	1.76	0.65
1:A:227:GLU:HG3	2:C:1:NAG:H83	1.78	0.65
1:A:545:LYS:CG	1:A:546:GLY:H	2.10	0.65
1:A:918:PHE:CE2	1:A:934:VAL:HG11	2.31	0.65
1:A:468:PHE:CD2	1:A:469:LEU:HG	2.32	0.65
1:B:382:THR:O	1:B:489:ASN:HA	1.96	0.65
1:B:466:LYS:HB2	1:B:474:PHE:CD2	2.32	0.65
1:A:461:ILE:HG13	1:A:462:LEU:N	2.11	0.65
1:A:626:ASP:HA	1:A:657:LYS:HB2	1.78	0.65
1:B:433:SER:O	1:B:545:LYS:HD3	1.97	0.65
1:B:784:LEU:HD22	1:B:785:ASN:H	1.62	0.65
1:A:197:THR:HG23	1:A:266:TYR:O	1.97	0.64
1:A:905:PHE:HB2	1:A:938:ILE:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ASP:OD1	1:A:655:ARG:HD3	1.96	0.64
1:A:784:LEU:HD22	1:A:785:ASN:H	1.61	0.64
1:B:69:LEU:HD23	1:B:147:GLN:HE21	1.63	0.64
1:B:236:MET:HB3	1:B:254:GLU:HB3	1.80	0.64
1:A:677:LEU:HB3	1:A:951:THR:HG21	1.80	0.64
1:A:386:TRP:CD1	1:A:446:ILE:HD13	2.33	0.64
1:A:441:GLU:HB2	1:A:445:GLN:OE1	1.98	0.64
1:B:152:VAL:HG21	1:B:156:LEU:HD21	1.79	0.64
1:A:457:LYS:HE3	1:A:630:TYR:CE2	2.33	0.64
1:B:195:ALA:HB3	1:B:268:VAL:HG22	1.79	0.64
1:B:401:LEU:HD12	1:B:417:PHE:CD2	2.33	0.64
1:B:457:LYS:HE3	1:B:630:TYR:CE2	2.33	0.64
1:B:659:ARG:HD2	1:B:690:GLU:OE1	1.98	0.64
1:B:777:TRP:HB2	1:B:786:ILE:HD11	1.79	0.64
3:E:3:MAN:H3	3:E:4:MAN:H5	1.78	0.64
1:B:727:LEU:HD11	1:B:763:HIS:HB2	1.79	0.64
1:B:86:LEU:HD21	1:B:268:VAL:HG23	1.80	0.64
1:B:863:ALA:HB1	1:B:904:HIS:HE1	1.62	0.64
1:B:75:PRO:HG2	1:B:216:PHE:HB3	1.80	0.64
1:B:461:ILE:HG13	1:B:462:LEU:N	2.11	0.64
1:A:777:TRP:HB2	1:A:786:ILE:HD11	1.80	0.64
1:A:797:VAL:O	1:A:800:GLN:HG2	1.97	0.64
1:B:386:TRP:CD1	1:B:446:ILE:HD13	2.33	0.64
1:B:537:MET:HE2	1:B:589:PRO:HG3	1.78	0.64
1:B:833:HIS:HB2	1:B:836:LYS:HG3	1.79	0.63
1:A:299:ALA:O	1:A:303:SER:OG	2.16	0.63
1:A:817:SER:O	1:A:821:GLN:HG3	1.99	0.63
1:B:122:LEU:CB	1:B:137:LEU:HD21	2.28	0.63
1:B:323:LEU:HD11	1:B:342:ILE:HD12	1.80	0.63
1:A:563:GLN:O	1:A:563:GLN:HG3	1.98	0.63
1:A:718:ILE:HD12	1:A:949:LEU:HD11	1.79	0.63
1:B:915:LYS:O	1:B:919:GLU:HG2	1.97	0.63
1:A:537:MET:HE2	1:A:589:PRO:HG3	1.80	0.63
1:B:364:VAL:O	1:B:368:ILE:HG13	1.98	0.63
1:B:605:LEU:HD12	1:B:606:LYS:H	1.63	0.63
1:B:677:LEU:HB3	1:B:951:THR:CG2	2.29	0.63
1:A:122:LEU:CB	1:A:137:LEU:HD21	2.29	0.62
1:B:56:ALA:O	1:B:57:THR:HG23	1.98	0.62
1:A:410:GLU:O	1:A:412:GLN:HG3	1.99	0.62
1:B:332:ALA:HB3	1:B:333:PRO:HD3	1.81	0.62
1:B:905:PHE:HB2	1:B:938:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:GLU:O	1:A:583:ARG:CB	2.47	0.62
1:A:915:LYS:O	1:A:919:GLU:HG2	1.98	0.62
1:B:141:SER:HA	1:B:148:ILE:HG22	1.81	0.62
1:A:457:LYS:HE3	1:A:630:TYR:HE2	1.63	0.62
1:B:812:TYR:CE1	1:B:821:GLN:HB3	2.35	0.62
1:B:122:LEU:HB3	1:B:137:LEU:HD21	1.82	0.62
1:B:412:GLN:OE1	1:B:746:TRP:HD1	1.82	0.62
1:B:465:LEU:HD13	1:B:538:MET:SD	2.38	0.61
1:B:481:TYR:O	1:B:485:PHE:HD2	1.83	0.61
1:B:646:GLN:HA	1:B:646:GLN:HE21	1.63	0.61
1:A:400:GLU:O	1:A:404:VAL:HG23	2.01	0.61
1:B:299:ALA:O	1:B:303:SER:OG	2.17	0.61
1:A:945:LEU:HD22	1:A:949:LEU:HD22	1.81	0.61
1:B:777:TRP:HB2	1:B:786:ILE:CD1	2.30	0.61
1:B:457:LYS:HE3	1:B:630:TYR:HE2	1.63	0.61
1:B:475:GLN:O	1:B:479:ILE:HG12	2.01	0.61
1:A:727:LEU:HD21	1:A:761:LEU:HB3	1.82	0.61
1:B:400:GLU:O	1:B:404:VAL:HG23	2.00	0.61
1:B:448:GLU:OE2	1:B:928:LEU:HA	2.00	0.61
1:A:69:LEU:HD23	1:A:147:GLN:HE21	1.65	0.61
1:A:152:VAL:HG21	1:A:156:LEU:HD21	1.81	0.61
1:A:448:GLU:OE2	1:A:928:LEU:HA	2.01	0.61
1:A:873:TRP:CZ2	1:A:877:ARG:HD3	2.35	0.61
1:A:236:MET:HB3	1:A:254:GLU:HB3	1.83	0.61
1:A:309:PHE:C	1:A:309:PHE:CD2	2.79	0.61
1:B:945:LEU:HD22	1:B:949:LEU:HD22	1.83	0.61
1:A:442:THR:HG22	1:A:445:GLN:NE2	2.16	0.61
1:A:647:LEU:HD11	1:A:683:MET:HE3	1.81	0.61
1:B:205:ARG:NH2	1:B:212:ASP:HB3	2.07	0.61
1:A:298:TYR:CZ	1:A:361:LYS:HD2	2.36	0.61
1:A:323:LEU:HD11	1:A:342:ILE:HD12	1.83	0.60
1:A:99:VAL:HG12	1:A:100:LEU:H	1.65	0.60
1:B:325:LEU:HD12	1:B:325:LEU:N	2.16	0.60
1:A:220:PHE:O	1:A:256:THR:HG23	2.01	0.60
1:A:838:LEU:HD23	1:A:871:LEU:HD21	1.83	0.60
1:B:313:TYR:HE2	1:B:478:ILE:HD11	1.66	0.60
1:A:605:LEU:HD12	1:A:606:LYS:H	1.66	0.60
1:A:860:HIS:HD2	1:A:860:HIS:O	1.83	0.60
1:B:442:THR:HG22	1:B:445:GLN:NE2	2.17	0.60
1:A:205:ARG:NH2	1:A:212:ASP:HB3	2.11	0.60
1:B:99:VAL:HG12	1:B:100:LEU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD21	1:A:268:VAL:HG23	1.83	0.60
1:A:528:LEU:HB3	1:A:529:GLY:CA	2.31	0.60
1:A:863:ALA:HB1	1:A:904:HIS:HE1	1.66	0.60
1:B:545:LYS:CG	1:B:546:GLY:N	2.65	0.60
1:A:141:SER:HA	1:A:148:ILE:HG22	1.84	0.60
1:A:227:GLU:HB3	1:A:229:ARG:HG2	1.84	0.60
1:A:156:LEU:HD12	1:A:162:TYR:CE1	2.37	0.60
1:B:464:MET:HG3	1:B:629:GLY:HA2	1.83	0.60
1:A:122:LEU:HB3	1:A:137:LEU:HD21	1.82	0.60
1:A:407:THR:C	1:A:409:PRO:HD3	2.27	0.60
1:B:332:ALA:O	1:B:345:ARG:NH1	2.34	0.60
1:B:763:HIS:O	1:B:767:ILE:HG22	2.01	0.60
1:A:286:ILE:CG2	1:A:296:THR:HB	2.32	0.59
1:B:62:PHE:CE1	1:B:142:TYR:HB2	2.37	0.59
1:B:158:PRO:HB2	1:B:159:HIS:HD2	1.67	0.59
1:A:442:THR:O	1:A:446:ILE:HG13	2.03	0.59
1:A:183:THR:HA	1:A:192:ARG:O	2.03	0.59
1:B:309:PHE:C	1:B:309:PHE:CD2	2.79	0.59
1:B:431:ASN:HA	1:B:565:ARG:HH22	1.67	0.59
1:B:624:ASN:HD21	1:B:629:GLY:H	1.50	0.59
1:A:158:PRO:HB2	1:A:159:HIS:HD2	1.67	0.59
1:B:552:VAL:HG12	1:B:561:LEU:HD23	1.85	0.59
1:B:647:LEU:HD11	1:B:683:MET:HE3	1.84	0.59
1:A:56:ALA:HB1	1:A:57:THR:CA	2.27	0.59
1:A:731:LYS:N	1:A:732:PRO:HD2	2.16	0.59
1:A:763:HIS:O	1:A:767:ILE:HG22	2.02	0.59
1:A:833:HIS:HB2	1:A:836:LYS:HG3	1.83	0.59
1:A:325:LEU:N	1:A:325:LEU:HD12	2.17	0.59
1:A:412:GLN:OE1	1:A:746:TRP:HD1	1.85	0.59
1:A:545:LYS:CG	1:A:546:GLY:N	2.66	0.59
1:B:286:ILE:CG2	1:B:296:THR:HB	2.32	0.59
1:A:486:SER:HB3	1:A:487:TYR:CD2	2.38	0.59
1:B:714:ASN:O	1:B:716:SER:N	2.36	0.59
1:A:475:GLN:O	1:A:479:ILE:HG12	2.01	0.59
1:A:398:TYR:OH	1:A:466:LYS:HD3	2.03	0.59
1:A:442:THR:OG1	1:A:443:PRO:HD2	2.01	0.59
1:A:659:ARG:HD2	1:A:690:GLU:OE1	2.01	0.59
1:B:56:ALA:HA	1:B:62:PHE:HB2	1.84	0.59
1:B:464:MET:HE1	1:B:541:TRP:CE2	2.38	0.59
1:B:855:LEU:HD22	1:B:859:LEU:HD22	1.83	0.59
1:B:918:PHE:CZ	1:B:934:VAL:HG11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:GLU:O	1:B:412:GLN:HG3	2.03	0.58
1:B:604:ILE:H	1:B:604:ILE:CD1	2.06	0.58
1:A:566:PHE:CE2	1:A:632:ILE:HD12	2.38	0.58
1:A:855:LEU:HD22	1:A:859:LEU:HD22	1.86	0.58
1:B:407:THR:C	1:B:409:PRO:HD3	2.28	0.58
1:A:646:GLN:HA	1:A:646:GLN:HE21	1.67	0.58
1:A:466:LYS:HB2	1:A:474:PHE:CD2	2.38	0.58
1:B:466:LYS:O	1:B:466:LYS:HG3	2.04	0.58
1:A:313:TYR:HE2	1:A:478:ILE:HD11	1.69	0.58
1:B:355:THR:HG21	1:B:820:GLU:CB	2.29	0.58
1:A:481:TYR:O	1:A:485:PHE:HD2	1.87	0.58
1:B:220:PHE:O	1:B:256:THR:HG23	2.04	0.58
1:B:889:LEU:HD21	1:B:925:GLY:HA2	1.86	0.58
1:A:60:GLU:HB3	8:A:1153:HOH:O	2.04	0.57
1:A:431:ASN:HA	1:A:565:ARG:HH22	1.68	0.57
1:A:889:LEU:HD13	1:A:928:LEU:HD21	1.85	0.57
1:B:156:LEU:HD12	1:B:162:TYR:CE1	2.38	0.57
1:B:486:SER:HB3	1:B:487:TYR:CD2	2.38	0.57
1:B:731:LYS:N	1:B:732:PRO:HD2	2.18	0.57
1:A:918:PHE:CZ	1:A:934:VAL:HG11	2.39	0.57
1:B:106:GLN:HE21	1:B:155:LYS:NZ	2.02	0.57
1:A:604:ILE:H	1:A:604:ILE:CD1	2.12	0.57
1:B:710:MET:O	1:B:713:ARG:O	2.22	0.57
1:B:442:THR:O	1:B:446:ILE:HG13	2.04	0.57
1:A:75:PRO:HG2	1:A:216:PHE:HB3	1.86	0.57
1:A:567:LEU:HD11	1:A:581:GLN:N	2.20	0.57
1:B:85:ASN:HB3	1:B:88:SER:HB3	1.86	0.57
1:A:466:LYS:HG3	1:A:466:LYS:O	2.04	0.57
1:A:666:VAL:O	1:A:670:VAL:HG23	2.05	0.57
1:B:272:HIS:CE1	1:B:290:PRO:HB3	2.40	0.57
1:B:566:PHE:CE2	1:B:632:ILE:HD12	2.40	0.57
1:B:727:LEU:O	1:B:731:LYS:HB2	2.03	0.57
1:A:677:LEU:HB3	1:A:951:THR:CG2	2.35	0.57
1:B:544:GLN:NE2	1:B:584:TYR:HD1	2.03	0.57
1:A:786:ILE:HG21	1:A:791:LEU:HA	1.87	0.56
1:A:828:LEU:HB3	1:A:840:LEU:HD11	1.87	0.56
1:B:282:VAL:HG21	1:B:318:TYR:HD2	1.68	0.56
1:B:333:PRO:CG	4:B:1005:LYS:HE3	2.35	0.56
1:B:398:TYR:OH	1:B:466:LYS:HD3	2.05	0.56
1:A:272:HIS:CE1	1:A:290:PRO:HB3	2.39	0.56
1:B:889:LEU:HD13	1:B:928:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:GLN:O	1:B:926:SER:HA	2.06	0.56
1:A:332:ALA:O	1:A:345:ARG:NH1	2.37	0.56
1:A:528:LEU:HB3	1:A:529:GLY:HA2	1.86	0.56
1:A:714:ASN:O	1:A:716:SER:N	2.38	0.56
1:A:777:TRP:HB2	1:A:786:ILE:CD1	2.35	0.56
1:B:442:THR:OG1	1:B:443:PRO:HD2	2.06	0.56
1:B:730:PHE:C	1:B:732:PRO:HD2	2.31	0.56
1:A:693:SER:N	1:A:694:PRO:HD2	2.21	0.56
1:A:419:ASN:HD22	1:A:419:ASN:H	1.54	0.56
1:B:792:LYS:HG2	1:B:826:TYR:CD2	2.40	0.56
1:A:730:PHE:C	1:A:732:PRO:HD2	2.30	0.56
1:B:421:CYS:O	1:B:424:VAL:HG12	2.04	0.56
1:A:67:LEU:HA	1:A:145:HIS:CD2	2.40	0.56
1:A:792:LYS:HG2	1:A:826:TYR:CD2	2.40	0.56
1:A:464:MET:HE1	1:A:541:TRP:CE2	2.41	0.56
1:B:929:ASP:HA	8:B:1106:HOH:O	2.05	0.56
1:A:731:LYS:N	1:A:732:PRO:CD	2.68	0.56
1:B:666:VAL:O	1:B:670:VAL:HG23	2.05	0.56
1:B:828:LEU:HB3	1:B:840:LEU:HD11	1.88	0.56
1:B:928:LEU:HB2	1:B:930:ILE:HG22	1.87	0.56
1:A:332:ALA:HB3	1:A:333:PRO:HD3	1.88	0.56
1:A:257:VAL:HG23	1:A:258:LYS:O	2.06	0.55
1:B:182:SER:HB2	1:B:330:ASP:HB2	1.87	0.55
1:A:812:TYR:CE1	1:A:821:GLN:HB3	2.42	0.55
1:B:838:LEU:HD23	1:B:871:LEU:HD21	1.88	0.55
1:A:548:PRO:HG3	1:A:586:TRP:CE3	2.41	0.55
1:B:197:THR:HG23	1:B:266:TYR:O	2.07	0.55
1:B:924:GLN:O	1:B:925:GLY:C	2.48	0.55
1:A:819:ALA:O	1:A:823:LYS:HG3	2.06	0.55
1:A:877:ARG:HG3	1:A:917:PHE:CD1	2.41	0.55
1:B:693:SER:N	1:B:694:PRO:HD2	2.22	0.55
1:B:731:LYS:HE2	1:B:763:HIS:CE1	2.42	0.55
1:A:581:GLN:HG3	1:A:582:GLU:H	1.71	0.55
1:B:349:LEU:C	1:B:350:LEU:HD23	2.30	0.55
1:B:892:TYR:CE1	6:B:1010:MES:H52	2.42	0.55
1:A:421:CYS:O	1:A:424:VAL:HG12	2.06	0.55
1:B:89:LEU:HD13	1:B:181:LYS:HD3	1.87	0.55
1:A:533:GLU:O	1:A:533:GLU:CG	2.54	0.55
1:A:124:SER:HB2	1:A:131:MET:O	2.07	0.55
1:A:811:GLN:HA	1:A:811:GLN:NE2	2.21	0.55
1:B:921:LEU:O	1:B:922:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HA	1:B:145:HIS:CD2	2.39	0.55
1:B:424:VAL:HG21	1:B:457:LYS:HB2	1.88	0.55
1:B:777:TRP:HB2	1:B:784:LEU:HD12	1.89	0.54
1:A:552:VAL:HG12	1:A:561:LEU:HD23	1.89	0.54
1:B:227:GLU:HB3	1:B:229:ARG:HG2	1.90	0.54
1:B:257:VAL:HG23	1:B:258:LYS:O	2.07	0.54
1:B:819:ALA:O	1:B:823:LYS:HG3	2.08	0.54
1:A:113:LYS:HG2	1:A:206:MET:HG2	1.90	0.54
1:A:229:ARG:NH2	1:B:190:GLU:OE2	2.34	0.54
1:A:710:MET:CB	1:A:719:SER:HB3	2.37	0.54
1:A:624:ASN:HB2	1:A:631:TYR:CE2	2.42	0.54
1:A:624:ASN:HD21	1:A:629:GLY:H	1.56	0.54
1:B:624:ASN:HB2	1:B:631:TYR:CE2	2.42	0.54
1:B:183:THR:HA	1:B:192:ARG:O	2.07	0.54
1:B:786:ILE:HG21	1:B:791:LEU:HA	1.89	0.54
1:B:838:LEU:O	1:B:842:GLU:HG3	2.08	0.54
1:A:258:LYS:HG2	2:D:1:NAG:O6	2.07	0.54
1:A:581:GLN:HB3	1:A:584:TYR:HE2	1.72	0.54
1:A:738:SER:O	1:A:751:ARG:CD	2.56	0.54
1:B:487:TYR:HA	8:B:1104:HOH:O	2.08	0.54
1:B:877:ARG:HG3	1:B:917:PHE:CD1	2.42	0.54
1:A:349:LEU:C	1:A:350:LEU:HD23	2.33	0.54
1:A:566:PHE:CD2	1:A:632:ILE:HD12	2.43	0.54
1:B:56:ALA:HB1	1:B:61:ARG:C	2.32	0.54
1:B:236:MET:HE3	1:B:256:THR:CA	2.30	0.54
1:B:496:TRP:CE3	1:B:496:TRP:HA	2.43	0.54
1:A:62:PHE:CE1	1:A:142:TYR:HB2	2.42	0.54
1:A:182:SER:HB2	1:A:330:ASP:HB2	1.89	0.54
1:A:435:PRO:HA	8:A:1143:HOH:O	2.08	0.54
1:B:811:GLN:HA	1:B:811:GLN:NE2	2.22	0.54
1:B:56:ALA:CB	1:B:61:ARG:CA	2.81	0.53
1:B:388:ASP:CG	1:B:492:ASN:HB2	2.33	0.53
1:A:85:ASN:HB3	1:A:88:SER:HB3	1.91	0.53
1:A:928:LEU:HB2	1:A:930:ILE:HG22	1.90	0.53
1:B:731:LYS:N	1:B:732:PRO:CD	2.70	0.53
1:A:650:ASN:OD1	5:A:1007:NAG:N2	2.41	0.53
1:A:123:GLN:HG2	1:A:133:PRO:HA	1.90	0.53
1:B:62:PHE:CD1	1:B:142:TYR:HB2	2.43	0.53
1:B:634:HIS:HE1	1:B:675:LEU:CD1	2.22	0.53
1:A:710:MET:O	1:A:713:ARG:O	2.27	0.53
1:A:870:GLN:O	1:A:871:LEU:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:HG2	1:A:246:GLY:N	2.23	0.53
1:B:405:ASN:O	1:B:409:PRO:HG3	2.09	0.53
1:B:640:TRP:CZ3	1:B:666:VAL:HG22	2.44	0.53
1:B:738:SER:O	1:B:751:ARG:CD	2.57	0.53
1:A:286:ILE:HG21	1:A:296:THR:HB	1.91	0.53
1:B:710:MET:CB	1:B:719:SER:HB3	2.37	0.53
1:B:934:VAL:O	1:B:938:ILE:HG13	2.08	0.53
1:A:838:LEU:O	1:A:842:GLU:HG3	2.09	0.52
2:F:1:NAG:H61	2:F:2:NAG:H82	1.89	0.52
1:A:429:SER:C	1:A:430:LEU:HD23	2.33	0.52
1:B:285:SER:HB2	1:B:324:ASP:OD1	2.10	0.52
1:B:615:PRO:O	1:B:616:GLU:CB	2.58	0.52
1:A:186:THR:HG23	1:A:190:GLU:O	2.08	0.52
1:B:56:ALA:CB	1:B:62:PHE:H	2.10	0.52
1:A:401:LEU:C	1:A:401:LEU:HD23	2.35	0.52
1:A:528:LEU:CB	1:A:529:GLY:CA	2.87	0.52
1:B:557:CYS:O	1:B:613:ASP:HA	2.10	0.52
1:A:118:THR:O	1:A:119:ASN:CB	2.58	0.52
1:A:123:GLN:NE2	1:A:133:PRO:HB3	2.25	0.52
1:A:925:GLY:O	1:A:926:SER:C	2.53	0.52
1:B:100:LEU:HD13	1:B:161:LYS:HG2	1.90	0.52
1:B:805:TRP:HH2	1:B:839:LYS:HD3	1.75	0.52
1:A:109:ILE:HD11	1:A:149:ALA:HB2	1.91	0.52
1:A:202:THR:O	1:A:202:THR:OG1	2.27	0.52
1:A:634:HIS:HE1	1:A:675:LEU:CD1	2.23	0.52
1:B:363:TRP:O	1:B:366:ARG:HB2	2.09	0.52
1:B:860:HIS:HD2	1:B:860:HIS:O	1.93	0.52
1:B:923:ALA:O	1:B:924:GLN:HB2	2.10	0.51
1:A:355:THR:HG21	1:A:820:GLU:CB	2.33	0.51
1:B:605:LEU:HD12	1:B:607:SER:H	1.75	0.51
1:B:665:ASP:O	1:B:669:LEU:HG	2.10	0.51
1:A:528:LEU:HD23	1:A:529:GLY:CA	2.34	0.51
1:B:56:ALA:HB1	1:B:62:PHE:N	2.25	0.51
1:B:186:THR:HG23	1:B:190:GLU:O	2.10	0.51
1:B:419:ASN:HD22	1:B:419:ASN:H	1.55	0.51
1:A:485:PHE:O	1:A:486:SER:C	2.52	0.51
1:B:429:SER:C	1:B:430:LEU:HD23	2.36	0.51
1:B:545:LYS:HG2	1:B:546:GLY:N	2.26	0.51
1:B:677:LEU:HG	1:B:681:LEU:HD23	1.90	0.51
1:A:282:VAL:HG21	1:A:318:TYR:HD2	1.75	0.51
1:A:615:PRO:O	1:A:616:GLU:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HG	1:A:681:LEU:HD23	1.93	0.51
1:B:863:ALA:HA	1:B:869:GLN:HA	1.92	0.51
1:A:293:ARG:NH2	3:E:3:MAN:O2	2.40	0.51
1:A:934:VAL:O	1:A:938:ILE:HG13	2.11	0.51
1:B:431:ASN:HA	1:B:565:ARG:NH2	2.25	0.51
1:B:777:TRP:HH2	1:B:811:GLN:HG2	1.76	0.51
1:A:345:ARG:NH2	1:A:853:GLN:HB2	2.26	0.51
1:A:496:TRP:HA	1:A:496:TRP:CE3	2.46	0.51
4:B:1005:LYS:HB3	6:B:1010:MES:O1S	2.11	0.51
1:A:589:PRO:C	1:A:590:LEU:HD23	2.36	0.50
1:A:919:GLU:O	1:A:922:GLU:HB2	2.11	0.50
1:B:553:LYS:HB2	1:B:636:GLU:OE2	2.11	0.50
1:B:479:ILE:O	1:B:483:LYS:HG3	2.11	0.50
1:B:681:LEU:HB3	1:B:955:TRP:CZ2	2.46	0.50
1:B:428:ASP:OD2	1:B:457:LYS:HD2	2.11	0.50
1:B:545:LYS:HG3	1:B:546:GLY:H	1.75	0.50
1:B:892:TYR:CD1	6:B:1010:MES:H71	2.47	0.50
1:A:431:ASN:HA	1:A:565:ARG:NH2	2.26	0.50
1:A:442:THR:CG2	1:A:445:GLN:HG3	2.41	0.50
1:A:777:TRP:HB2	1:A:784:LEU:HD12	1.92	0.50
1:A:935:LEU:O	1:A:939:THR:HG23	2.10	0.50
1:A:69:LEU:HD22	1:A:109:ILE:HG22	1.92	0.50
1:A:191:THR:HB	1:B:191:THR:H	1.76	0.50
1:A:405:ASN:O	1:A:409:PRO:HG3	2.12	0.50
1:A:860:HIS:O	1:A:860:HIS:CD2	2.65	0.50
1:A:860:HIS:C	1:A:860:HIS:CD2	2.89	0.50
1:A:911:LEU:O	1:A:915:LYS:HB2	2.12	0.50
1:B:924:GLN:O	1:B:926:SER:CA	2.60	0.50
1:A:651:HIS:C	1:A:651:HIS:CD2	2.89	0.50
1:A:219:ASN:OD1	1:A:258:LYS:HD3	2.11	0.50
1:A:388:ASP:CG	1:A:492:ASN:HB2	2.37	0.50
1:A:917:PHE:CE2	1:A:921:LEU:HD11	2.46	0.50
1:B:411:LEU:HA	1:B:745:VAL:HG21	1.93	0.50
1:B:845:MET:SD	1:B:855:LEU:HD11	2.52	0.50
1:A:662:LEU:HB3	1:A:683:MET:CE	2.41	0.50
1:B:442:THR:CG2	1:B:445:GLN:HG3	2.41	0.49
1:B:566:PHE:CD2	1:B:632:ILE:HD12	2.46	0.49
1:A:500:SER:HB3	1:A:534:VAL:HB	1.94	0.49
1:A:557:CYS:O	1:A:613:ASP:HA	2.12	0.49
1:A:681:LEU:HB3	1:A:955:TRP:CZ2	2.46	0.49
1:A:863:ALA:HA	1:A:869:GLN:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:HG2	1:B:206:MET:HG2	1.94	0.49
1:B:362:LEU:HD13	1:B:411:LEU:HB3	1.94	0.49
1:B:436:ILE:HD11	1:B:458:GLY:N	2.27	0.49
1:B:479:ILE:HG22	1:B:483:LYS:HE3	1.94	0.49
1:A:464:MET:HG3	1:A:629:GLY:HA2	1.93	0.49
1:A:545:LYS:HG3	1:A:546:GLY:H	1.76	0.49
1:B:548:PRO:HG3	1:B:586:TRP:CE3	2.47	0.49
1:B:654:LEU:HA	8:B:1121:HOH:O	2.13	0.49
1:B:898:ILE:HG22	1:B:899:SER:N	2.26	0.49
1:A:75:PRO:CG	1:A:211:PHE:CD1	2.92	0.49
1:A:235:ASN:O	1:A:322:LYS:HE3	2.13	0.49
1:A:372:LEU:N	1:A:372:LEU:HD23	2.27	0.49
1:A:414:ASP:O	8:A:1101:HOH:O	2.19	0.49
1:A:693:SER:OG	1:A:750:LEU:HD22	2.13	0.49
1:B:67:LEU:HB3	1:B:145:HIS:CD2	2.47	0.49
1:B:245:GLU:HG2	1:B:246:GLY:N	2.27	0.49
1:B:917:PHE:CE2	1:B:921:LEU:HD11	2.47	0.49
1:B:918:PHE:CE2	1:B:934:VAL:CG1	2.95	0.49
1:B:741:ASP:OD2	1:B:787:PRO:CB	2.48	0.49
1:B:889:LEU:HD21	1:B:925:GLY:CA	2.42	0.49
1:B:440:ALA:HA	8:B:1117:HOH:O	2.11	0.49
1:B:860:HIS:C	1:B:860:HIS:CD2	2.90	0.49
1:B:877:ARG:HA	1:B:917:PHE:CE1	2.48	0.49
1:B:821:GLN:O	1:B:822:ASN:C	2.55	0.49
1:B:873:TRP:CE2	1:B:877:ARG:HD3	2.47	0.49
1:B:108:ILE:HB	1:B:150:LEU:HB2	1.94	0.49
1:B:640:TRP:CH2	1:B:666:VAL:HG22	2.47	0.49
1:A:366[B]:ARG:HE	1:A:400:GLU:CD	2.20	0.48
1:B:286:ILE:HG21	1:B:296:THR:HB	1.94	0.48
1:B:634:HIS:CE1	1:B:675:LEU:HD13	2.48	0.48
1:B:347:THR:HG22	1:B:818:SER:HB2	1.94	0.48
1:B:397:LYS:HB3	1:B:459:ALA:HB2	1.95	0.48
1:A:362:LEU:HD13	1:A:411:LEU:HB3	1.94	0.48
1:B:223:LYS:HD3	1:B:252:HIS:CE1	2.48	0.48
1:A:108:ILE:HB	1:A:150:LEU:HB2	1.94	0.48
1:A:407:THR:O	1:A:409:PRO:HD3	2.14	0.48
1:B:69:LEU:HD22	1:B:109:ILE:HG22	1.94	0.48
1:B:118:THR:O	1:B:119:ASN:CB	2.62	0.48
1:B:401:LEU:HD23	1:B:401:LEU:C	2.38	0.48
1:B:452:GLU:CD	1:B:452:GLU:N	2.71	0.48
1:B:537:MET:HA	1:B:587:HIS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:TYR:HE1	1:B:723:LYS:HB2	1.78	0.48
1:A:347:THR:HG22	1:A:818:SER:HB2	1.94	0.48
1:A:411:LEU:HA	1:A:745:VAL:HG21	1.96	0.48
1:A:479:ILE:O	1:A:483:LYS:HG3	2.13	0.48
1:A:544:GLN:NE2	1:A:584:TYR:HD1	2.10	0.48
1:A:877:ARG:HA	1:A:917:PHE:CE1	2.48	0.48
1:A:926:SER:HA	1:A:927:HIS:HA	1.60	0.48
1:B:243:GLU:HA	1:B:249:LEU:HD23	1.94	0.48
1:B:491:LYS:O	1:B:494:ASP:HB2	2.14	0.48
1:B:565:ARG:O	1:B:567:LEU:HD12	2.14	0.48
1:A:245:GLU:CG	1:A:246:GLY:N	2.75	0.48
1:A:319:PRO:HB2	1:A:320:LEU:HD23	1.96	0.48
1:A:777:TRP:HH2	1:A:811:GLN:HG2	1.79	0.48
1:B:109:ILE:HD11	1:B:149:ALA:HB2	1.96	0.48
1:B:395:PHE:HE2	1:B:495:LEU:HD21	1.78	0.48
1:A:565:ARG:HD2	1:A:584:TYR:CE2	2.48	0.48
1:B:757:LEU:CD1	1:B:761:LEU:HD22	2.44	0.48
1:A:653:LEU:HD21	5:A:1007:NAG:H82	1.94	0.48
1:B:911:LEU:O	1:B:915:LYS:HB2	2.13	0.48
1:A:62:PHE:CD1	1:A:142:TYR:HB2	2.49	0.48
1:A:380:LEU:HG	1:A:486:SER:HA	1.95	0.48
1:A:491:LYS:HB2	1:A:491:LYS:HE3	1.61	0.48
1:A:534:VAL:O	1:A:535:LYS:C	2.56	0.48
1:A:845:MET:SD	1:A:855:LEU:HD11	2.53	0.48
1:B:359:SER:O	1:B:360:ASP:C	2.56	0.48
1:B:380:LEU:HG	1:B:486:SER:HA	1.95	0.48
1:B:552:VAL:HG12	1:B:561:LEU:CD2	2.42	0.48
1:B:589:PRO:C	1:B:590:LEU:HD23	2.38	0.48
1:B:870:GLN:O	1:B:871:LEU:C	2.56	0.48
1:A:285:SER:HB2	1:A:324:ASP:OD1	2.14	0.47
1:A:538:MET:HA	1:A:541:TRP:HD1	1.79	0.47
1:A:845:MET:O	1:A:846:GLU:C	2.57	0.47
1:B:75:PRO:CG	1:B:211:PHE:CD1	2.92	0.47
1:B:790:VAL:O	1:B:794:VAL:HG23	2.14	0.47
1:B:500:SER:HB3	1:B:534:VAL:HB	1.96	0.47
1:B:604:ILE:HD12	1:B:604:ILE:N	2.14	0.47
1:B:634:HIS:HE1	1:B:675:LEU:HD13	1.80	0.47
1:B:935:LEU:O	1:B:939:THR:HG23	2.14	0.47
1:B:182:SER:CB	1:B:330:ASP:HB2	2.44	0.47
1:A:56:ALA:CB	1:A:57:THR:CA	2.89	0.47
1:A:398:TYR:CD2	1:A:398:TYR:C	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:THR:HG22	1:A:445:GLN:CD	2.40	0.47
1:B:668:GLN:HA	1:B:668:GLN:OE1	2.14	0.47
1:A:100:LEU:HD13	1:A:161:LYS:HG2	1.96	0.47
1:A:559:LEU:HD12	1:A:612:LEU:O	2.14	0.47
1:A:605:LEU:HD12	1:A:607:SER:H	1.79	0.47
1:B:119:ASN:O	1:B:166:MET:HA	2.13	0.47
1:B:236:MET:HE1	1:B:320:LEU:HD22	1.96	0.47
1:B:243:GLU:O	1:B:244:LEU:HD23	2.14	0.47
1:B:245:GLU:CG	1:B:246:GLY:N	2.78	0.47
1:B:496:TRP:HA	1:B:496:TRP:HE3	1.79	0.47
2:D:1:NAG:H62	2:D:2:NAG:O5	2.15	0.47
1:A:407:THR:OG1	1:A:408:TYR:HD2	1.98	0.47
1:A:545:LYS:HG2	1:A:546:GLY:N	2.29	0.47
1:B:342:ILE:HG22	1:B:344:TYR:CE1	2.48	0.47
1:B:651:HIS:C	1:B:651:HIS:CD2	2.92	0.47
1:B:655:ARG:HB2	1:B:658:ASP:OD2	2.14	0.47
1:B:661:GLY:O	1:B:664:HIS:HB3	2.14	0.47
1:A:452:GLU:CD	1:A:452:GLU:N	2.72	0.47
1:A:640:TRP:CZ3	1:A:666:VAL:HG22	2.50	0.47
1:A:791:LEU:HD11	1:A:795:TYR:CZ	2.50	0.47
1:A:898:ILE:HG22	1:A:899:SER:N	2.29	0.47
1:B:178:GLY:O	1:B:197:THR:HA	2.15	0.47
1:B:309:PHE:HD2	1:B:310:TYR:N	2.13	0.47
1:B:345:ARG:NH2	1:B:853:GLN:HB2	2.29	0.47
1:B:442:THR:HG22	1:B:445:GLN:CD	2.40	0.47
1:B:538:MET:HA	1:B:541:TRP:HD1	1.79	0.47
1:B:587:HIS:CE1	1:B:606:LYS:HD2	2.49	0.47
1:B:845:MET:O	1:B:846:GLU:C	2.57	0.47
1:A:110:LEU:HD12	1:A:148:ILE:HG13	1.97	0.47
1:A:146:GLU:OE1	1:A:205:ARG:HD2	2.15	0.47
1:A:274:LEU:HD21	1:A:293:ARG:HE	1.79	0.47
1:A:792:LYS:HB2	8:A:1144:HOH:O	2.15	0.47
1:B:360:ASP:O	1:B:361:LYS:C	2.58	0.47
1:B:693:SER:O	1:B:697:LEU:HB2	2.15	0.47
1:B:791:LEU:HD11	1:B:795:TYR:CZ	2.50	0.47
1:B:949:LEU:N	1:B:950:PRO:HD2	2.30	0.47
1:A:922:GLU:HG2	1:A:926:SER:OG	2.14	0.47
1:B:205:ARG:HH21	1:B:212:ASP:CB	2.11	0.47
1:A:90:ASP:CB	1:A:171:LYS:HA	2.46	0.46
1:B:309:PHE:CD2	1:B:310:TYR:N	2.84	0.46
1:B:370:HIS:C	1:B:370:HIS:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:TYR:O	1:A:479:ILE:HD11	2.14	0.46
1:A:763:HIS:NE2	1:A:765:PRO:HG2	2.30	0.46
1:A:856:ALA:O	1:A:857:ALA:C	2.58	0.46
1:A:949:LEU:N	1:A:950:PRO:HD2	2.29	0.46
1:B:643:LEU:O	1:B:646:GLN:HB3	2.15	0.46
1:B:763:HIS:NE2	1:B:765:PRO:HG2	2.29	0.46
1:B:905:PHE:O	1:B:938:ILE:HG23	2.14	0.46
1:A:67:LEU:HB3	1:A:145:HIS:CD2	2.49	0.46
1:A:119:ASN:O	1:A:166:MET:HA	2.15	0.46
1:B:407:THR:OG1	1:B:408:TYR:HD2	1.97	0.46
1:B:659:ARG:O	1:B:663:ILE:HG13	2.16	0.46
1:B:939:THR:O	1:B:943:LYS:HG3	2.16	0.46
1:A:74:ILE:HA	1:A:75:PRO:HD3	1.74	0.46
1:A:313:TYR:CE2	1:A:478:ILE:HD11	2.50	0.46
1:A:370:HIS:C	1:A:370:HIS:CD2	2.93	0.46
1:B:280:SER:HB2	1:B:317:TYR:HE1	1.80	0.46
1:B:534:VAL:O	1:B:535:LYS:C	2.58	0.46
1:B:911:LEU:HD11	1:B:939:THR:HG22	1.97	0.46
1:A:389:ILE:HD12	1:A:392:LYS:HE3	1.98	0.46
1:B:110:LEU:HD12	1:B:148:ILE:HG13	1.96	0.46
1:B:723:LYS:O	1:B:727:LEU:HD23	2.15	0.46
1:A:236:MET:HE3	1:A:256:THR:CA	2.35	0.46
1:A:359:SER:O	1:A:360:ASP:C	2.58	0.46
1:A:723:LYS:O	1:A:727:LEU:HD23	2.16	0.46
1:A:812:TYR:HB2	1:A:824:ILE:HG21	1.98	0.46
1:B:122:LEU:HD11	1:B:162:TYR:CB	2.37	0.46
1:B:398:TYR:CD2	1:B:398:TYR:C	2.94	0.46
1:B:594:THR:HG21	1:B:614:LEU:HD11	1.98	0.46
1:B:843:LEU:HD22	1:B:849:VAL:HB	1.98	0.46
1:A:428:ASP:OD2	1:A:457:LYS:HD2	2.15	0.46
1:A:436:ILE:HD11	1:A:458:GLY:N	2.31	0.46
1:A:651:HIS:CD2	1:A:652:THR:N	2.84	0.46
1:B:313:TYR:CE2	1:B:478:ILE:HD11	2.48	0.46
1:B:696:LEU:HD23	1:B:750:LEU:HD21	1.98	0.46
1:B:924:GLN:OE1	1:B:924:GLN:HA	2.15	0.46
3:E:3:MAN:H3	3:E:4:MAN:C5	2.43	0.46
1:A:416:TYR:O	1:A:417:PHE:C	2.59	0.46
1:B:64:TRP:CD2	1:B:70:PRO:HG3	2.51	0.46
1:B:387:ASN:HB3	1:B:438:LYS:O	2.15	0.46
1:B:591:THR:O	1:B:592:TYR:HB3	2.16	0.46
1:A:182:SER:CB	1:A:330:ASP:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:HE2	1:A:238:LYS:HB3	1.76	0.46
1:A:395:PHE:HE2	1:A:495:LEU:HD21	1.80	0.46
1:A:604:ILE:O	1:A:605:LEU:CB	2.63	0.46
1:A:934:VAL:CG1	1:A:935:LEU:N	2.77	0.46
1:A:479:ILE:HG22	1:A:483:LYS:HE3	1.97	0.45
1:A:884:LEU:HD21	1:A:889:LEU:HD23	1.98	0.45
1:A:921:LEU:O	1:A:922:GLU:HB2	2.16	0.45
1:B:421:CYS:HA	1:B:424:VAL:HG12	1.97	0.45
1:B:662:LEU:O	1:B:663:ILE:C	2.59	0.45
1:A:424:VAL:HG21	1:A:457:LYS:HB2	1.98	0.45
1:A:536:GLU:O	1:A:540:THR:HG22	2.15	0.45
1:A:634:HIS:CE1	1:A:675:LEU:HD13	2.51	0.45
1:A:661:GLY:O	1:A:664:HIS:HB3	2.16	0.45
1:B:200:GLU:HA	1:B:201:PRO:HA	1.64	0.45
1:B:351:PHE:CE1	1:B:361:LYS:HB2	2.51	0.45
1:B:389:ILE:HD12	1:B:392:LYS:HE3	1.99	0.45
1:B:568:GLN:O	1:B:569:GLY:O	2.34	0.45
1:A:647:LEU:CD1	1:A:683:MET:HE3	2.45	0.45
1:A:668:GLN:OE1	1:A:668:GLN:HA	2.16	0.45
1:A:873:TRP:CE2	1:A:877:ARG:HD3	2.51	0.45
1:B:140:LEU:O	1:B:148:ILE:HA	2.16	0.45
1:B:386:TRP:HB3	1:B:446:ILE:HG23	1.99	0.45
1:B:545:LYS:HG2	1:B:546:GLY:H	1.77	0.45
1:B:313:TYR:O	1:B:479:ILE:HD11	2.16	0.45
1:B:416:TYR:O	1:B:417:PHE:C	2.60	0.45
1:B:549:LEU:HB2	1:B:566:PHE:HD2	1.82	0.45
1:B:726:LEU:HD23	1:B:726:LEU:HA	1.84	0.45
1:A:245:GLU:CD	1:A:246:GLY:H	2.25	0.45
1:A:393:GLU:OE1	1:A:455:TYR:CE2	2.70	0.45
1:A:581:GLN:HB3	1:A:584:TYR:CE2	2.51	0.45
1:B:67:LEU:CA	1:B:145:HIS:CD2	2.99	0.45
1:B:240:LYS:HB2	1:B:240:LYS:HE3	1.60	0.45
1:B:274:LEU:HD21	1:B:293:ARG:HE	1.81	0.45
1:B:693:SER:OG	1:B:750:LEU:HD22	2.16	0.45
1:B:763:HIS:C	1:B:765:PRO:HD2	2.42	0.45
1:A:64:TRP:CD2	1:A:70:PRO:HG3	2.52	0.45
1:A:236:MET:HE1	1:A:320:LEU:HD22	1.97	0.45
1:A:243:GLU:HA	1:A:249:LEU:HD23	1.98	0.45
1:A:591:THR:O	1:A:592:TYR:HB3	2.17	0.45
1:A:697:LEU:HD12	1:A:697:LEU:HA	1.73	0.45
1:A:860:HIS:O	1:A:864:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:HB2	1:B:61:ARG:HA	1.97	0.45
1:B:393:GLU:OE1	1:B:455:TYR:CE2	2.69	0.45
1:B:491:LYS:HE3	1:B:491:LYS:HB2	1.61	0.45
1:B:536:GLU:O	1:B:540:THR:HG22	2.17	0.45
1:A:91:PHE:CE2	1:A:170:ALA:HB3	2.52	0.45
1:B:138:LYS:HD2	1:B:151:LEU:HD12	1.99	0.45
1:B:647:LEU:O	1:B:651:HIS:HB3	2.17	0.45
1:B:777:TRP:HA	1:B:784:LEU:HB3	1.99	0.45
1:B:784:LEU:HD13	1:B:786:ILE:HD12	1.98	0.45
1:A:223:LYS:HD3	1:A:252:HIS:CE1	2.51	0.45
1:A:475:GLN:O	1:A:478:ILE:HG12	2.17	0.45
1:A:594:THR:HG21	1:A:614:LEU:HD11	1.99	0.45
1:A:643:LEU:O	1:A:646:GLN:HB3	2.17	0.45
1:A:655:ARG:O	1:A:658:ASP:HB2	2.16	0.45
1:A:884:LEU:HD12	1:A:884:LEU:HA	1.67	0.45
1:B:60:GLU:HB2	1:B:61:ARG:CA	2.47	0.45
1:B:104:ALA:CB	1:B:158:PRO:HD3	2.39	0.45
1:B:273:SER:HA	1:B:286:ILE:O	2.17	0.45
1:B:651:HIS:CD2	1:B:652:THR:N	2.85	0.45
1:A:62:PHE:HA	1:A:63:PRO:HD3	1.67	0.45
1:A:140:LEU:O	1:A:148:ILE:HA	2.17	0.45
1:A:243:GLU:O	1:A:244:LEU:HD23	2.17	0.45
1:A:294:ASN:HD22	1:A:294:ASN:HA	1.64	0.45
1:A:301:GLN:NE2	1:A:408:TYR:OH	2.50	0.45
1:A:360:ASP:O	1:A:361:LYS:C	2.59	0.45
1:A:537:MET:HA	1:A:587:HIS:HB2	1.99	0.45
1:A:565:ARG:O	1:A:567:LEU:HD12	2.16	0.45
1:A:589:PRO:O	1:A:590:LEU:HD23	2.17	0.45
1:A:843:LEU:HD22	1:A:849:VAL:HB	1.97	0.45
1:A:907:SER:HB2	1:A:909:ASP:OD2	2.17	0.45
6:A:1009:MES:H32	6:A:1009:MES:H82	1.70	0.45
1:B:158:PRO:CB	1:B:159:HIS:HD2	2.30	0.45
1:B:436:ILE:HA	1:B:453:VAL:CG1	2.47	0.45
1:B:889:LEU:HD12	1:B:889:LEU:O	2.17	0.45
1:B:922:GLU:HA	1:B:922:GLU:OE2	2.17	0.45
1:A:535:LYS:O	1:A:536:GLU:C	2.60	0.44
1:A:568:GLN:O	1:A:569:GLY:O	2.35	0.44
1:B:146:GLU:OE1	1:B:205:ARG:HD2	2.17	0.44
1:B:366:ARG:HD2	1:B:413:PHE:CE1	2.52	0.44
1:B:592:TYR:OH	1:B:612:LEU:HD21	2.17	0.44
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:TRP:O	1:A:877:ARG:HB2	2.18	0.44
1:A:939:THR:O	1:A:943:LYS:HG3	2.17	0.44
1:B:275:SER:HB3	1:B:283:LYS:HE2	1.99	0.44
1:A:67:LEU:HD12	1:A:67:LEU:C	2.43	0.44
1:A:138:LYS:HD2	1:A:151:LEU:HD12	1.99	0.44
1:A:196:VAL:HG22	1:A:197:THR:N	2.33	0.44
1:A:387:ASN:HB3	1:A:438:LYS:O	2.18	0.44
1:A:491:LYS:O	1:A:494:ASP:HB2	2.17	0.44
1:B:812:TYR:HB2	1:B:824:ILE:HG21	2.00	0.44
1:A:168:PHE:N	1:A:168:PHE:CD1	2.85	0.44
1:A:421:CYS:HA	1:A:424:VAL:HG12	1.99	0.44
1:A:763:HIS:C	1:A:765:PRO:HD2	2.42	0.44
1:A:796:SER:HA	1:A:827:ALA:HB1	1.98	0.44
1:A:918:PHE:CE2	1:A:934:VAL:CG1	2.98	0.44
1:A:922:GLU:HA	1:A:926:SER:HB2	1.98	0.44
1:B:355:THR:O	1:B:355:THR:HG22	2.17	0.44
1:B:647:LEU:CD1	1:B:683:MET:HE3	2.45	0.44
1:B:863:ALA:HB1	1:B:904:HIS:CE1	2.48	0.44
1:A:496:TRP:HA	1:A:496:TRP:HE3	1.83	0.44
1:A:557:CYS:O	1:A:614:LEU:N	2.48	0.44
1:A:693:SER:O	1:A:697:LEU:HB2	2.18	0.44
1:B:55:VAL:O	1:B:56:ALA:HB2	2.18	0.44
1:B:106:GLN:HG3	1:B:155:LYS:HD3	1.99	0.44
1:A:124:SER:CB	1:A:131:MET:H	2.30	0.44
1:A:910:LYS:HA	1:A:910:LYS:HD3	1.83	0.44
1:B:245:GLU:CD	1:B:246:GLY:H	2.26	0.44
1:B:337:GLU:OE2	4:B:1005:LYS:N	2.51	0.44
2:C:1:NAG:H62	2:C:2:NAG:C1	2.48	0.44
1:A:309:PHE:CD2	1:A:310:TYR:N	2.86	0.44
1:A:316:ILE:HG12	1:A:483:LYS:HE2	2.00	0.44
1:A:397:LYS:O	1:A:400:GLU:HB2	2.18	0.44
1:A:655:ARG:HB2	1:A:658:ASP:OD2	2.18	0.44
1:B:553:LYS:O	1:B:559:LEU:HA	2.17	0.44
1:B:113:LYS:O	1:B:114:ASP:C	2.60	0.44
1:B:646:GLN:HE21	1:B:646:GLN:CA	2.28	0.44
1:B:838:LEU:HD13	1:B:838:LEU:C	2.43	0.44
1:A:416:TYR:C	1:A:416:TYR:CD2	2.95	0.44
1:A:611:THR:HG22	1:A:612:LEU:N	2.33	0.44
1:A:763:HIS:CG	1:A:765:PRO:HD2	2.53	0.44
1:B:90:ASP:HA	1:B:172:LEU:H	1.83	0.44
1:B:485:PHE:O	1:B:486:SER:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HD12	1:A:68:ARG:N	2.33	0.43
1:A:390:TRP:CZ2	1:A:391:LEU:HD23	2.53	0.43
1:A:553:LYS:HB2	1:A:636:GLU:OE2	2.18	0.43
1:A:665:ASP:O	1:A:669:LEU:HG	2.18	0.43
1:A:858:LEU:HD12	1:A:858:LEU:O	2.18	0.43
1:A:922:GLU:OE2	1:A:926:SER:HB2	2.17	0.43
1:B:62:PHE:HA	1:B:63:PRO:HD3	1.68	0.43
1:B:74:ILE:HA	1:B:75:PRO:HD3	1.76	0.43
1:A:158:PRO:CB	1:A:159:HIS:HD2	2.30	0.43
1:A:553:LYS:O	1:A:559:LEU:HA	2.18	0.43
1:B:416:TYR:C	1:B:416:TYR:CD2	2.96	0.43
1:B:624:ASN:HD21	1:B:629:GLY:N	2.13	0.43
1:B:907:SER:HB2	1:B:909:ASP:OD2	2.18	0.43
1:A:205:ARG:HH21	1:A:212:ASP:CB	2.16	0.43
1:A:565:ARG:HD3	1:A:581:GLN:HB2	1.99	0.43
1:B:551:VAL:CG1	1:B:634:HIS:HB3	2.37	0.43
1:B:774:PHE:HB2	1:B:794:VAL:CG1	2.48	0.43
1:B:884:LEU:HD12	1:B:884:LEU:HA	1.70	0.43
1:A:324:ASP:C	1:A:325:LEU:HD12	2.43	0.43
1:B:69:LEU:CD2	1:B:147:GLN:HE21	2.31	0.43
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.61	0.43
1:A:757:LEU:CD1	1:A:761:LEU:HD22	2.49	0.43
1:B:90:ASP:CB	1:B:171:LYS:HA	2.48	0.43
1:B:197:THR:HB	1:B:199:PHE:CZ	2.54	0.43
1:B:417:PHE:CE1	1:B:421:CYS:SG	3.11	0.43
1:B:623:PHE:HB2	1:B:633:VAL:HG11	2.01	0.43
1:B:664:HIS:O	1:B:668:GLN:HG2	2.17	0.43
1:B:707:TYR:C	1:B:707:TYR:CD2	2.96	0.43
1:B:796:SER:HA	1:B:827:ALA:HB1	2.01	0.43
1:A:641:ASP:OD1	1:A:641:ASP:N	2.51	0.43
1:A:821:GLN:O	1:A:822:ASN:C	2.60	0.43
1:A:835:GLU:CD	1:A:835:GLU:H	2.25	0.43
1:B:168:PHE:N	1:B:168:PHE:CD1	2.86	0.43
1:B:237:PRO:HG3	1:B:322:LYS:CG	2.49	0.43
1:B:271:PHE:CD2	1:B:326:ILE:HD11	2.53	0.43
1:B:416:TYR:O	1:B:418:LEU:N	2.52	0.43
1:B:884:LEU:HD21	1:B:889:LEU:HD23	2.01	0.43
1:A:113:LYS:O	1:A:114:ASP:C	2.61	0.43
1:A:934:VAL:HG12	1:A:935:LEU:N	2.34	0.43
1:B:67:LEU:C	1:B:67:LEU:HD12	2.44	0.43
1:B:640:TRP:O	1:B:644:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:MET:HG3	1:B:718:ILE:HB	1.99	0.43
1:B:860:HIS:O	1:B:864:ARG:HG3	2.18	0.43
1:B:909:ASP:O	1:B:913:GLU:HG3	2.19	0.43
1:A:122:LEU:HD11	1:A:162:TYR:CB	2.38	0.43
1:A:288:ALA:O	1:A:289:SER:C	2.61	0.43
1:A:318:TYR:HA	1:A:319:PRO:HD3	1.75	0.43
1:A:797:VAL:C	1:A:799:ALA:H	2.26	0.43
1:B:91:PHE:CE2	1:B:170:ALA:HB3	2.53	0.43
1:B:179:PHE:CD1	1:B:197:THR:HG22	2.54	0.43
1:B:227:GLU:OE1	1:B:229:ARG:HD3	2.19	0.43
1:B:533:GLU:C	1:B:534:VAL:HG23	2.44	0.43
1:B:833:HIS:O	1:B:836:LYS:HB2	2.19	0.43
1:B:836:LYS:O	1:B:839:LYS:HB3	2.19	0.43
1:A:197:THR:HB	1:A:199:PHE:CZ	2.53	0.43
1:A:640:TRP:O	1:A:644:ILE:HG13	2.19	0.43
1:B:324:ASP:C	1:B:325:LEU:HD12	2.43	0.43
1:B:422:PHE:HA	1:B:425:ILE:HD12	2.00	0.43
1:B:662:LEU:HB3	1:B:683:MET:CE	2.44	0.43
1:B:856:ALA:O	1:B:857:ALA:C	2.61	0.43
1:A:355:THR:O	1:A:355:THR:HG22	2.17	0.43
1:A:552:VAL:HG12	1:A:561:LEU:CD2	2.49	0.43
1:A:693:SER:O	1:A:694:PRO:C	2.60	0.43
1:B:491:LYS:H	1:B:494:ASP:HB2	1.84	0.43
1:B:588:ILE:HD11	1:B:631:TYR:CG	2.53	0.43
1:B:777:TRP:CH2	1:B:811:GLN:HG2	2.53	0.43
1:B:802:THR:HG22	1:B:806:ASN:ND2	2.34	0.43
1:A:549:LEU:HB2	1:A:566:PHE:HD2	1.84	0.42
1:A:625:VAL:C	1:A:627:SER:H	2.27	0.42
1:A:707:TYR:CD2	1:A:707:TYR:C	2.96	0.42
1:B:419:ASN:N	1:B:419:ASN:ND2	2.64	0.42
1:B:687:LEU:HD11	1:B:699:GLY:HA3	2.01	0.42
1:B:875:PHE:C	1:B:875:PHE:CD2	2.97	0.42
1:A:178:GLY:O	1:A:197:THR:HA	2.19	0.42
1:A:237:PRO:HG3	1:A:322:LYS:CG	2.50	0.42
1:A:273:SER:HA	1:A:286:ILE:O	2.19	0.42
1:B:535:LYS:O	1:B:536:GLU:C	2.61	0.42
1:A:196:VAL:CG2	1:A:197:THR:N	2.82	0.42
1:A:592:TYR:OH	1:A:612:LEU:HD21	2.19	0.42
1:A:646:GLN:HE21	1:A:646:GLN:CA	2.31	0.42
1:A:707:TYR:HE1	1:A:723:LYS:HB2	1.84	0.42
1:A:790:VAL:O	1:A:794:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:PHE:CZ	1:B:395:PHE:CD1	3.08	0.42
1:A:710:MET:HG3	1:A:718:ILE:HB	2.01	0.42
1:A:858:LEU:HD12	1:A:858:LEU:C	2.44	0.42
1:B:196:VAL:HG22	1:B:197:THR:N	2.34	0.42
1:B:604:ILE:O	1:B:605:LEU:CB	2.66	0.42
1:A:93:ALA:HB3	1:A:168:PHE:CE2	2.55	0.42
1:A:451:ASP:OD1	1:A:451:ASP:C	2.63	0.42
1:A:768:GLN:O	1:A:771:ALA:HB3	2.20	0.42
1:B:79:ASP:HB2	1:B:96:LYS:HB3	2.02	0.42
1:B:219:ASN:OD1	1:B:258:LYS:HD3	2.18	0.42
1:B:325:LEU:HB3	1:B:344:TYR:CE1	2.54	0.42
1:B:475:GLN:O	1:B:478:ILE:HG12	2.19	0.42
1:A:104:ALA:CB	1:A:158:PRO:HD3	2.43	0.42
1:A:693:SER:N	1:A:694:PRO:CD	2.82	0.42
1:A:774:PHE:HB2	1:A:794:VAL:CG1	2.50	0.42
1:A:863:ALA:HB1	1:A:904:HIS:CE1	2.51	0.42
1:B:559:LEU:HD12	1:B:612:LEU:O	2.19	0.42
1:A:227:GLU:OE1	1:A:229:ARG:HD3	2.20	0.42
1:A:284:VAL:HG11	1:A:303:SER:HB2	2.01	0.42
1:B:319:PRO:HB2	1:B:320:LEU:HD23	2.00	0.42
1:B:397:LYS:O	1:B:400:GLU:HB2	2.20	0.42
1:B:438:LYS:HG3	1:B:439:PRO:HD2	2.02	0.42
1:B:860:HIS:O	1:B:860:HIS:CD2	2.73	0.42
1:A:79:ASP:HB2	1:A:96:LYS:HB3	2.02	0.42
1:B:387:ASN:CB	1:B:438:LYS:O	2.68	0.42
1:B:496:TRP:CZ2	1:B:538:MET:HB3	2.55	0.42
1:B:565:ARG:HD2	1:B:584:TYR:CE2	2.54	0.42
1:B:586:TRP:C	1:B:588:ILE:H	2.28	0.42
1:B:870:GLN:HE22	1:B:910:LYS:HE3	1.85	0.42
1:B:889:LEU:HA	1:B:890:GLY:HA2	1.62	0.42
1:B:919:GLU:O	1:B:922:GLU:HB2	2.20	0.42
1:A:67:LEU:CA	1:A:145:HIS:CD2	3.01	0.42
1:A:79:ASP:O	1:A:95:GLU:HA	2.20	0.42
1:A:496:TRP:CZ2	1:A:538:MET:HB3	2.55	0.42
1:A:634:HIS:HE1	1:A:675:LEU:HD13	1.84	0.42
1:A:687:LEU:HD11	1:A:699:GLY:HA3	2.01	0.42
1:A:889:LEU:HA	1:A:890:GLY:HA2	1.60	0.42
1:B:284:VAL:HG11	1:B:303:SER:HB2	2.00	0.42
1:B:468:PHE:CE2	1:B:469:LEU:HG	2.55	0.42
1:B:636:GLU:H	1:B:636:GLU:HG3	1.62	0.42
1:B:858:LEU:HD12	1:B:858:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:THR:O	1:A:855:LEU:HB2	2.20	0.42
1:B:104:ALA:H	1:B:158:PRO:HG3	1.85	0.42
1:B:757:LEU:HD11	1:B:761:LEU:HD22	2.02	0.42
1:B:768:GLN:O	1:B:771:ALA:HB3	2.20	0.42
1:B:916:LEU:HD22	1:B:916:LEU:HA	1.85	0.42
1:A:784:LEU:HD13	1:A:786:ILE:HD12	2.02	0.41
1:A:889:LEU:O	1:A:889:LEU:HD12	2.20	0.41
1:B:95:GLU:OE1	1:B:209:PRO:HD2	2.21	0.41
1:B:238:LYS:HB3	1:B:238:LYS:HE2	1.72	0.41
1:B:372:LEU:N	1:B:372:LEU:HD23	2.34	0.41
1:B:390:TRP:CB	1:B:436:ILE:HG23	2.50	0.41
1:B:655:ARG:O	1:B:658:ASP:HB2	2.20	0.41
1:A:433:SER:HB3	1:A:545:LYS:HG3	2.02	0.41
1:A:662:LEU:O	1:A:663:ILE:C	2.63	0.41
1:A:741:ASP:OD2	1:A:787:PRO:CB	2.51	0.41
1:A:797:VAL:C	1:A:799:ALA:N	2.78	0.41
1:B:201:PRO:HD2	1:B:202:THR:HG23	2.01	0.41
1:B:817:SER:O	1:B:821:GLN:CG	2.65	0.41
1:A:374:HIS:CE1	1:A:392:LYS:HG2	2.56	0.41
1:A:386:TRP:HB3	1:A:446:ILE:HG23	2.02	0.41
1:A:397:LYS:HB3	1:A:459:ALA:HB2	2.02	0.41
1:A:647:LEU:O	1:A:651:HIS:HB3	2.19	0.41
1:A:761:LEU:O	1:A:762:ASN:HB2	2.21	0.41
1:B:79:ASP:O	1:B:95:GLU:HA	2.20	0.41
1:B:213:GLU:HB2	1:B:216:PHE:CD2	2.54	0.41
1:B:386:TRP:CB	1:B:446:ILE:HG23	2.50	0.41
1:A:309:PHE:HD2	1:A:310:TYR:N	2.17	0.41
1:A:314:PHE:O	1:A:316:ILE:HG13	2.21	0.41
1:A:381:VAL:HG13	1:A:485:PHE:CB	2.50	0.41
1:B:67:LEU:HD12	1:B:68:ARG:N	2.35	0.41
1:B:183:THR:HG22	1:B:193:ILE:HG12	2.02	0.41
1:B:763:HIS:CG	1:B:765:PRO:HD2	2.55	0.41
1:B:923:ALA:O	1:B:924:GLN:CB	2.67	0.41
1:A:200:GLU:HA	1:A:201:PRO:HA	1.69	0.41
1:A:215:LEU:HA	1:A:489:ASN:ND2	2.35	0.41
1:A:419:ASN:N	1:A:419:ASN:ND2	2.65	0.41
1:A:436:ILE:HA	1:A:453:VAL:CG1	2.50	0.41
1:A:700:LEU:HD23	1:A:700:LEU:HA	1.90	0.41
1:B:551:VAL:CG2	1:B:562:GLN:HB2	2.50	0.41
1:B:805:TRP:CH2	1:B:839:LYS:HD3	2.54	0.41
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:THR:O	1:B:409:PRO:HD3	2.21	0.41
1:B:559:LEU:HD12	1:B:612:LEU:HB3	2.02	0.41
1:B:589:PRO:O	1:B:590:LEU:HD23	2.20	0.41
1:B:797:VAL:C	1:B:799:ALA:H	2.29	0.41
1:A:219:ASN:OD1	1:A:258:LYS:CD	2.68	0.41
1:A:280:SER:HB2	1:A:317:TYR:HE1	1.85	0.41
1:A:777:TRP:CH2	1:A:811:GLN:HG2	2.56	0.41
1:B:93:ALA:HB3	1:B:168:PHE:CE2	2.55	0.41
1:B:374:HIS:CE1	1:B:392:LYS:HG2	2.55	0.41
1:B:770:ALA:CB	1:B:797:VAL:HG21	2.51	0.41
1:B:802:THR:HG23	1:B:836:LYS:CE	2.50	0.41
1:A:366[A]:ARG:HD3	1:A:400:GLU:OE1	2.21	0.41
1:A:442:THR:OG1	1:A:443:PRO:CD	2.68	0.41
1:B:385:TRP:CG	1:B:386:TRP:N	2.88	0.41
1:B:611:THR:HG22	1:B:612:LEU:N	2.36	0.41
1:B:959:ASN:C	1:B:961:ARG:N	2.77	0.41
1:A:533:GLU:O	1:A:534:VAL:C	2.62	0.41
1:A:688:GLN:HB3	1:A:729:TYR:CE2	2.46	0.41
1:A:802:THR:HG23	1:A:836:LYS:CE	2.51	0.41
1:B:196:VAL:CG2	1:B:197:THR:N	2.84	0.41
1:B:257:VAL:HB	2:F:1:NAG:O6	2.21	0.41
1:B:277:PHE:HA	1:B:282:VAL:O	2.21	0.41
1:B:301:GLN:NE2	1:B:408:TYR:OH	2.53	0.41
1:B:385:TRP:CD1	1:B:387:ASN:ND2	2.80	0.41
1:B:543:LEU:HB3	8:B:1101:HOH:O	2.20	0.41
1:B:660:VAL:HG13	1:B:698:GLU:OE1	2.21	0.41
1:B:858:LEU:HD12	1:B:858:LEU:C	2.46	0.41
1:B:934:VAL:CG1	1:B:935:LEU:N	2.80	0.41
1:A:130:TYR:C	1:A:130:TYR:CD2	2.99	0.41
1:A:551:VAL:CG1	1:A:634:HIS:HB3	2.37	0.41
1:A:959:ASN:C	1:A:961:ARG:N	2.76	0.41
1:B:215:LEU:HA	1:B:489:ASN:HD21	1.86	0.41
1:B:215:LEU:HA	1:B:489:ASN:ND2	2.36	0.41
1:B:236:MET:HG2	1:B:256:THR:HG22	2.03	0.41
1:B:381:VAL:HG13	1:B:485:PHE:CB	2.51	0.41
1:B:739:TRP:CZ2	1:B:755:LEU:HD22	2.56	0.41
1:A:415:ASP:HB2	1:A:746:TRP:CZ2	2.56	0.40
1:A:441:GLU:HA	1:A:441:GLU:OE2	2.21	0.40
1:A:659:ARG:O	1:A:663:ILE:HG13	2.21	0.40
1:B:59:GLY:C	1:B:60:GLU:HG2	2.46	0.40
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:HD22	8:B:1101:HOH:O	2.20	0.40
1:A:660:VAL:HG13	1:A:698:GLU:OE1	2.21	0.40
1:B:685:TYR:O	1:B:688:GLN:HG2	2.21	0.40
1:B:879:ASN:HD22	1:B:879:ASN:N	2.20	0.40
6:B:1010:MES:H81	6:B:1010:MES:H32	1.47	0.40
1:A:528:LEU:CG	1:A:529:GLY:HA2	2.51	0.40
1:A:635:TYR:H	1:A:640:TRP:NE1	2.18	0.40
1:A:655:ARG:HA	1:A:656:PRO:HD3	1.86	0.40
1:A:802:THR:HG22	1:A:806:ASN:ND2	2.35	0.40
1:B:106:GLN:HE21	1:B:155:LYS:HZ2	1.70	0.40
1:B:309:PHE:CE1	1:B:406:ALA:CB	3.04	0.40
1:B:873:TRP:O	1:B:877:ARG:HB2	2.21	0.40
1:A:90:ASP:HB3	1:A:171:LYS:HA	2.04	0.40
1:A:640:TRP:CH2	1:A:666:VAL:HG22	2.56	0.40
1:A:777:TRP:HA	1:A:784:LEU:HB3	2.03	0.40
1:B:727:LEU:HD12	1:B:731:LYS:HE3	2.04	0.40
1:B:801:THR:HG23	1:B:804:GLY:N	2.21	0.40
1:B:858:LEU:HD11	1:B:862:ILE:HD11	2.04	0.40
1:A:80:LEU:O	1:A:222:ILE:HA	2.21	0.40
1:A:277:PHE:HA	1:A:282:VAL:O	2.21	0.40
1:A:433:SER:C	1:A:545:LYS:HD3	2.45	0.40
1:A:486:SER:HB3	1:A:487:TYR:HD2	1.83	0.40
1:A:813:GLU:OE1	1:B:848:LYS:NZ	2.52	0.40
1:A:905:PHE:O	1:A:938:ILE:HG23	2.22	0.40
1:B:316:ILE:HG12	1:B:483:LYS:HE2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:SER:O	1:A:961:ARG:NH2[2_655]	2.11	0.09
1:B:320:LEU:O	1:B:961:ARG:NH1[2_556]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	863/967 (89%)	729 (84%)	108 (12%)	26 (3%)	3	22
1	B	851/967 (88%)	710 (83%)	114 (13%)	27 (3%)	3	20
All	All	1714/1934 (89%)	1439 (84%)	222 (13%)	53 (3%)	3	21

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	119	ASN
1	A	583	ARG
1	A	596	SER
1	A	603	HIS
1	A	604	ILE
1	A	605	LEU
1	A	616	GLU
1	A	715	ILE
1	A	922	GLU
1	B	119	ASN
1	B	569	GLY
1	B	596	SER
1	B	603	HIS
1	B	604	ILE
1	B	605	LEU
1	B	616	GLU
1	B	715	ILE
1	B	922	GLU
1	B	924	GLN
1	B	925	GLY
1	B	926	SER
1	A	546	GLY
1	B	417	PHE
1	B	534	VAL
1	B	546	GLY
1	A	100	LEU
1	A	417	PHE
1	A	545	LYS
1	A	619	SER
1	A	763	HIS
1	B	60	GLU
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	763	HIS
1	A	921	LEU
1	B	545	LYS
1	B	619	SER
1	B	765	PRO
1	A	59	GLY
1	A	471	GLU
1	A	649	GLN
1	A	765	PRO
1	B	56	ALA
1	B	649	GLN
1	B	921	LEU
1	B	615	PRO
1	A	615	PRO
1	A	99	VAL
1	A	133	PRO
1	B	99	VAL
1	B	453	VAL
1	A	72	VAL
1	A	925	GLY

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	768/870 (88%)	669 (87%)	99 (13%)	4 19
1	B	768/870 (88%)	672 (88%)	96 (12%)	4 20
All	All	1536/1740 (88%)	1341 (87%)	195 (13%)	4 20

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	72	VAL
1	A	73	VAL

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Mol	Chain	Res	Type
1	A	80	LEU
1	A	87	THR
1	A	99	VAL
1	A	110	LEU
1	A	113	LYS
1	A	117	ILE
1	A	121	THR
1	A	124	SER
1	A	125	GLU
1	A	137	LEU
1	A	160	LEU
1	A	166	MET
1	A	174	ASP
1	A	181	LYS
1	A	186	THR
1	A	193	ILE
1	A	196	VAL
1	A	202	THR
1	A	215	LEU
1	A	240	LYS
1	A	242	ILE
1	A	257	VAL
1	A	278	THR
1	A	294	ASN
1	A	303	SER
1	A	321	SER
1	A	352	ASP
1	A	361	LYS
1	A	364	VAL
1	A	367	VAL
1	A	372	LEU
1	A	383	MET
1	A	387	ASN
1	A	389	ILE
1	A	395	PHE
1	A	419	ASN
1	A	426	THR
1	A	436	ILE
1	A	444	THR
1	A	466	LYS
1	A	469	LEU
1	A	494	ASP

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Mol	Chain	Res	Type
1	A	528	LEU
1	A	533	GLU
1	A	540	THR
1	A	547	ILE
1	A	558	SER
1	A	559	LEU
1	A	582	GLU
1	A	585	LEU
1	A	588	ILE
1	A	591	THR
1	A	598	ASN
1	A	604	ILE
1	A	605	LEU
1	A	610	ASP
1	A	625	VAL
1	A	632	ILE
1	A	636	GLU
1	A	641	ASP
1	A	645	THR
1	A	646	GLN
1	A	652	THR
1	A	675	LEU
1	A	681	LEU
1	A	684	THR
1	A	697	LEU
1	A	701	SER
1	A	705	SER
1	A	722	LEU
1	A	750	LEU
1	A	751	ARG
1	A	761	LEU
1	A	766	CYS
1	A	769	LYS
1	A	773	LEU
1	A	784	LEU
1	A	791	LEU
1	A	825	LEU
1	A	828	LEU
1	A	852	THR
1	A	855	LEU
1	A	859	LEU
1	A	871	LEU

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Mol	Chain	Res	Type
1	A	877	ARG
1	A	881	THR
1	A	894	ILE
1	A	909	ASP
1	A	911	LEU
1	A	916	LEU
1	A	922	GLU
1	A	924	GLN
1	A	927	HIS
1	A	934	VAL
1	A	940	LYS
1	A	952	LEU
1	B	58	ASN
1	B	72	VAL
1	B	73	VAL
1	B	80	LEU
1	B	87	THR
1	B	99	VAL
1	B	110	LEU
1	B	113	LYS
1	B	117	ILE
1	B	121	THR
1	B	124	SER
1	B	137	LEU
1	B	160	LEU
1	B	166	MET
1	B	174	ASP
1	B	181	LYS
1	B	186	THR
1	B	193	ILE
1	B	196	VAL
1	B	202	THR
1	B	215	LEU
1	B	240	LYS
1	B	242	ILE
1	B	257	VAL
1	B	278	THR
1	B	294	ASN
1	B	303	SER
1	B	321	SER
1	B	325	LEU
1	B	352	ASP

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Mol	Chain	Res	Type
1	B	361	LYS
1	B	364	VAL
1	B	367	VAL
1	B	372	LEU
1	B	383	MET
1	B	387	ASN
1	B	389	ILE
1	B	395	PHE
1	B	419	ASN
1	B	426	THR
1	B	427	LYS
1	B	444	THR
1	B	466	LYS
1	B	494	ASP
1	B	540	THR
1	B	547	ILE
1	B	558	SER
1	B	559	LEU
1	B	570	VAL
1	B	585	LEU
1	B	588	ILE
1	B	591	THR
1	B	598	ASN
1	B	604	ILE
1	B	605	LEU
1	B	610	ASP
1	B	625	VAL
1	B	632	ILE
1	B	636	GLU
1	B	641	ASP
1	B	645	THR
1	B	646	GLN
1	B	652	THR
1	B	675	LEU
1	B	681	LEU
1	B	684	THR
1	B	697	LEU
1	B	705	SER
1	B	722	LEU
1	B	731	LYS
1	B	750	LEU
1	B	751	ARG

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Mol	Chain	Res	Type
1	B	761	LEU
1	B	766	CYS
1	B	769	LYS
1	B	773	LEU
1	B	784	LEU
1	B	791	LEU
1	B	825	LEU
1	B	828	LEU
1	B	852	THR
1	B	855	LEU
1	B	859	LEU
1	B	871	LEU
1	B	877	ARG
1	B	881	THR
1	B	894	ILE
1	B	909	ASP
1	B	911	LEU
1	B	916	LEU
1	B	922	GLU
1	B	927	HIS
1	B	929	ASP
1	B	934	VAL
1	B	940	LYS
1	B	952	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	77	HIS
1	A	145	HIS
1	A	147	GLN
1	A	159	HIS
1	A	252	HIS
1	A	294	ASN
1	A	301	GLN
1	A	419	ASN
1	A	447	GLN
1	A	463	ASN
1	A	489	ASN
1	A	544	GLN
1	A	554	GLN

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Mol	Chain	Res	Type
1	A	624	ASN
1	A	646	GLN
1	A	651	HIS
1	A	776	GLN
1	A	806	ASN
1	A	811	GLN
1	A	821	GLN
1	A	834	GLN
1	A	860	HIS
1	A	869	GLN
1	A	870	GLN
1	A	904	HIS
1	A	927	HIS
1	A	932	GLN
1	B	58	ASN
1	B	106	GLN
1	B	145	HIS
1	B	147	GLN
1	B	159	HIS
1	B	252	HIS
1	B	294	ASN
1	B	301	GLN
1	B	419	ASN
1	B	447	GLN
1	B	463	ASN
1	B	489	ASN
1	B	544	GLN
1	B	624	ASN
1	B	646	GLN
1	B	651	HIS
1	B	664	HIS
1	B	776	GLN
1	B	806	ASN
1	B	811	GLN
1	B	821	GLN
1	B	834	GLN
1	B	869	GLN
1	B	870	GLN
1	B	904	HIS
1	B	912	GLN
1	B	927	HIS
1	B	932	GLN

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Mol	Chain	Res	Type
1	B	959	ASN

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](#)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.84	0	17,19,21	2.50	9 (52%)
2	NAG	C	2	2	14,14,15	0.41	0	17,19,21	1.53	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.65	0	17,19,21	1.61	3 (17%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	1.20	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.39	0	17,19,21	1.44	2 (11%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	1.02	1 (5%)
3	MAN	E	3	3	11,11,12	0.70	0	15,15,17	0.88	0
3	MAN	E	4	3	11,11,12	0.59	0	15,15,17	0.57	0
2	NAG	F	1	1,2	14,14,15	0.50	0	17,19,21	0.83	0
2	NAG	F	2	2	14,14,15	0.55	0	17,19,21	1.11	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
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	4.81	118.64	112.19
2	D	1	NAG	C1-O5-C5	4.31	117.96	112.19
2	C	1	NAG	O5-C1-C2	-4.20	104.79	111.29
2	C	1	NAG	C3-C4-C5	-4.14	102.73	110.23
2	C	1	NAG	C1-O5-C5	-3.81	107.08	112.19
2	C	1	NAG	O5-C5-C6	3.61	114.68	107.66
3	E	1	NAG	C4-C3-C2	-3.60	105.75	111.02
3	E	1	NAG	C1-O5-C5	3.47	116.83	112.19
2	F	2	NAG	C1-O5-C5	3.34	116.66	112.19
2	D	1	NAG	C2-N2-C7	-3.29	118.49	122.90
2	C	1	NAG	C2-N2-C7	-3.22	118.58	122.90
3	E	2	NAG	C1-O5-C5	3.21	116.49	112.19
2	D	2	NAG	O5-C1-C2	3.01	115.94	111.29
2	C	1	NAG	O4-C4-C3	2.93	117.28	110.38
2	C	1	NAG	O5-C5-C4	-2.80	104.03	110.83
2	D	2	NAG	C1-C2-N2	-2.60	106.33	110.43
2	C	1	NAG	O7-C7-C8	-2.52	117.58	122.05
2	C	1	NAG	O7-C7-N2	2.11	125.71	121.98
2	D	1	NAG	O4-C4-C5	2.02	114.30	109.32
2	C	2	NAG	C6-C5-C4	-2.00	108.10	113.02

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2

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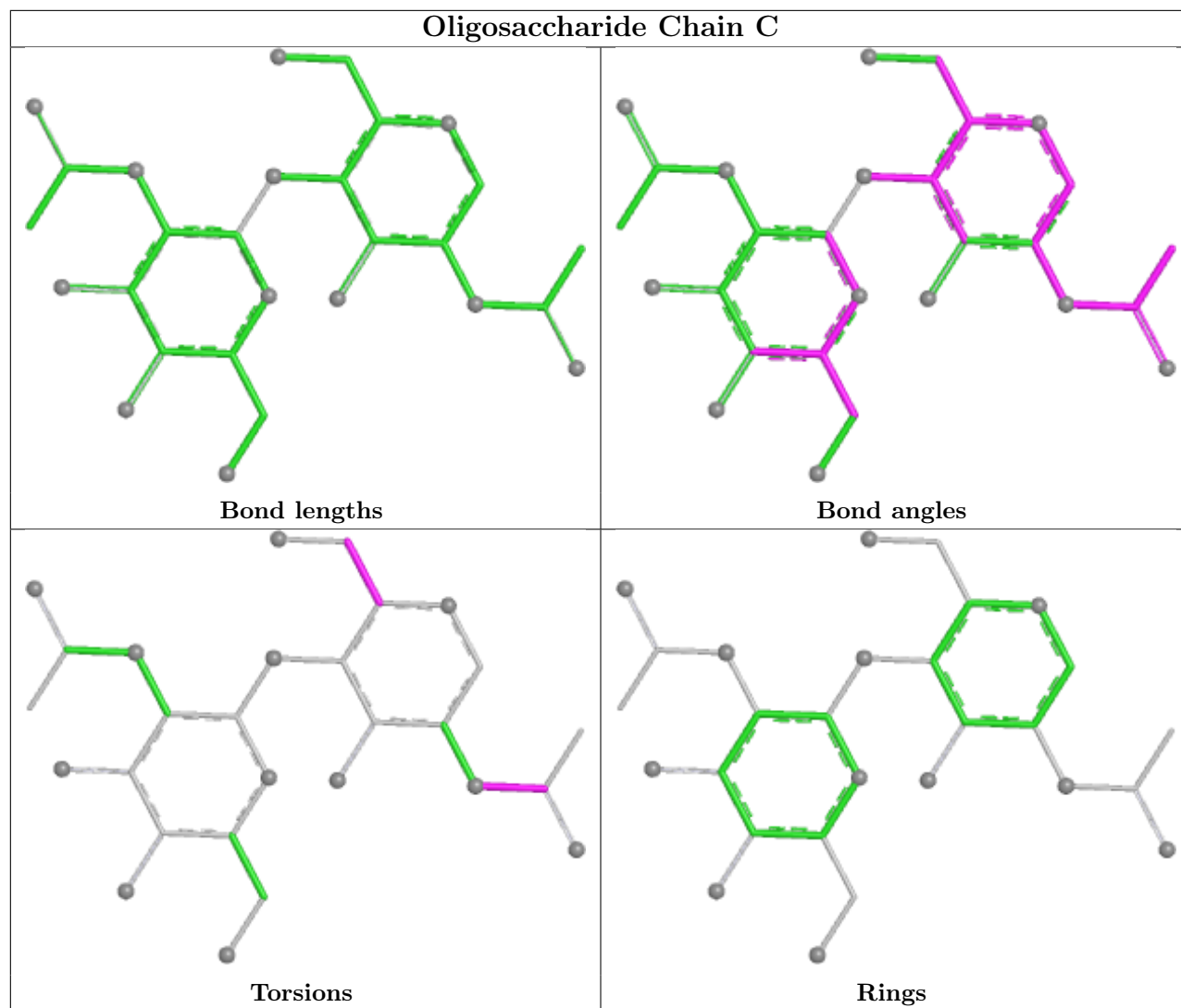
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	E	3	MAN	C4-C5-C6-O6
3	E	3	MAN	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6

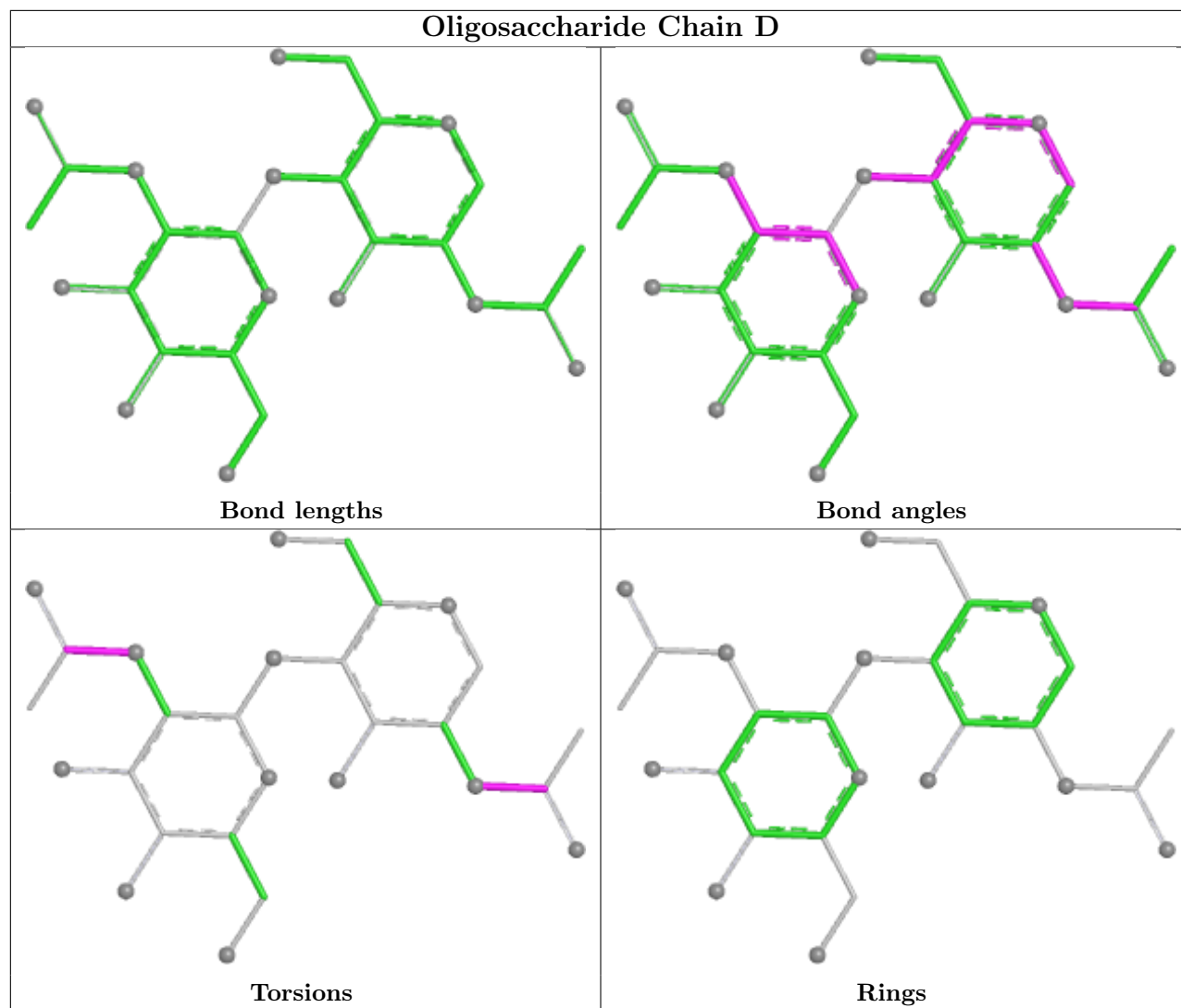
There are no ring outliers.

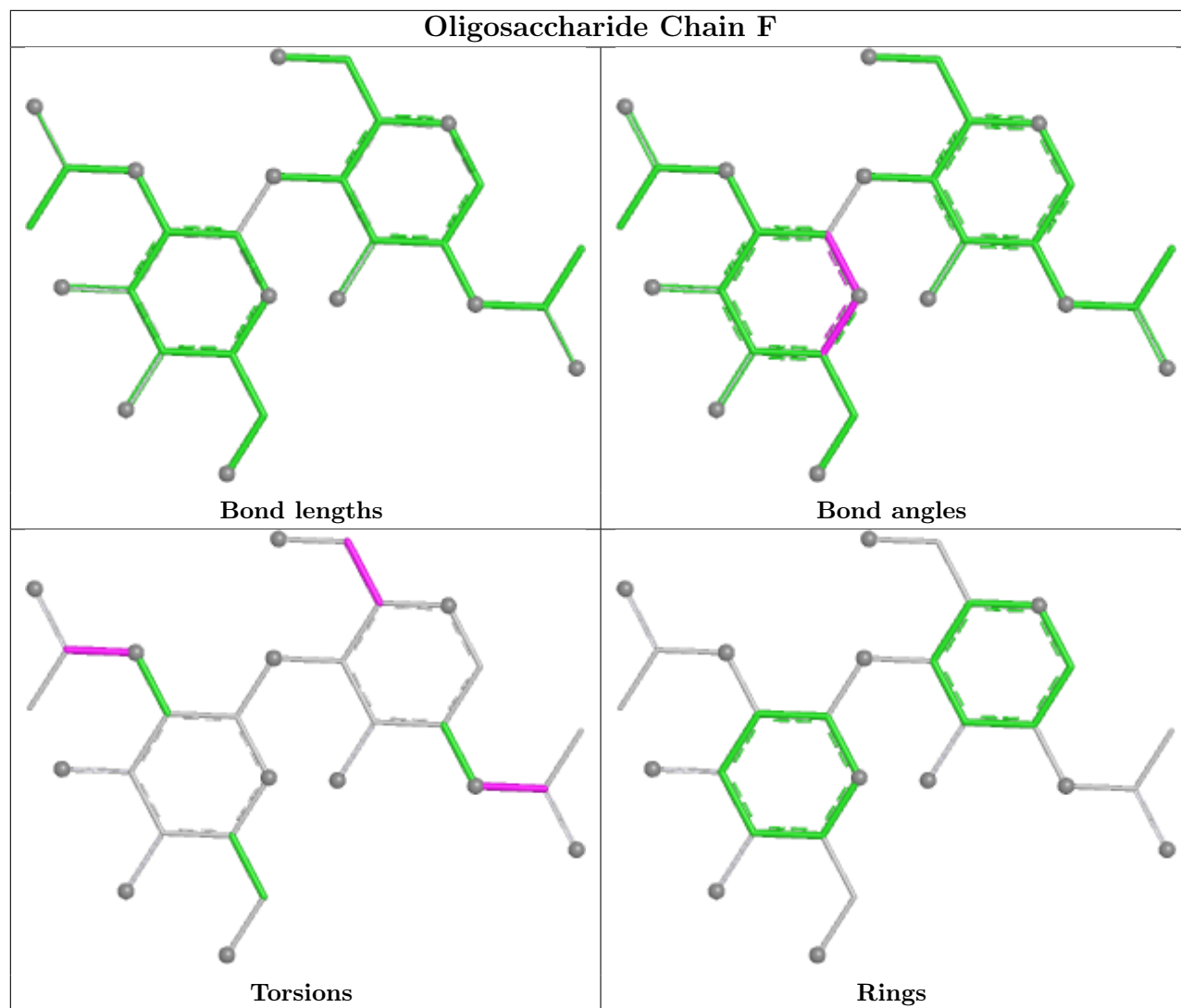
8 monomers are involved in 14 short contacts:

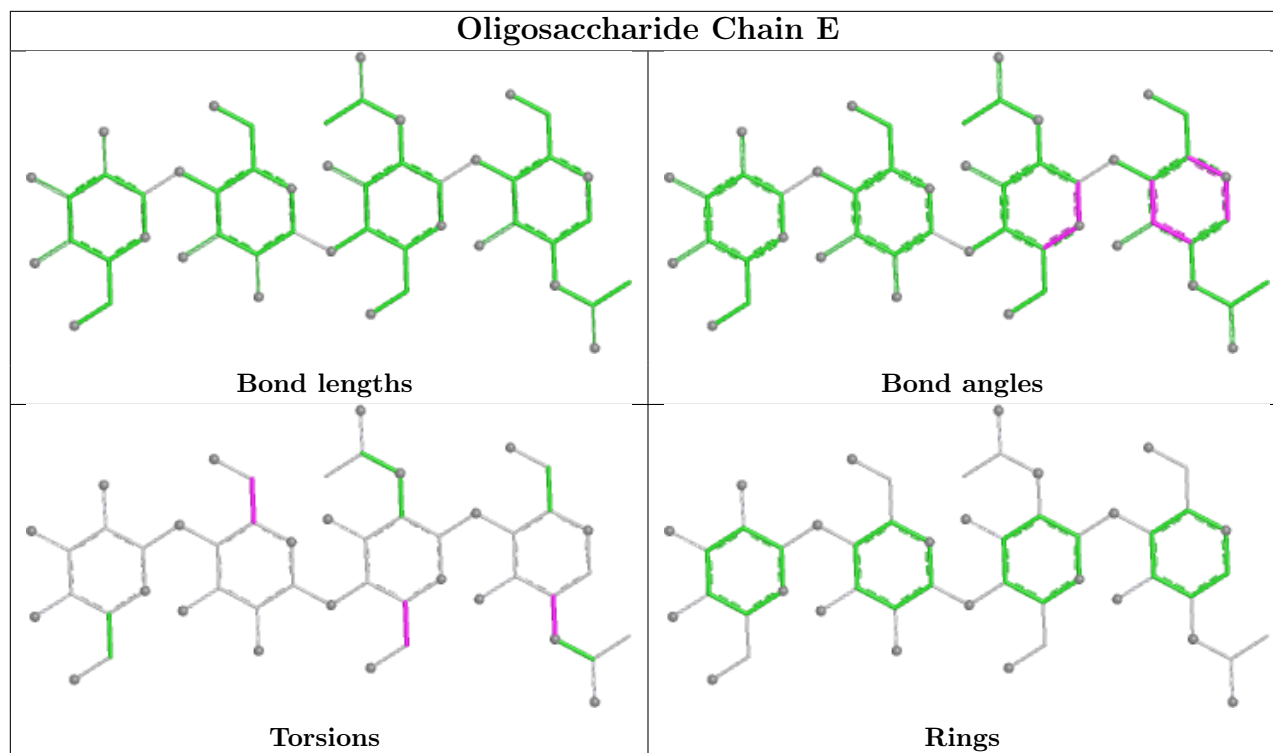
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	MAN	5	0
2	F	2	NAG	1	0
2	C	2	NAG	1	0
2	D	2	NAG	1	0
2	D	1	NAG	2	0
3	E	4	MAN	4	0
2	C	1	NAG	5	0
2	F	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
6	MES	B	1010	-	12,12,12	2.27	1 (8%)	15,16,16	2.57	7 (46%)
5	NAG	A	1006	1	14,14,15	0.53	0	17,19,21	1.40	2 (11%)
6	MES	A	1009	-	12,12,12	2.26	1 (8%)	15,16,16	2.54	6 (40%)
4	LYS	B	1005	7	8,9,9	0.96	1 (12%)	7,10,10	0.93	1 (14%)
4	LYS	A	1001	7	8,9,9	0.90	1 (12%)	7,10,10	0.68	0
5	NAG	A	1008	1	14,14,15	0.47	0	17,19,21	0.81	0
5	NAG	B	1009	1	14,14,15	0.43	0	17,19,21	1.30	2 (11%)
5	NAG	A	1007	1	14,14,15	0.61	0	17,19,21	2.07	5 (29%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MES	B	1010	-	-	5/6/14/14	0/1/1/1
5	NAG	A	1006	1	-	4/6/23/26	0/1/1/1
6	MES	A	1009	-	-	3/6/14/14	0/1/1/1
4	LYS	B	1005	7	-	5/9/9/9	-
4	LYS	A	1001	7	-	5/9/9/9	-
5	NAG	A	1008	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1007	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1010	MES	C8-S	-7.53	1.67	1.77
6	A	1009	MES	C8-S	-7.51	1.67	1.77
4	B	1005	LYS	OXT-C	-2.51	1.22	1.30
4	A	1001	LYS	OXT-C	-2.37	1.23	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1010	MES	C5-N4-C3	4.93	119.45	108.84
6	A	1009	MES	C5-N4-C3	4.92	119.44	108.84
6	B	1010	MES	C6-C5-N4	-4.42	103.41	110.12
5	A	1007	NAG	C1-O5-C5	4.19	117.80	112.19
5	A	1007	NAG	C3-C4-C5	-4.18	102.64	110.23
5	A	1006	NAG	C1-O5-C5	3.98	117.53	112.19
5	A	1007	NAG	C2-N2-C7	-3.85	117.75	122.90
6	A	1009	MES	C6-C5-N4	-3.75	104.42	110.12
5	B	1009	NAG	C1-O5-C5	3.63	117.06	112.19
6	A	1009	MES	C7-N4-C3	3.63	120.90	111.24
6	B	1010	MES	C7-N4-C5	3.48	120.51	111.24
6	B	1010	MES	C2-C3-N4	-3.38	104.98	110.12
6	A	1009	MES	C2-C3-N4	-3.33	105.06	110.12
6	B	1010	MES	C7-N4-C3	3.30	120.03	111.24
6	A	1009	MES	O1S-S-C8	3.19	111.54	106.73
6	A	1009	MES	C7-N4-C5	3.16	119.65	111.24
5	A	1007	NAG	O5-C5-C6	2.56	112.64	107.66
5	B	1009	NAG	C4-C3-C2	-2.38	107.53	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1006	NAG	C2-N2-C7	-2.35	119.75	122.90
4	B	1005	LYS	OXT-C-O	-2.29	118.88	124.08
5	A	1007	NAG	O4-C4-C5	2.29	114.96	109.32
6	B	1010	MES	O1S-S-C8	2.21	110.06	106.73
6	B	1010	MES	O3S-S-C8	2.04	109.99	106.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1005	LYS	C-CA-CB-CG
5	A	1006	NAG	C8-C7-N2-C2
5	A	1006	NAG	O7-C7-N2-C2
5	A	1008	NAG	C8-C7-N2-C2
5	A	1008	NAG	O7-C7-N2-C2
6	A	1009	MES	C8-C7-N4-C3
6	B	1010	MES	C8-C7-N4-C3
6	B	1010	MES	C7-C8-S-O1S
6	B	1010	MES	C7-C8-S-O3S
5	A	1007	NAG	O5-C5-C6-O6
5	B	1009	NAG	O5-C5-C6-O6
5	A	1008	NAG	O5-C5-C6-O6
4	B	1005	LYS	OXT-C-CA-N
5	A	1007	NAG	C4-C5-C6-O6
5	A	1008	NAG	C4-C5-C6-O6
5	B	1009	NAG	C4-C5-C6-O6
5	A	1006	NAG	O5-C5-C6-O6
6	A	1009	MES	N4-C7-C8-S
6	B	1010	MES	C7-C8-S-O2S
6	A	1009	MES	C8-C7-N4-C5
6	B	1010	MES	C8-C7-N4-C5
4	A	1001	LYS	OXT-C-CA-CB
5	A	1006	NAG	C4-C5-C6-O6
4	A	1001	LYS	CA-CB-CG-CD
4	A	1001	LYS	O-C-CA-CB
4	B	1005	LYS	O-C-CA-CB
4	A	1001	LYS	C-CA-CB-CG
4	B	1005	LYS	OXT-C-CA-CB
4	B	1005	LYS	O-C-CA-N
4	A	1001	LYS	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1010	MES	4	0
6	A	1009	MES	1	0
4	B	1005	LYS	4	0
5	A	1007	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	869/967 (89%)	-0.27	3 (0%) 90 81	22, 67, 111, 147	4 (0%)
1	B	859/967 (88%)	-0.26	3 (0%) 90 81	34, 70, 116, 146	0
All	All	1728/1934 (89%)	-0.27	6 (0%) 90 81	22, 68, 114, 147	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	SER	4.7
1	B	558	SER	2.8
1	A	102	SER	2.7
1	B	639	GLY	2.6
1	B	500	SER	2.3
1	A	781	SER	2.1

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

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

6.3 Carbohydrates [i](#)

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

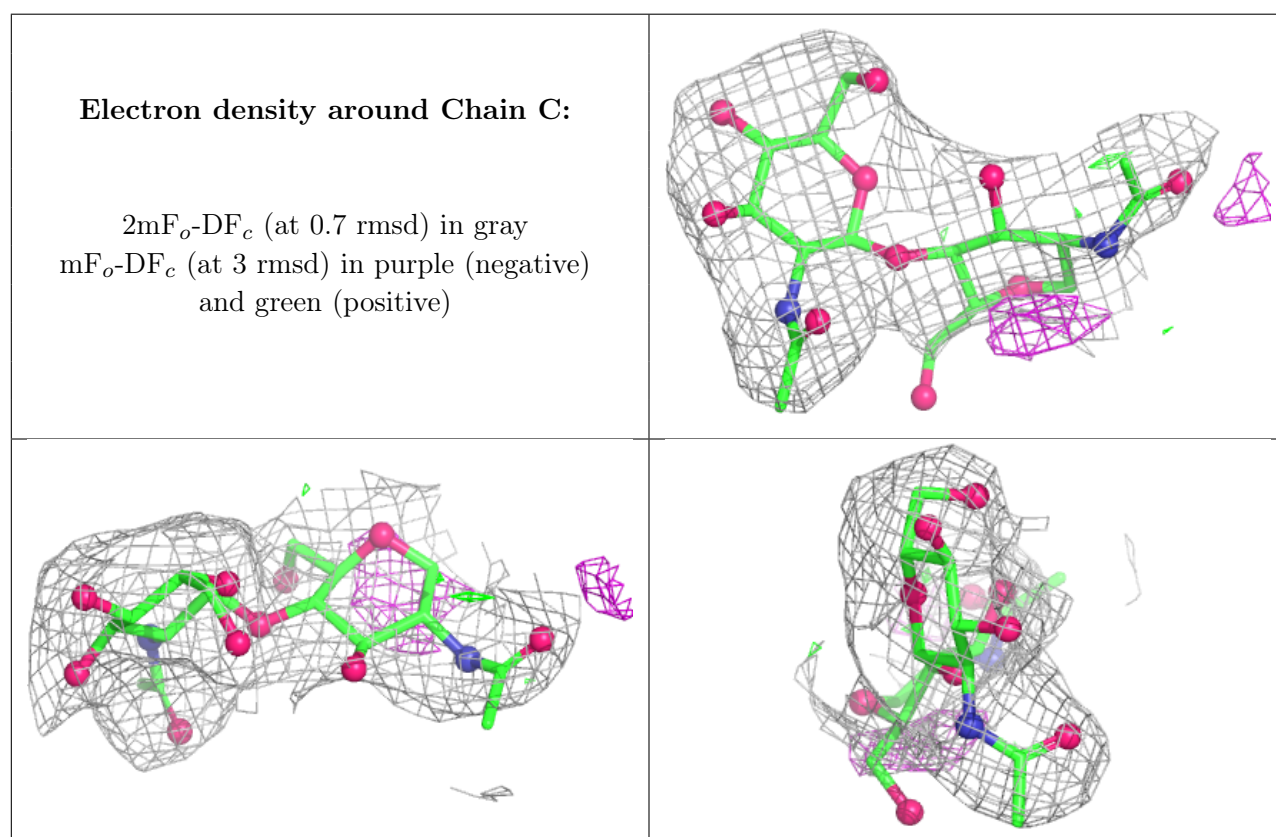
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.69	0.13	60,81,88,99	0
3	MAN	E	4	11/12	0.73	0.12	96,113,135,142	0
2	NAG	C	1	14/15	0.77	0.14	64,79,83,87	0

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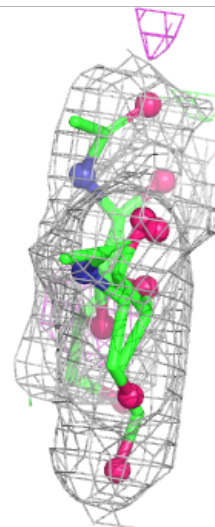
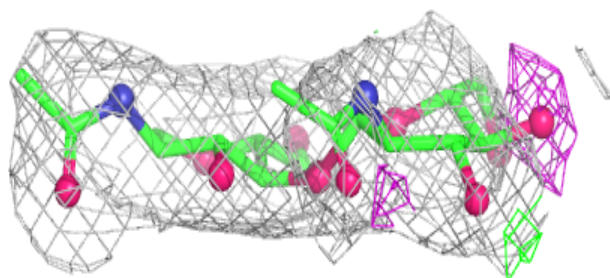
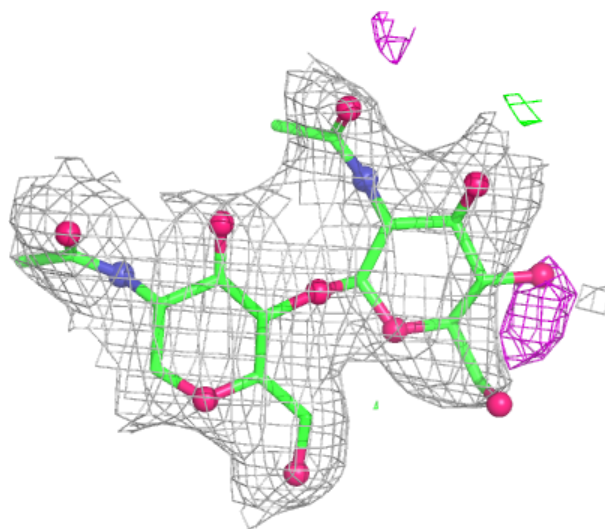
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	E	3	11/12	0.78	0.09	72,97,108,112	0
2	NAG	F	2	14/15	0.81	0.09	84,113,127,133	0
2	NAG	F	1	14/15	0.83	0.08	68,91,111,112	0
2	NAG	C	2	14/15	0.86	0.07	65,82,87,91	0
3	NAG	E	1	14/15	0.88	0.08	56,73,85,87	0
3	NAG	E	2	14/15	0.89	0.08	50,77,92,102	0
2	NAG	D	1	14/15	0.91	0.07	46,53,69,70	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



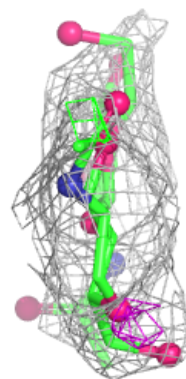
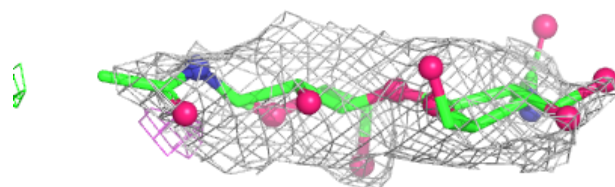
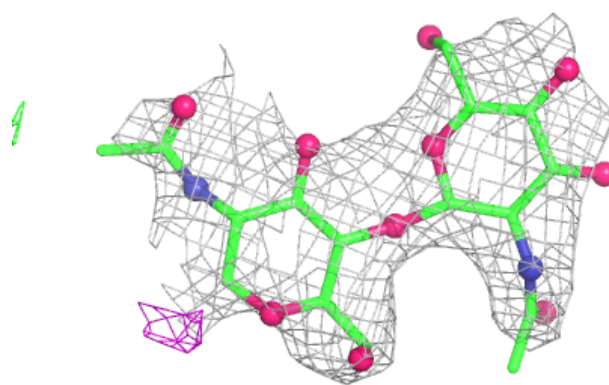
Electron density around Chain D:

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

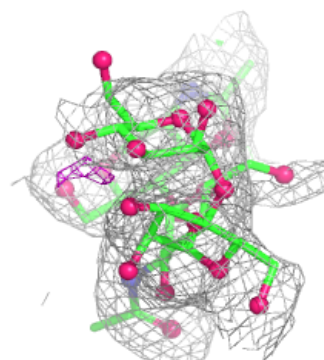
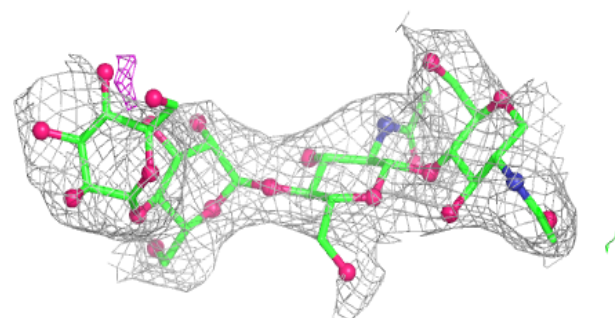
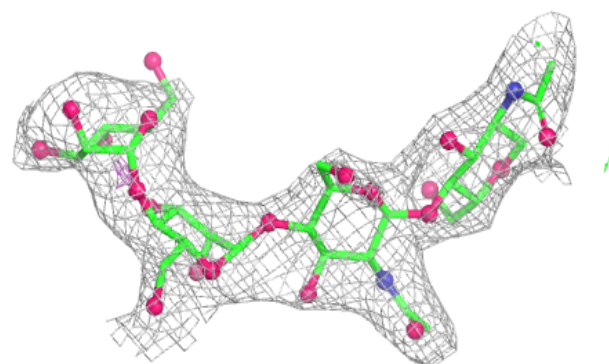


Electron density around Chain F:

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

**Electron density around Chain E:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	1009	14/15	0.66	0.11	76,101,110,112	0
5	NAG	A	1008	14/15	0.70	0.10	96,107,114,117	0
6	MES	A	1009	12/12	0.75	0.13	57,72,86,95	12
5	NAG	A	1007	14/15	0.78	0.13	88,104,121,130	0
6	MES	B	1010	12/12	0.79	0.20	57,65,73,84	12
4	LYS	B	1005	10/10	0.84	0.14	46,59,65,69	0
5	NAG	A	1006	14/15	0.90	0.07	62,85,87,88	0
4	LYS	A	1001	10/10	0.94	0.09	34,45,52,53	0
7	ZN	A	1010	1/1	0.99	0.05	32,32,32,32	0
7	ZN	B	1006	1/1	0.99	0.04	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.