



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:09 AM UTC

PDB ID : 2XWB / pdb_00002xwb
Title : Crystal Structure of Complement C3b in complex with Factors B and D
Authors : Forneris, F.; Ricklin, D.; Wu, J.; Tzekou, A.; Wallace, R.S.; Lambris, J.D.; Gros, P.
Deposited on : 2010-11-01
Resolution : 3.49 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

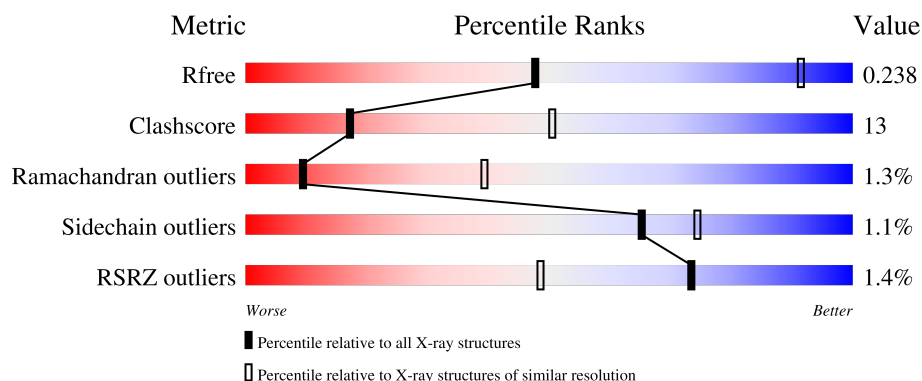
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	642	 69% 30% .
1	C	642	 68% 29% .
2	B	912	 70% 27% ..
2	D	912	 70% 28% ..
3	F	732	 72% 23% ..

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Mol	Chain	Length	Quality of chain
3	H	732	
4	I	228	
4	J	228	
5	E	2	
5	G	2	
5	K	2	
6	L	3	
6	M	3	

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
5	NAG	K	1	-	-	X	-
8	NAG	F	1747	X	-	-	-
9	GOL	J	1229	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 39285 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 COMPLEMENT C3B BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			
1	C	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			
2	D	901	Total	C	N	O	S	0	0	0
			7197	4563	1210	1386	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	991	GLU	GLN	SEE REMARK 999	UNP P01024
D	991	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	714	Total	C	N	O	S	0	0	0
			5627	3536	979	1079	33			
3	H	711	Total	C	N	O	S	0	0	0
			5608	3523	976	1076	33			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	254	GLY	ASP	engineered mutation	UNP P00751
F	260	ASP	ASN	engineered mutation	UNP P00751

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Chain	Residue	Modelled	Actual	Comment	Reference
F	740	ALA	-	expression tag	UNP P00751
F	741	ALA	-	expression tag	UNP P00751
H	254	GLY	ASP	engineered mutation	UNP P00751
H	260	ASP	ASN	engineered mutation	UNP P00751
H	740	ALA	-	expression tag	UNP P00751
H	741	ALA	-	expression tag	UNP P00751

- Molecule 4 is a protein called COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			
4	J	228	Total	C	N	O	S	0	0	0
			1710	1058	325	317	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	183	ALA	SER	engineered mutation	UNP P00746
J	183	ALA	SER	engineered mutation	UNP P00746

- Molecule 5 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
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

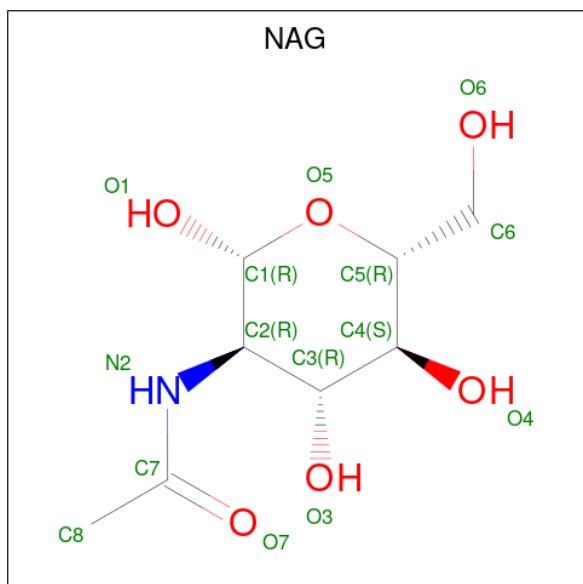


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	H	1	Total	Mg	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



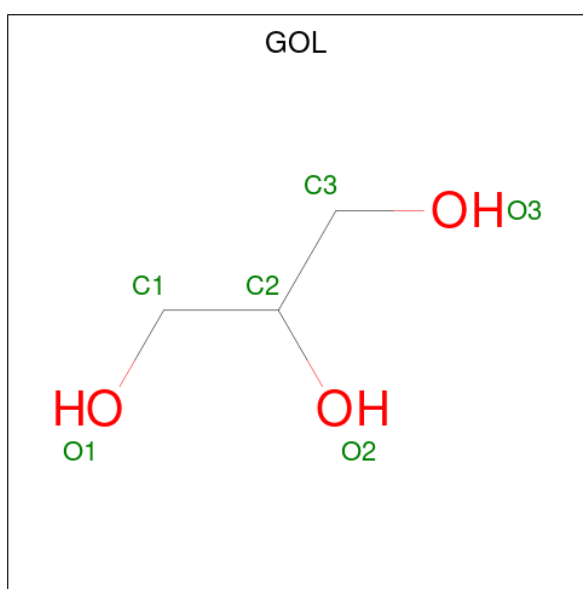
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	H	1	Total	C	N	O	0	0
			14	8	1	5		
8	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	I	1	Total	C	O	0	0
			6	3	3		
9	J	1	Total	C	O	0	0
			6	3	3		

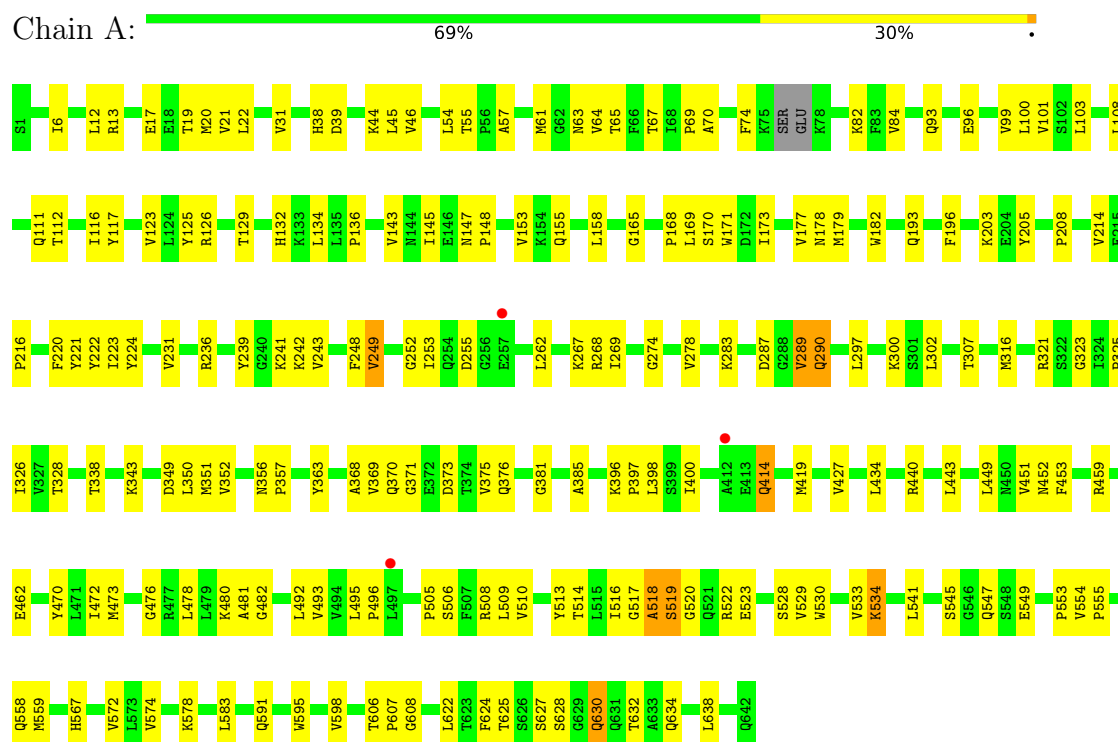
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	2	Total	O	0	0
			2	2		
10	H	2	Total	O	0	0
			2	2		

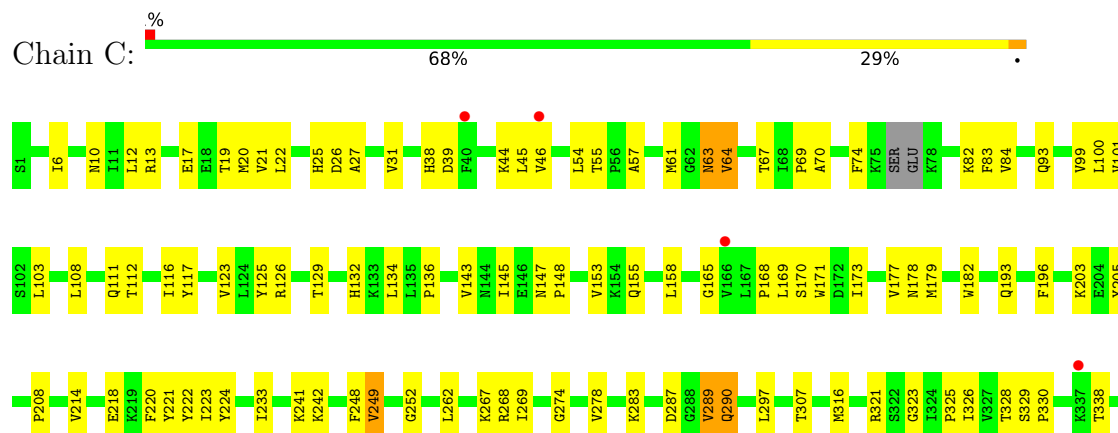
3 Residue-property plots

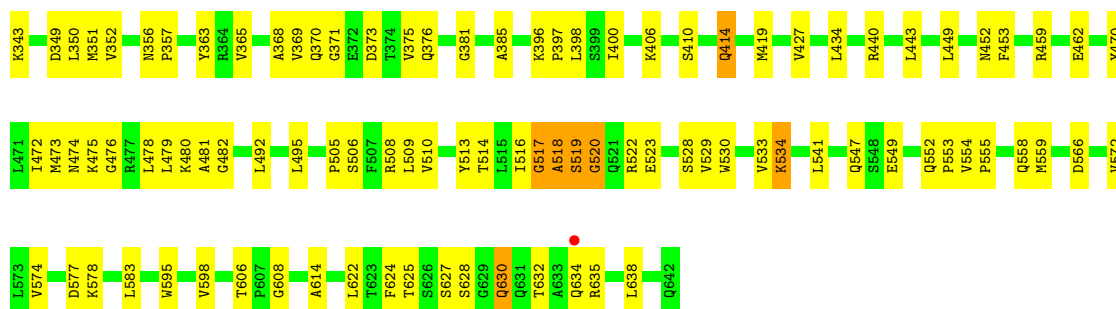
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: COMPLEMENT C3B BETA CHAIN

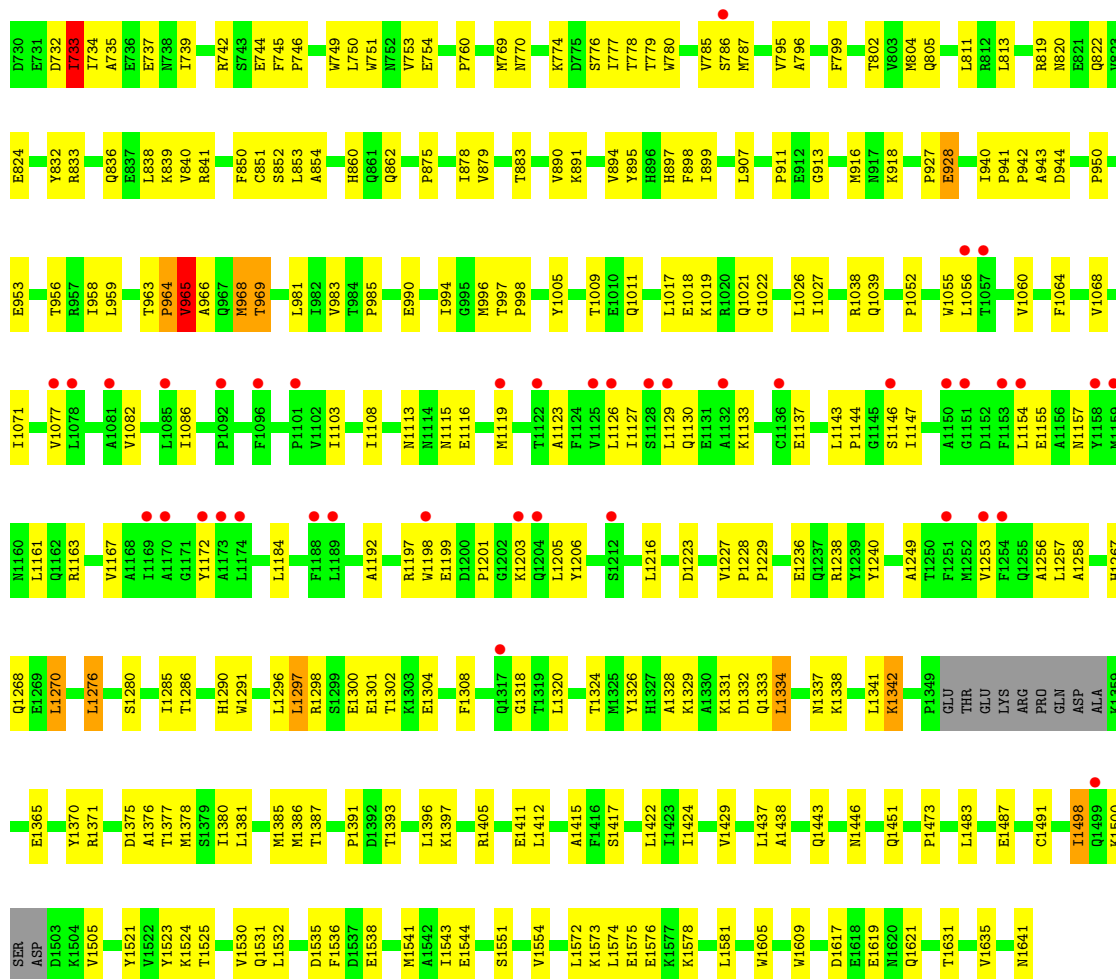


• Molecule 1: COMPLEMENT C3B BETA CHAIN

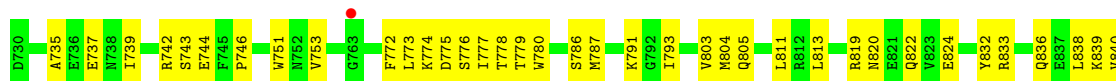


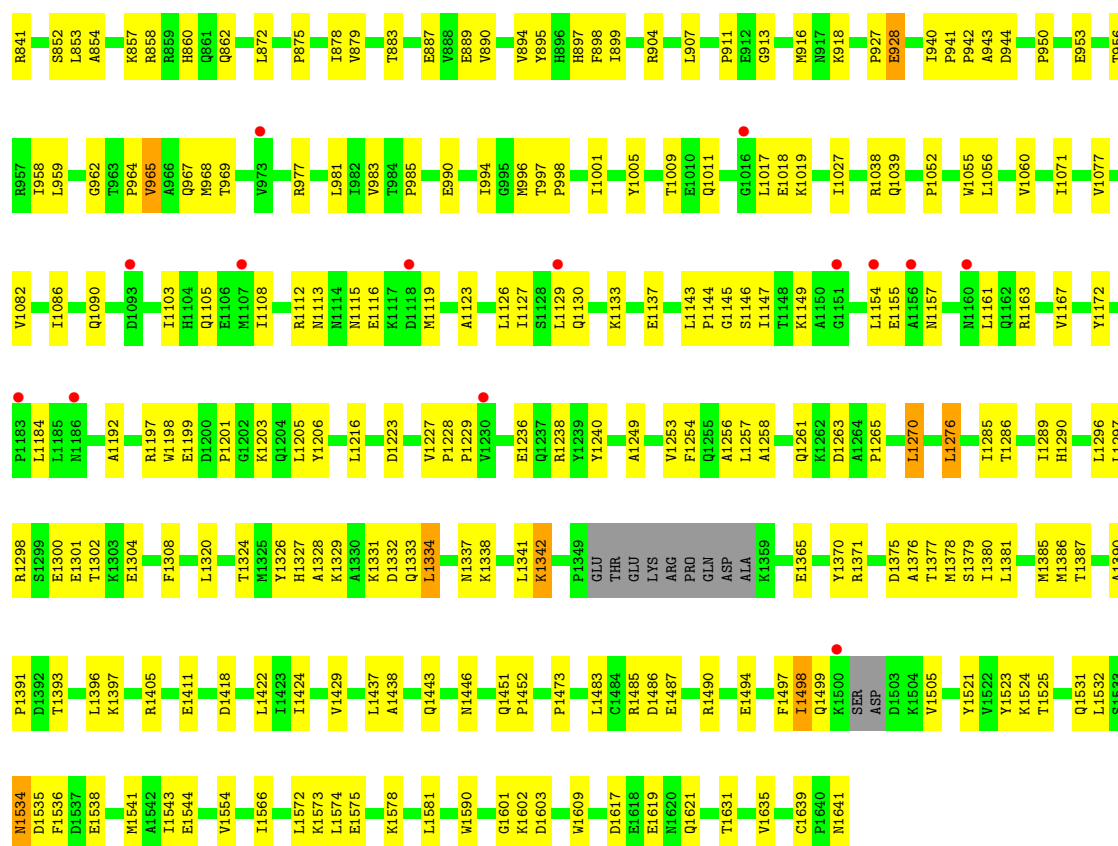


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN



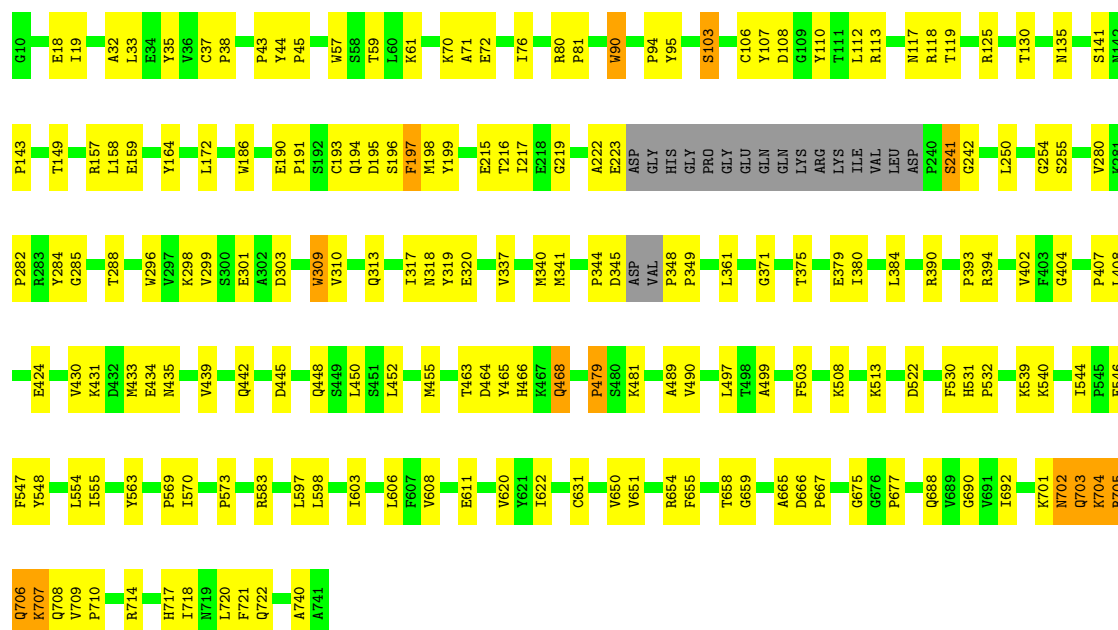
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN





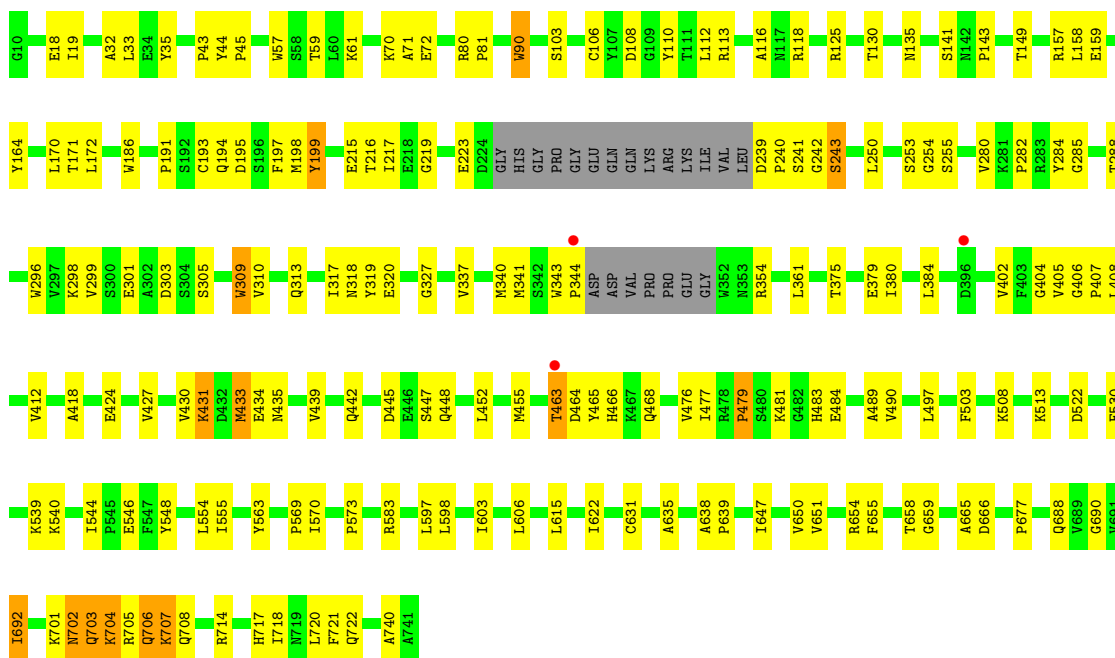
- Molecule 3: COMPLEMENT FACTOR B

Chain F: 72% 23% 5%

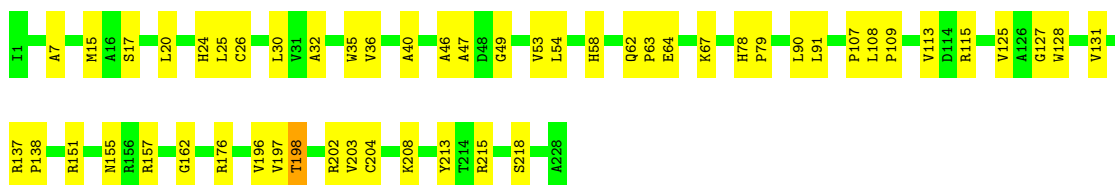


- Molecule 3: COMPLEMENT FACTOR B

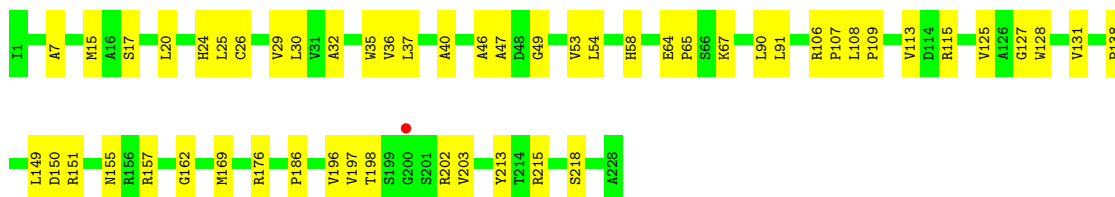
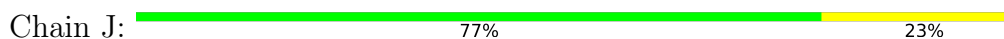
Chain H: 72% 23% . .



• Molecule 4: COMPLEMENT FACTOR D



• Molecule 4: COMPLEMENT FACTOR D



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

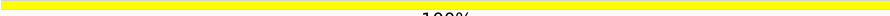


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

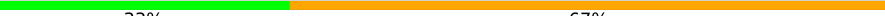
MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

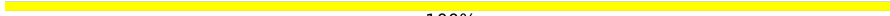
MAG1
MAG2

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%

MAG1
MAG2
BMA3

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	108.28Å 135.78Å 149.97Å 95.47° 110.69° 113.39°	Depositor
Resolution (Å)	65.95 – 3.49 65.95 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.95-3.49) 91.0 (65.95-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.189 , 0.244 0.186 , 0.238	Depositor DCC
R_{free} test set	4098 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	39285	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: NAG, MG, BMA, GOL

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	0.24	0/5092	0.69	0/6917
1	C	0.25	0/5092	0.71	5/6917 (0.1%)
2	B	0.25	0/7340	0.68	3/9936 (0.0%)
2	D	0.24	0/7340	0.66	0/9936
3	F	0.25	0/5754	0.67	0/7786
3	H	0.27	1/5733 (0.0%)	0.67	0/7758
4	I	0.25	0/1745	0.70	0/2376
4	J	0.25	0/1745	0.71	0/2376
All	All	0.25	1/39841 (0.0%)	0.68	8/54002 (0.0%)

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
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	116	ALA	C-N	8.45	1.45	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	964	PRO	CA-C-O	-6.28	113.94	121.48
1	C	63	ASN	O-C-N	6.27	129.28	122.64
1	C	64	VAL	N-CA-C	5.57	116.33	108.36
1	C	63	ASN	CA-C-N	-5.52	115.97	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ASN	C-N-CA	-5.52	115.97	122.93
2	B	964	PRO	CA-C-N	5.47	131.55	121.70
2	B	964	PRO	C-N-CA	5.47	131.55	121.70
1	C	63	ASN	CB-CA-C	-5.03	103.93	111.73

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	964	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4992	0	5055	147	0
1	C	4992	0	5056	154	0
2	B	7197	0	7124	209	0
2	D	7197	0	7124	198	0
3	F	5627	0	5476	130	0
3	H	5608	0	5456	126	0
4	I	1710	0	1698	33	0
4	J	1710	0	1698	33	0
5	E	28	0	25	2	0
5	G	28	0	25	1	0
5	K	28	0	25	10	0
6	L	39	0	34	1	0
6	M	39	0	34	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
8	D	14	0	13	0	0
8	F	28	0	26	1	0
8	H	28	0	26	0	0
9	I	6	0	8	3	0
9	J	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	2	0	0	0	0
10	H	2	0	0	1	0
All	All	39285	0	38911	982	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 13.

All (982) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ASN:HD21	5:K:1:NAG:C1	1.35	1.30
1:A:69:PRO:HA	1:A:70:ALA:HB3	1.36	1.06
1:C:69:PRO:HA	1:C:70:ALA:HB3	1.37	1.03
3:H:430:VAL:HG21	3:H:433:MET:HE2	1.45	0.96
2:B:733:ILE:HD11	2:B:841:ARG:HH21	1.32	0.94
3:F:430:VAL:HG21	3:F:433:MET:HE2	1.50	0.94
1:A:628:SER:HB2	1:A:630:GLN:HE22	1.32	0.93
3:F:222:ALA:N	3:F:223:GLU:HA	1.82	0.93
1:C:628:SER:HB2	1:C:630:GLN:HE22	1.32	0.92
3:H:706:GLN:O	3:H:708:GLN:N	2.08	0.87
3:F:705:ARG:HG2	3:F:705:ARG:HH11	1.37	0.87
2:B:1331:LYS:HA	2:B:1332:ASP:HB2	1.56	0.87
2:B:733:ILE:HG22	2:B:895:TYR:HA	1.55	0.87
2:D:1331:LYS:HA	2:D:1332:ASP:HB2	1.58	0.86
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.41	0.84
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.42	0.84
2:D:840:VAL:HG22	2:D:894:VAL:HG12	1.58	0.83
1:C:517:GLY:O	1:C:518:ALA:O	1.97	0.83
1:C:158:LEU:HD21	1:C:169:LEU:HD21	1.60	0.81
3:H:706:GLN:O	3:H:706:GLN:HG3	1.81	0.80
1:A:158:LEU:HD21	1:A:169:LEU:HD21	1.63	0.79
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.63	0.79
2:D:1205:LEU:HD12	2:D:1249:ALA:HB2	1.65	0.78
3:H:489:ALA:HB2	3:H:677:PRO:HG3	1.64	0.78
3:F:489:ALA:HB2	3:F:677:PRO:HG3	1.65	0.78
2:B:1205:LEU:HD12	2:B:1249:ALA:HB2	1.65	0.78
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.65	0.77
3:H:539:LYS:HB3	3:H:544:ILE:HB	1.68	0.76
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.21	0.75
3:F:361:LEU:HD21	3:F:402:VAL:HG22	1.69	0.75
3:F:539:LYS:HB3	3:F:544:ILE:HB	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:H	1:C:223:ILE:HD12	1.52	0.75
3:H:361:LEU:HD21	3:H:402:VAL:HG22	1.69	0.75
1:C:168:PRO:HB3	3:H:108:ASP:HB3	1.69	0.74
1:A:100:LEU:HD21	1:A:638:LEU:HD23	1.70	0.74
3:H:705:ARG:O	3:H:707:LYS:N	2.21	0.74
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.70	0.74
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.70	0.74
1:C:443:LEU:HD21	1:C:449:LEU:HD13	1.70	0.73
4:J:150:ASP:HA	9:J:1229:GOL:H2	1.69	0.73
1:C:268:ARG:HB2	2:D:1378:MET:HE1	1.70	0.73
2:B:850:PHE:HZ	2:B:907:LEU:HD21	1.53	0.73
2:B:964:PRO:HA	2:B:965:VAL:HG12	1.71	0.73
1:A:223:ILE:HD12	1:A:223:ILE:H	1.52	0.72
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.70	0.72
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.71	0.72
1:C:63:ASN:CG	5:K:1:NAG:C1	2.61	0.72
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.25	0.72
3:F:299:VAL:H	3:F:340:MET:HE3	1.55	0.72
1:C:100:LEU:HD21	1:C:638:LEU:HD23	1.72	0.71
3:F:143:PRO:HG3	3:F:186:TRP:CE2	2.25	0.71
2:B:1333:GLN:HA	2:B:1334:LEU:CB	2.21	0.70
3:H:508:LYS:HA	3:H:508:LYS:HE2	1.73	0.70
1:A:414:GLN:HE21	1:A:414:GLN:HA	1.56	0.70
1:C:414:GLN:HE21	1:C:414:GLN:HA	1.57	0.70
4:J:151:ARG:H	9:J:1229:GOL:H11	1.56	0.70
1:A:547:GLN:HE22	1:A:559:MET:HA	1.56	0.70
1:C:480:LYS:HA	5:K:1:NAG:H81	1.73	0.70
2:D:1333:GLN:HA	2:D:1334:LEU:CB	2.20	0.70
2:B:1103:ILE:HD12	2:B:1103:ILE:H	1.56	0.70
1:C:547:GLN:HE22	1:C:559:MET:HA	1.56	0.69
1:C:63:ASN:HD21	5:K:1:NAG:C2	2.03	0.69
1:A:268:ARG:HB2	2:B:1378:MET:HE1	1.72	0.69
3:F:195:ASP:HB2	3:F:198:MET:HE3	1.72	0.69
1:A:443:LEU:HD21	1:A:449:LEU:HD13	1.73	0.69
2:D:858:ARG:HH22	2:D:1494:GLU:HA	1.56	0.69
3:H:143:PRO:HG3	3:H:186:TRP:CE2	2.28	0.69
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.73	0.68
3:F:508:LYS:HE2	3:F:508:LYS:HA	1.76	0.68
3:F:705:ARG:HG2	3:F:705:ARG:NH1	2.03	0.68
3:H:195:ASP:HB2	3:H:198:MET:HE3	1.74	0.68
3:F:706:GLN:O	3:F:708:GLN:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:VAL:HG22	2:B:795:VAL:HG12	1.74	0.67
1:C:55:THR:HG22	1:C:57:ALA:H	1.59	0.67
3:H:299:VAL:H	3:H:340:MET:HE3	1.58	0.67
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.76	0.67
1:C:443:LEU:HD11	1:C:449:LEU:HD22	1.76	0.67
1:A:351:MET:HE2	1:A:351:MET:HA	1.76	0.66
2:D:1333:GLN:HA	2:D:1334:LEU:HB3	1.77	0.66
1:C:518:ALA:O	1:C:520:GLY:N	2.28	0.66
2:D:804:MET:HG2	2:D:805:GLN:H	1.60	0.66
3:F:464:ASP:O	3:F:465:TYR:HB2	1.95	0.66
2:B:1333:GLN:HA	2:B:1334:LEU:HB3	1.78	0.66
1:C:351:MET:HE2	1:C:351:MET:HA	1.77	0.65
2:D:967:GLN:HG2	2:D:968:MET:H	1.61	0.65
1:C:241:LYS:HE2	2:D:804:MET:HE1	1.78	0.65
2:B:819:ARG:HH12	2:B:1487:GLU:HG2	1.60	0.65
2:B:819:ARG:NH1	2:B:1487:GLU:HG2	2.12	0.65
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.77	0.65
4:J:32:ALA:HB3	4:J:35:TRP:HB2	1.78	0.65
2:D:857:LYS:HD2	2:D:1602:LYS:HE2	1.79	0.65
4:I:64:GLU:HB2	4:I:67:LYS:HG3	1.78	0.64
4:J:64:GLU:HB2	4:J:67:LYS:HG3	1.78	0.64
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.64
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.32	0.64
2:B:1280:SER:HA	3:F:390:ARG:HD3	1.80	0.64
1:A:268:ARG:HH11	2:B:1378:MET:HE3	1.62	0.64
1:C:268:ARG:HH11	2:D:1378:MET:HE3	1.63	0.64
2:B:927:PRO:O	2:B:928:GLU:HB2	1.98	0.63
1:C:208:PRO:HD3	1:C:583:LEU:HD11	1.80	0.63
3:H:318:ASN:HD21	3:H:320:GLU:HG2	1.64	0.63
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.80	0.63
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.63	0.63
1:C:606:THR:HG22	1:C:608:GLY:H	1.63	0.63
4:I:32:ALA:HB3	4:I:35:TRP:HB2	1.79	0.63
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.81	0.63
2:D:1490:ARG:HD2	2:D:1590:TRP:CZ3	2.33	0.63
1:A:606:THR:HG22	1:A:608:GLY:H	1.63	0.63
2:B:819:ARG:HE	2:B:883:THR:HG23	1.63	0.63
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.81	0.63
1:A:69:PRO:HA	1:A:70:ALA:CB	2.17	0.62
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.11	0.62
1:C:19:THR:HB	1:C:478:LEU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:927:PRO:O	2:D:928:GLU:HB2	1.98	0.62
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.82	0.62
3:F:337:VAL:HG12	3:F:341:MET:HE3	1.82	0.62
1:C:69:PRO:HA	1:C:70:ALA:CB	2.18	0.62
1:A:19:THR:HB	1:A:478:LEU:HB2	1.81	0.62
3:H:598:LEU:HA	3:H:603:ILE:HD13	1.81	0.62
2:B:916:MET:HE2	2:B:916:MET:HA	1.81	0.62
1:C:368:ALA:HB2	1:C:376:GLN:HG2	1.82	0.62
1:A:452:ASN:HB3	1:A:492:LEU:HD11	1.82	0.62
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.65	0.62
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.64	0.62
2:B:943:ALA:HB2	2:B:1324:THR:HG21	1.82	0.61
1:C:45:LEU:HD23	1:C:45:LEU:H	1.65	0.61
2:D:916:MET:HE2	2:D:916:MET:HA	1.83	0.61
2:D:1531:GLN:HB2	2:D:1538:GLU:HB2	1.82	0.61
2:D:819:ARG:HE	2:D:883:THR:HG23	1.64	0.61
1:A:208:PRO:HD3	1:A:583:LEU:HD11	1.83	0.61
2:D:958:ILE:HG21	2:D:1276:LEU:HD13	1.83	0.61
3:F:705:ARG:O	3:F:707:LYS:N	2.34	0.61
1:C:452:ASN:HB3	1:C:492:LEU:HD11	1.83	0.61
4:I:108:LEU:HD12	4:I:109:PRO:HD2	1.83	0.60
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.66	0.60
3:H:113:ARG:HH22	3:H:141:SER:HB2	1.65	0.60
1:A:45:LEU:HD23	1:A:45:LEU:H	1.65	0.60
2:B:958:ILE:HG21	2:B:1276:LEU:HD13	1.84	0.60
3:F:598:LEU:HA	3:F:603:ILE:HD13	1.83	0.60
4:J:108:LEU:HD12	4:J:109:PRO:HD2	1.82	0.60
3:H:239:ASP:CB	3:H:240:PRO:HD2	2.32	0.60
2:B:853:LEU:HB2	2:B:860:HIS:CD2	2.37	0.59
2:D:943:ALA:HB2	2:D:1324:THR:HG21	1.84	0.59
1:A:368:ALA:HB2	1:A:376:GLN:HG2	1.83	0.59
2:D:1113:ASN:HB3	2:D:1163:ARG:HH12	1.67	0.59
1:C:479:LEU:O	5:K:1:NAG:H83	2.03	0.59
2:D:853:LEU:HB2	2:D:860:HIS:CD2	2.37	0.59
1:A:396:LYS:HD2	1:A:397:PRO:HD2	1.83	0.59
3:H:442:GLN:HE22	4:J:176:ARG:HH22	1.50	0.59
1:C:126:ARG:HG3	2:D:751:TRP:CZ2	2.38	0.58
2:D:1534:ASN:O	2:D:1566:ILE:HG13	2.04	0.58
3:F:631:CYS:SG	3:F:714:ARG:HD2	2.43	0.58
3:H:318:ASN:ND2	3:H:320:GLU:HG2	2.18	0.58
2:D:1276:LEU:HG	2:D:1285:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:811:LEU:HD22	2:D:890:VAL:HG22	1.85	0.58
1:C:193:GLN:CD	1:C:193:GLN:H	2.11	0.58
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.14	0.58
1:A:193:GLN:H	1:A:193:GLN:CD	2.11	0.58
1:C:6:ILE:HD11	1:C:20:MET:HG2	1.86	0.58
3:F:285:GLY:HA3	3:F:340:MET:HE1	1.86	0.58
3:F:690:GLY:HA2	3:F:718:ILE:O	2.04	0.58
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.86	0.57
1:A:352:VAL:HB	1:A:385:ALA:HB3	1.86	0.57
1:C:396:LYS:HD2	1:C:397:PRO:HD2	1.85	0.57
2:D:1385:MET:HE2	2:D:1385:MET:HA	1.86	0.57
1:C:400:ILE:HD13	1:C:419:MET:HE3	1.87	0.57
3:F:433:MET:C	3:F:435:ASN:H	2.13	0.57
1:A:221:TYR:HD2	1:A:326:ILE:HG23	1.70	0.57
2:B:1113:ASN:HB3	2:B:1163:ARG:HH12	1.69	0.57
3:H:563:TYR:CZ	3:H:569:PRO:HG3	2.40	0.57
1:C:514:THR:OG1	1:C:522:ARG:HD2	2.04	0.57
4:J:131:VAL:HG13	4:J:138:PRO:HG3	1.86	0.57
1:A:168:PRO:HB3	3:F:108:ASP:HB3	1.87	0.57
1:C:289:VAL:HG21	1:C:297:LEU:HD21	1.86	0.57
2:D:997:THR:N	2:D:998:PRO:HD2	2.20	0.57
2:B:811:LEU:HD22	2:B:890:VAL:HG22	1.86	0.57
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.86	0.57
1:A:514:THR:OG1	1:A:522:ARG:HD2	2.05	0.56
2:B:883:THR:HG21	2:B:911:PRO:HG3	1.85	0.56
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.87	0.56
3:H:622:ILE:HA	3:H:658:THR:HG22	1.87	0.56
4:I:131:VAL:HG13	4:I:138:PRO:HG3	1.87	0.56
1:C:63:ASN:ND2	5:K:1:NAG:O5	2.34	0.56
2:D:744:GLU:C	2:D:746:PRO:HD3	2.31	0.56
2:D:804:MET:HG2	2:D:805:GLN:N	2.19	0.56
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.86	0.56
1:A:289:VAL:HG21	1:A:297:LEU:HD21	1.87	0.56
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.86	0.56
4:J:20:LEU:HD11	4:J:49:GLY:HA3	1.87	0.56
1:A:6:ILE:HD11	1:A:20:MET:HG2	1.87	0.56
4:I:20:LEU:HD11	4:I:49:GLY:HA3	1.87	0.56
1:C:480:LYS:HA	5:K:1:NAG:C8	2.36	0.56
3:H:690:GLY:HA2	3:H:718:ILE:O	2.06	0.56
5:E:1:NAG:C1	5:E:1:NAG:O4	2.52	0.56
2:B:1302:THR:HG22	2:B:1304:GLU:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:O	1:A:290:GLN:HG2	2.06	0.56
2:B:997:THR:N	2:B:998:PRO:HD2	2.20	0.56
2:B:1376:ALA:HB3	2:B:1429:VAL:HG23	1.88	0.56
1:C:134:LEU:HD11	1:C:598:VAL:HG21	1.87	0.56
2:D:1238:ARG:HG2	2:D:1240:TYR:OH	2.06	0.56
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.88	0.55
3:F:622:ILE:HA	3:F:658:THR:HG22	1.88	0.55
3:H:172:LEU:HD11	3:H:191:PRO:HB3	1.88	0.55
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.22	0.55
1:C:289:VAL:O	1:C:290:GLN:HG2	2.06	0.55
2:D:1302:THR:HG22	2:D:1304:GLU:H	1.70	0.55
2:B:1331:LYS:CA	2:B:1332:ASP:HB2	2.32	0.55
1:C:221:TYR:HD2	1:C:326:ILE:HG23	1.70	0.55
3:H:597:LEU:HD12	3:H:721:PHE:HZ	1.72	0.55
1:A:363:TYR:HD1	1:A:381:GLY:HA2	1.72	0.55
1:C:61:MET:HE1	1:C:482:GLY:HA2	1.89	0.55
2:D:1017:LEU:C	2:D:1019:LYS:H	2.15	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.87	0.55
2:D:889:GLU:HB2	2:D:904:ARG:HG3	1.89	0.55
3:H:285:GLY:HA3	3:H:340:MET:HE1	1.87	0.55
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.89	0.55
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.89	0.55
2:D:742:ARG:HH12	2:D:777:ILE:HG13	1.72	0.55
1:C:241:LYS:HG3	2:D:832:TYR:CE1	2.42	0.55
1:C:363:TYR:HD1	1:C:381:GLY:HA2	1.72	0.55
2:D:911:PRO:HD2	2:D:1327:HIS:HE1	1.72	0.55
1:A:400:ILE:HD13	1:A:419:MET:HE3	1.88	0.54
1:C:352:VAL:HB	1:C:385:ALA:HB3	1.88	0.54
3:F:113:ARG:HH22	3:F:141:SER:HB2	1.71	0.54
1:A:517:GLY:O	1:A:518:ALA:O	2.25	0.54
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.88	0.54
3:F:563:TYR:CZ	3:F:569:PRO:HG3	2.41	0.54
3:H:433:MET:C	3:H:435:ASN:H	2.15	0.54
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.90	0.54
2:B:1238:ARG:HG2	2:B:1240:TYR:OH	2.07	0.54
3:H:659:GLY:HA2	3:H:666:ASP:HB2	1.90	0.54
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.88	0.54
2:B:964:PRO:HA	2:B:965:VAL:CG1	2.36	0.54
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.23	0.54
3:F:172:LEU:HD11	3:F:191:PRO:HB3	1.90	0.54
4:I:157:ARG:HD3	4:I:157:ARG:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.72	0.54
2:D:956:THR:HG23	2:D:1324:THR:HG22	1.90	0.54
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.43	0.54
2:D:1376:ALA:HB3	2:D:1429:VAL:HG23	1.90	0.54
3:F:216:THR:HG22	3:F:216:THR:O	2.08	0.54
3:H:631:CYS:SG	3:H:714:ARG:HD2	2.48	0.54
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.90	0.54
2:D:1370:TYR:CD1	2:D:1376:ALA:HB2	2.43	0.54
3:F:573:PRO:HB3	3:F:721:PHE:CZ	2.43	0.54
3:F:18:GLU:HG2	3:F:70:LYS:NZ	2.23	0.54
2:B:956:THR:HG23	2:B:1324:THR:HG22	1.90	0.53
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.43	0.53
3:F:468:GLN:HG2	3:F:608:VAL:HG21	1.88	0.53
3:H:284:TYR:HB2	3:H:310:VAL:HG21	1.90	0.53
2:B:1276:LEU:HG	2:B:1285:ILE:HB	1.89	0.53
1:C:578:LYS:HG3	2:D:779:THR:O	2.09	0.53
3:F:284:TYR:HB2	3:F:310:VAL:HG21	1.88	0.53
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.74	0.53
2:B:1005:TYR:HD1	2:B:1258:ALA:HB2	1.73	0.53
3:F:149:THR:HG22	3:F:193:CYS:SG	2.48	0.53
2:D:894:VAL:HG23	2:D:897:HIS:HB2	1.91	0.53
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.53
2:D:1203:LYS:HG3	2:D:1206:TYR:CE2	2.44	0.53
3:H:573:PRO:HB3	3:H:721:PHE:CZ	2.43	0.53
4:J:197:VAL:HG22	4:J:213:TYR:HE2	1.73	0.53
1:A:134:LEU:HD11	1:A:598:VAL:HG21	1.90	0.53
2:B:776:SER:HB2	2:B:780:TRP:HZ2	1.72	0.53
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.91	0.53
3:F:503:PHE:CZ	3:F:555:ILE:HD11	2.43	0.53
3:F:659:GLY:HA2	3:F:666:ASP:HB2	1.91	0.53
5:K:1:NAG:O6	5:K:2:NAG:N2	2.36	0.53
2:D:959:LEU:HD11	2:D:1297:LEU:HD22	1.91	0.53
3:H:219:GLY:HA2	3:H:455:MET:CE	2.39	0.53
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.52
2:B:1017:LEU:C	2:B:1019:LYS:H	2.17	0.52
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.44	0.52
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.89	0.52
2:D:1197:ARG:HE	2:D:1199:GLU:CD	2.17	0.52
3:F:348:PRO:N	3:F:349:PRO:HD3	2.24	0.52
3:F:442:GLN:HE22	4:I:176:ARG:HH22	1.58	0.52
2:B:742:ARG:NH1	2:B:777:ILE:HG13	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:GLU:C	2:B:746:PRO:HD3	2.34	0.52
1:C:126:ARG:HG3	2:D:751:TRP:HZ2	1.74	0.52
2:D:894:VAL:CG2	2:D:899:ILE:HB	2.40	0.52
3:H:239:ASP:HB3	3:H:240:PRO:HD2	1.92	0.52
3:H:706:GLN:C	3:H:708:GLN:H	2.10	0.52
2:B:742:ARG:HH12	2:B:777:ILE:HG13	1.74	0.52
2:B:965:VAL:HG21	2:B:1268:GLN:HE21	1.75	0.52
2:B:1572:LEU:HB3	2:B:1574:LEU:HG	1.91	0.52
2:D:950:PRO:HD3	2:D:1329:LYS:HE2	1.92	0.52
3:H:18:GLU:HG2	3:H:70:LYS:NZ	2.25	0.52
2:B:1203:LYS:HG3	2:B:1206:TYR:CE2	2.44	0.52
2:D:1525:THR:HB	2:D:1541:MET:HB3	1.92	0.52
3:F:407:PRO:HB2	3:F:408:LEU:HD22	1.91	0.52
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.44	0.52
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.10	0.52
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.10	0.52
4:I:196:VAL:O	4:I:198:THR:HG22	2.09	0.52
4:J:157:ARG:HD3	4:J:157:ARG:C	2.34	0.52
1:A:307:THR:HG21	1:A:316:MET:HE3	1.92	0.52
3:F:701:LYS:O	3:F:702:ASN:C	2.53	0.52
3:H:337:VAL:HG12	3:H:341:MET:HE3	1.92	0.52
3:H:503:PHE:CZ	3:H:555:ILE:HD11	2.44	0.52
4:I:24:HIS:CE1	4:I:128:TRP:HB2	2.45	0.52
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.92	0.52
2:D:1331:LYS:CA	2:D:1332:ASP:HB2	2.34	0.52
3:H:216:THR:HG22	3:H:216:THR:O	2.09	0.52
1:C:74:PHE:C	1:C:82:LYS:HZ3	2.18	0.51
2:D:1133:LYS:O	2:D:1137:GLU:HB2	2.10	0.51
2:B:819:ARG:HH12	2:B:1487:GLU:CG	2.23	0.51
2:D:967:GLN:HG2	2:D:968:MET:N	2.25	0.51
3:H:464:ASP:C	3:H:466:HIS:H	2.19	0.51
4:J:24:HIS:CE1	4:J:128:TRP:HB2	2.45	0.51
1:C:84:VAL:HG13	1:C:101:VAL:HG21	1.92	0.51
1:C:223:ILE:HD13	1:C:328:THR:HG22	1.92	0.51
1:A:13:ARG:NH1	1:A:132:HIS:HB3	2.25	0.51
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.76	0.51
2:D:773:LEU:HD13	2:D:803:VAL:HG21	1.91	0.51
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	1.92	0.51
2:D:1498:ILE:HA	2:D:1602:LYS:O	2.11	0.51
4:J:113:VAL:HG12	4:J:115:ARG:HG3	1.93	0.51
4:J:149:LEU:O	9:J:1229:GOL:H31	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:HE1	1:A:482:GLY:HA2	1.93	0.51
2:B:1575:GLU:HB2	2:B:1578:LYS:HD2	1.93	0.51
4:I:197:VAL:HG22	4:I:213:TYR:HE2	1.75	0.51
2:B:894:VAL:CG2	2:B:899:ILE:HB	2.41	0.51
2:B:918:LYS:HZ3	2:B:944:ASP:HB3	1.76	0.51
1:C:136:PRO:HG3	2:D:787:MET:SD	2.50	0.51
2:D:1103:ILE:HD12	2:D:1103:ILE:H	1.74	0.51
3:F:215:GLU:C	3:F:217:ILE:H	2.19	0.51
3:F:463:THR:O	3:F:466:HIS:HB2	2.11	0.51
1:A:223:ILE:HD13	1:A:328:THR:HG22	1.91	0.51
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.93	0.51
1:C:147:ASN:HA	1:C:182:TRP:CE3	2.46	0.51
2:D:1341:LEU:C	2:D:1342:LYS:HD3	2.36	0.51
3:H:215:GLU:C	3:H:217:ILE:H	2.19	0.51
3:H:242:GLY:O	3:H:243:SER:HB2	2.11	0.51
3:H:253:SER:HB3	10:H:2001:HOH:O	2.11	0.51
2:B:1530:VAL:HG23	2:B:1576:GLU:HG2	1.92	0.51
1:C:13:ARG:NH1	1:C:132:HIS:HB3	2.26	0.51
3:H:250:LEU:HB3	3:H:288:THR:HG22	1.92	0.51
3:H:407:PRO:HB2	3:H:408:LEU:HD22	1.93	0.51
1:A:74:PHE:C	1:A:82:LYS:HZ3	2.18	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
2:B:1197:ARG:HE	2:B:1199:GLU:CD	2.19	0.51
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.46	0.51
2:B:950:PRO:HD3	2:B:1329:LYS:HE2	1.93	0.51
2:D:1572:LEU:HB3	2:D:1574:LEU:HG	1.92	0.51
3:F:309:TRP:HZ3	3:F:313:GLN:CD	2.18	0.51
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.93	0.50
1:C:307:THR:HG21	1:C:316:MET:HE3	1.92	0.50
2:D:1498:ILE:HG12	2:D:1603:ASP:HA	1.93	0.50
4:I:113:VAL:HG12	4:I:115:ARG:HG3	1.92	0.50
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.47	0.50
2:D:1532:LEU:O	2:D:1532:LEU:HD12	2.11	0.50
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.46	0.50
2:B:1133:LYS:O	2:B:1137:GLU:HB2	2.12	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.30	0.50
2:D:1113:ASN:HB3	2:D:1163:ARG:NH1	2.26	0.50
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.47	0.50
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.12	0.50
3:H:606:LEU:C	3:H:606:LEU:HD12	2.37	0.50
1:A:470:TYR:HB2	1:A:509:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1286:THR:HG22	3:H:665:ALA:HB3	1.93	0.50
4:J:196:VAL:O	4:J:198:THR:HG22	2.12	0.50
2:D:787:MET:HE1	2:D:793:ILE:HB	1.94	0.50
3:H:424:GLU:OE2	3:H:583:ARG:HD3	2.11	0.50
1:A:96:GLU:OE2	2:B:1021:GLN:HG2	2.12	0.50
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.47	0.50
3:H:303:ASP:HB3	3:H:309:TRP:CD1	2.47	0.50
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.93	0.49
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.27	0.49
2:D:743:SER:HB3	2:D:904:ARG:NH1	2.27	0.49
2:B:833:ARG:HD3	2:B:836:GLN:HE21	1.76	0.49
2:B:1333:GLN:HB3	2:B:1334:LEU:C	2.37	0.49
3:F:303:ASP:HB3	3:F:309:TRP:CD1	2.47	0.49
3:H:298:LYS:HB3	3:H:301:GLU:HG3	1.94	0.49
1:A:147:ASN:HA	1:A:182:TRP:CE3	2.47	0.49
2:B:746:PRO:HG2	2:B:774:LYS:HE3	1.94	0.49
1:C:126:ARG:CZ	1:C:572:VAL:HB	2.43	0.49
2:D:1535:ASP:O	2:D:1536:PHE:HB2	2.12	0.49
3:F:298:LYS:HB3	3:F:301:GLU:HG3	1.94	0.49
1:C:153:VAL:HG12	2:D:1297:LEU:HD12	1.94	0.49
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.43	0.49
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	1.94	0.49
2:B:1341:LEU:C	2:B:1342:LYS:HD3	2.37	0.49
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.93	0.49
3:F:606:LEU:C	3:F:606:LEU:HD12	2.38	0.49
3:H:309:TRP:HZ3	3:H:313:GLN:CD	2.21	0.49
3:H:570:ILE:HD13	3:H:688:GLN:HB2	1.94	0.49
2:B:735:ALA:HB1	2:B:737:GLU:OE1	2.12	0.49
1:C:6:ILE:HD11	1:C:20:MET:CG	2.42	0.49
3:F:296:TRP:CE2	3:F:317:ILE:HG22	2.47	0.49
4:I:40:ALA:HA	4:I:91:LEU:HB2	1.95	0.49
1:C:518:ALA:O	1:C:519:SER:C	2.54	0.49
2:D:1333:GLN:HB3	2:D:1334:LEU:C	2.37	0.49
2:B:751:TRP:HB3	3:F:107:TYR:CD1	2.48	0.49
3:H:149:THR:HG22	3:H:193:CYS:SG	2.53	0.49
4:J:29:VAL:HB	4:J:186:PRO:HG3	1.95	0.49
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.94	0.49
2:D:1381:LEU:HB2	2:D:1424:ILE:O	2.13	0.49
3:F:424:GLU:OE2	3:F:583:ARG:HD3	2.12	0.49
4:I:25:LEU:HG	4:I:26:CYS:SG	2.52	0.49
2:B:1381:LEU:HB2	2:B:1424:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.94	0.49
3:F:597:LEU:HD12	3:F:721:PHE:HZ	1.76	0.49
4:J:40:ALA:HA	4:J:91:LEU:HB2	1.94	0.49
1:A:136:PRO:HG3	2:B:787:MET:SD	2.53	0.48
3:H:298:LYS:HZ2	3:H:340:MET:HA	1.78	0.48
2:B:850:PHE:CZ	2:B:907:LEU:HD21	2.42	0.48
2:D:1285:ILE:HG21	2:D:1300:GLU:HG3	1.95	0.48
2:D:1333:GLN:H	2:D:1333:GLN:CD	2.21	0.48
3:F:570:ILE:HD13	3:F:688:GLN:HB2	1.96	0.48
3:H:118:ARG:NH1	3:H:130:THR:HA	2.29	0.48
2:B:1333:GLN:CD	2:B:1333:GLN:H	2.21	0.48
2:D:1119:MET:HG3	2:D:1161:LEU:HD21	1.95	0.48
3:F:479:PRO:C	3:F:481:LYS:H	2.21	0.48
3:H:476:VAL:HB	3:H:484:GLU:HB3	1.95	0.48
1:A:478:LEU:HD21	1:A:622:LEU:HD21	1.94	0.48
1:A:624:PHE:H	1:A:632:THR:CG2	2.27	0.48
2:B:940:ILE:HD12	2:B:1308:PHE:CE2	2.49	0.48
2:B:1113:ASN:HB3	2:B:1163:ARG:NH1	2.27	0.48
1:C:373:ASP:C	1:C:375:VAL:H	2.22	0.48
3:H:158:LEU:O	3:H:159:GLU:HB2	2.13	0.48
4:I:36:VAL:HG21	4:I:53:VAL:HG11	1.95	0.48
3:F:241:SER:CB	3:F:242:GLY:HA3	2.43	0.48
3:H:701:LYS:O	3:H:702:ASN:C	2.55	0.48
1:A:242:LYS:HB3	1:A:274:GLY:HA3	1.96	0.48
1:A:369:VAL:HG12	1:A:371:GLY:H	1.79	0.48
1:A:373:ASP:C	1:A:375:VAL:H	2.21	0.48
1:A:624:PHE:H	1:A:632:THR:HG21	1.78	0.48
2:B:1331:LYS:HA	2:B:1332:ASP:CB	2.26	0.48
3:F:250:LEU:HB3	3:F:288:THR:HG22	1.95	0.48
6:L:1:NAG:H61	6:L:2:NAG:HN2	1.79	0.48
1:A:323:GLY:O	1:A:325:PRO:HD3	2.13	0.48
2:B:927:PRO:O	2:B:928:GLU:CB	2.62	0.48
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.14	0.48
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.94	0.48
2:B:1103:ILE:HD12	2:B:1103:ILE:N	2.27	0.48
2:B:1301:GLU:HG2	3:F:157:ARG:NH1	2.29	0.48
2:B:1531:GLN:C	2:B:1532:LEU:HD12	2.39	0.48
1:C:6:ILE:HG22	1:C:625:THR:O	2.13	0.48
2:D:907:LEU:HD23	2:D:907:LEU:H	1.78	0.48
2:D:985:PRO:HG3	2:D:996:MET:HA	1.96	0.48
2:D:990:GLU:O	2:D:994:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PRO:HD3	1:A:182:TRP:CE2	2.49	0.47
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.96	0.47
1:C:470:TYR:HB2	1:C:509:LEU:HD21	1.96	0.47
2:D:883:THR:HG21	2:D:911:PRO:HG3	1.96	0.47
3:F:19:ILE:HG13	3:F:71:ALA:C	2.39	0.47
3:H:706:GLN:O	3:H:706:GLN:CG	2.55	0.47
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.49	0.47
2:B:968:MET:O	2:B:969:THR:HB	2.14	0.47
1:C:148:PRO:HD3	1:C:182:TRP:CE2	2.49	0.47
1:C:177:VAL:HG22	1:C:178:ASN:N	2.29	0.47
1:C:242:LYS:HB3	1:C:274:GLY:HA3	1.96	0.47
2:D:916:MET:HG3	2:D:1328:ALA:CB	2.44	0.47
2:D:1005:TYR:HD1	2:D:1258:ALA:HB2	1.79	0.47
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.94	0.47
3:F:433:MET:HG3	3:F:434:GLU:N	2.29	0.47
1:A:338:THR:HG21	1:A:419:MET:HE1	1.95	0.47
1:C:45:LEU:HB2	1:C:46:VAL:HB	1.97	0.47
2:D:1543:ILE:HD12	2:D:1554:VAL:HG21	1.95	0.47
1:A:177:VAL:HG22	1:A:178:ASN:N	2.29	0.47
1:A:179:MET:HG3	1:A:203:LYS:HA	1.96	0.47
2:B:732:ASP:O	2:B:733:ILE:HG12	2.15	0.47
2:B:1483:LEU:HD11	2:B:1536:PHE:HB3	1.95	0.47
1:C:624:PHE:H	1:C:632:THR:HG21	1.79	0.47
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.15	0.47
3:H:296:TRP:CE2	3:H:317:ILE:HG22	2.50	0.47
4:J:36:VAL:HG21	4:J:53:VAL:HG11	1.96	0.47
2:B:1581:LEU:HB2	2:B:1609:TRP:HE3	1.79	0.47
1:C:630:GLN:H	1:C:630:GLN:NE2	2.13	0.47
2:D:918:LYS:NZ	2:D:944:ASP:HB3	2.29	0.47
2:D:927:PRO:O	2:D:928:GLU:CB	2.62	0.47
1:A:6:ILE:HD11	1:A:20:MET:CG	2.43	0.47
1:A:31:VAL:HG13	1:A:54:LEU:HB2	1.96	0.47
1:A:578:LYS:HG3	2:B:779:THR:O	2.15	0.47
2:B:940:ILE:HD11	2:B:1320:LEU:HD21	1.97	0.47
1:C:624:PHE:H	1:C:632:THR:CG2	2.28	0.47
2:D:1263:ASP:O	2:D:1265:PRO:HD3	2.14	0.47
3:F:404:GLY:O	3:F:430:VAL:HG22	2.14	0.47
3:H:703:GLN:O	3:H:704:LYS:HB2	2.14	0.47
1:A:177:VAL:HG22	1:A:178:ASN:H	1.80	0.47
2:B:739:ILE:HB	2:B:891:LYS:HD3	1.95	0.47
2:B:965:VAL:O	2:B:965:VAL:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLY:O	1:C:325:PRO:HD3	2.13	0.47
2:D:1443:GLN:HE21	2:D:1446:ASN:HA	1.79	0.47
3:F:118:ARG:NH1	3:F:130:THR:HA	2.30	0.47
4:J:197:VAL:HG22	4:J:213:TYR:CE2	2.50	0.47
2:B:966:ALA:HA	2:B:1267:HIS:HA	1.97	0.47
2:B:1119:MET:HG3	2:B:1161:LEU:HD21	1.96	0.47
3:F:344:PRO:O	3:F:345:ASP:HB2	2.15	0.47
3:H:435:ASN:O	3:H:439:VAL:HG23	2.14	0.47
4:J:215:ARG:NH1	4:J:218:SER:HB2	2.30	0.47
2:B:1531:GLN:HB2	2:B:1538:GLU:HB2	1.95	0.47
1:C:179:MET:HG3	1:C:203:LYS:HA	1.97	0.47
1:C:369:VAL:HG12	1:C:371:GLY:H	1.80	0.47
2:D:822:GLN:HA	2:D:879:VAL:HG22	1.97	0.47
2:D:1575:GLU:HB2	2:D:1578:LYS:HD2	1.96	0.47
3:F:654:ARG:HG3	3:F:722:GLN:HB3	1.97	0.47
3:H:254:GLY:HA2	3:H:319:TYR:OH	2.14	0.47
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.97	0.47
2:B:804:MET:HG2	2:B:805:GLN:N	2.30	0.47
2:D:894:VAL:HG22	2:D:899:ILE:HB	1.97	0.47
2:D:1581:LEU:HB2	2:D:1609:TRP:HE3	1.80	0.47
3:H:59:THR:HG23	3:H:61:LYS:HG2	1.96	0.47
3:H:219:GLY:HA2	3:H:455:MET:HE2	1.96	0.47
3:H:433:MET:O	3:H:434:GLU:HB2	2.15	0.47
2:B:1285:ILE:HG21	2:B:1300:GLU:HG3	1.98	0.46
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.96	0.46
2:D:872:LEU:HD13	2:D:1418:ASP:HB3	1.96	0.46
3:F:158:LEU:O	3:F:159:GLU:HB2	2.14	0.46
1:C:338:THR:HG21	1:C:419:MET:HE1	1.96	0.46
3:F:503:PHE:HB2	3:F:530:PHE:HZ	1.80	0.46
3:H:433:MET:HG3	3:H:434:GLU:N	2.30	0.46
4:I:151:ARG:H	9:I:1229:GOL:H11	1.80	0.46
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.15	0.46
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.14	0.46
3:H:44:TYR:HB3	3:H:72:GLU:O	2.15	0.46
1:A:6:ILE:HG22	1:A:625:THR:O	2.15	0.46
1:A:45:LEU:HB2	1:A:46:VAL:HB	1.97	0.46
1:A:453:PHE:HE1	1:A:495:LEU:HB2	1.80	0.46
2:B:822:GLN:HA	2:B:879:VAL:HG22	1.97	0.46
2:B:985:PRO:HG3	2:B:996:MET:HA	1.97	0.46
4:J:169:MET:HB2	9:J:1229:GOL:O3	2.15	0.46
2:B:1119:MET:SD	2:B:1157:ASN:HB2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:916:MET:HG3	2:D:1328:ALA:HB3	1.98	0.46
3:H:375:THR:O	3:H:379:GLU:HG3	2.15	0.46
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.46
1:A:583:LEU:N	1:A:583:LEU:HD12	2.31	0.46
1:A:630:GLN:NE2	1:A:630:GLN:H	2.13	0.46
2:B:735:ALA:C	2:B:737:GLU:H	2.23	0.46
1:C:112:THR:HG22	1:C:125:TYR:HB3	1.98	0.46
2:D:965:VAL:HG22	2:D:965:VAL:O	2.15	0.46
2:D:1119:MET:SD	2:D:1157:ASN:HB2	2.55	0.46
3:F:59:THR:HG23	3:F:61:LYS:HG2	1.96	0.46
3:F:435:ASN:O	3:F:439:VAL:HG23	2.16	0.46
1:A:12:LEU:HG	1:A:99:VAL:HG11	1.97	0.46
1:C:31:VAL:HG13	1:C:54:LEU:HB2	1.97	0.46
2:D:833:ARG:HD3	2:D:836:GLN:HE21	1.80	0.46
3:H:688:GLN:HG2	3:H:720:LEU:HD11	1.98	0.46
4:I:197:VAL:HG22	4:I:213:TYR:CE2	2.51	0.46
4:J:25:LEU:HG	4:J:26:CYS:SG	2.55	0.46
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.98	0.46
1:C:558:GLN:HG2	2:D:772:PHE:CE2	2.51	0.46
2:D:940:ILE:HD11	2:D:1320:LEU:HD21	1.98	0.46
3:F:90:TRP:H	3:F:90:TRP:CD1	2.33	0.46
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.81	0.46
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.56	0.46
2:D:940:ILE:HD12	2:D:1308:PHE:CE2	2.50	0.46
2:D:1639:CYS:O	3:H:327:GLY:HA2	2.16	0.46
2:B:894:VAL:HG22	2:B:899:ILE:HB	1.98	0.46
2:B:913:GLY:O	2:B:1331:LYS:HE3	2.16	0.46
2:B:1617:ASP:C	2:B:1619:GLU:H	2.24	0.46
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.97	0.46
1:C:223:ILE:HD12	1:C:223:ILE:N	2.25	0.46
3:H:404:GLY:O	3:H:430:VAL:HG22	2.15	0.46
3:H:503:PHE:HB2	3:H:530:PHE:HZ	1.81	0.46
2:B:1525:THR:HB	2:B:1541:MET:HB3	1.97	0.45
3:F:95:TYR:HE2	8:F:1743:NAG:HN2	1.65	0.45
3:F:164:TYR:CD1	3:F:191:PRO:HG2	2.52	0.45
3:F:706:GLN:C	3:F:708:GLN:H	2.23	0.45
3:H:171:THR:HG23	3:H:412:VAL:HG22	1.99	0.45
1:A:223:ILE:HD12	1:A:223:ILE:N	2.26	0.45
1:A:268:ARG:HD3	2:B:1378:MET:CE	2.47	0.45
1:A:628:SER:HB2	1:A:630:GLN:NE2	2.16	0.45
2:B:918:LYS:NZ	2:B:944:ASP:HB3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1443:GLN:HE21	2:B:1446:ASN:HA	1.80	0.45
1:A:45:LEU:HA	1:A:46:VAL:HA	1.72	0.45
1:A:112:THR:HG22	1:A:125:TYR:HB3	1.98	0.45
1:A:268:ARG:HH11	2:B:1378:MET:CE	2.29	0.45
1:A:356:ASN:HB3	1:A:357:PRO:HD2	1.97	0.45
1:C:614:ALA:HB1	1:C:632:THR:HA	1.99	0.45
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.45
3:H:654:ARG:HG3	3:H:722:GLN:HB3	1.98	0.45
4:I:215:ARG:NH1	4:I:218:SER:HB2	2.31	0.45
3:H:354:ARG:HD2	3:H:354:ARG:C	2.42	0.45
1:C:177:VAL:HG22	1:C:178:ASN:H	1.80	0.45
1:C:398:LEU:HD22	1:C:400:ILE:HD11	1.98	0.45
2:D:742:ARG:NH1	2:D:777:ILE:HG13	2.32	0.45
2:D:1617:ASP:C	2:D:1619:GLU:H	2.24	0.45
3:H:33:LEU:C	3:H:33:LEU:HD12	2.41	0.45
3:H:464:ASP:HB2	3:H:615:LEU:HD12	1.98	0.45
2:B:1286:THR:HG22	3:F:665:ALA:HB3	1.99	0.45
1:C:222:TYR:HE2	1:C:224:TYR:HB2	1.82	0.45
1:C:453:PHE:HE1	1:C:495:LEU:HB2	1.82	0.45
1:C:541:LEU:HD22	2:D:786:SER:CB	2.46	0.45
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.82	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.15	0.45
3:F:655:PHE:HA	3:F:717:HIS:O	2.16	0.45
3:F:703:GLN:O	3:F:704:LYS:HB2	2.15	0.45
1:A:222:TYR:HE2	1:A:224:TYR:HB2	1.81	0.45
1:A:248:PHE:HE2	2:B:1378:MET:HE2	1.81	0.45
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.97	0.45
2:B:1017:LEU:O	2:B:1018:GLU:HB3	2.16	0.45
2:D:1163:ARG:O	2:D:1167:VAL:HG23	2.17	0.45
3:H:90:TRP:H	3:H:90:TRP:CD1	2.35	0.45
2:B:733:ILE:HD11	2:B:841:ARG:NH2	2.15	0.45
2:B:819:ARG:HE	2:B:883:THR:CG2	2.27	0.45
2:B:990:GLU:O	2:B:994:ILE:HG13	2.17	0.45
2:D:852:SER:HB3	2:D:878:ILE:HG22	1.98	0.45
3:F:298:LYS:HZ2	3:F:340:MET:HA	1.82	0.45
3:H:477:ILE:HG13	3:H:483:HIS:CE1	2.51	0.45
3:H:544:ILE:HD13	3:H:650:VAL:HG12	1.98	0.45
2:B:732:ASP:CG	2:B:733:ILE:H	2.24	0.45
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.17	0.45
2:B:1236:GLU:HA	2:B:1238:ARG:NH2	2.31	0.45
2:B:1581:LEU:HB2	2:B:1609:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ILE:H	1:C:223:ILE:CD1	2.26	0.45
2:D:1105:GLN:O	2:D:1112:ARG:HD2	2.16	0.45
3:F:318:ASN:ND2	3:F:320:GLU:HG2	2.31	0.45
3:H:170:LEU:HD23	3:H:193:CYS:HB3	1.98	0.45
3:H:452:LEU:HD12	3:H:455:MET:HG3	1.99	0.45
5:K:1:NAG:O6	5:K:2:NAG:C1	2.64	0.45
2:B:907:LEU:HD23	2:B:907:LEU:H	1.82	0.45
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.45
2:D:1497:PHE:HA	2:D:1601:GLY:O	2.15	0.45
2:D:1631:THR:O	2:D:1635:VAL:HG23	2.17	0.45
3:F:345:ASP:O	3:F:348:PRO:HD2	2.16	0.45
3:F:688:GLN:HG2	3:F:720:LEU:HD11	1.99	0.45
2:B:840:VAL:HG12	2:B:841:ARG:N	2.33	0.44
2:B:854:ALA:HB2	2:B:860:HIS:HB3	1.99	0.44
2:B:1641:ASN:OXT	3:F:255:SER:HB3	2.17	0.44
1:C:6:ILE:HD12	1:C:21:VAL:O	2.17	0.44
2:D:819:ARG:HE	2:D:883:THR:CG2	2.28	0.44
2:D:918:LYS:HZ3	2:D:944:ASP:HB3	1.82	0.44
2:D:1301:GLU:HG2	3:H:157:ARG:NH1	2.32	0.44
3:F:125:ARG:HH21	3:F:194:GLN:HE22	1.65	0.44
1:C:63:ASN:HD22	5:K:1:NAG:C1	2.06	0.44
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.99	0.44
2:D:1483:LEU:HB3	2:D:1490:ARG:HG2	2.00	0.44
2:D:1581:LEU:HB2	2:D:1609:TRP:CE3	2.53	0.44
3:F:375:THR:O	3:F:379:GLU:HG3	2.17	0.44
3:H:32:ALA:HA	3:H:57:TRP:HZ3	1.83	0.44
3:H:199:TYR:CE1	3:H:431:LYS:HD3	2.51	0.44
3:H:655:PHE:HA	3:H:717:HIS:O	2.16	0.44
4:I:17:SER:HB3	4:I:54:LEU:HB3	1.98	0.44
2:B:833:ARG:HD2	2:B:838:LEU:HD21	1.99	0.44
2:B:916:MET:HG3	2:B:1328:ALA:CB	2.47	0.44
2:B:1551:SER:HB3	3:F:371:GLY:HA3	1.99	0.44
3:F:110:TYR:CE1	3:F:135:ASN:HB3	2.52	0.44
3:F:544:ILE:HD13	3:F:650:VAL:HG12	1.98	0.44
3:F:546:GLU:HB3	3:F:548:TYR:CE1	2.52	0.44
1:A:93:GLN:HE21	1:A:627:SER:HB2	1.82	0.44
2:D:1103:ILE:HD12	2:D:1103:ILE:N	2.31	0.44
2:D:1365:GLU:HA	2:D:1438:ALA:HB2	1.99	0.44
3:F:433:MET:O	3:F:434:GLU:HB2	2.17	0.44
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.99	0.44
1:C:39:ASP:CG	1:C:44:LYS:HB3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LEU:N	1:C:583:LEU:HD12	2.33	0.44
2:D:941:PRO:HA	2:D:942:PRO:HD3	1.90	0.44
3:F:513:LYS:HB3	3:F:522:ASP:HB3	1.99	0.44
4:J:15:MET:HE2	4:J:127:GLY:HA2	2.00	0.44
2:B:964:PRO:HA	2:B:965:VAL:CB	2.47	0.44
2:B:1276:LEU:HD23	2:B:1276:LEU:H	1.83	0.44
2:D:1017:LEU:O	2:D:1018:GLU:HB3	2.17	0.44
1:A:39:ASP:CG	1:A:44:LYS:HB3	2.42	0.44
1:A:116:ILE:HG12	1:A:205:TYR:CE2	2.52	0.44
1:A:398:LEU:HD22	1:A:400:ILE:HD11	1.99	0.44
2:B:733:ILE:HG13	2:B:734:ILE:N	2.31	0.44
1:C:356:ASN:HB3	1:C:357:PRO:HD2	1.99	0.44
2:D:840:VAL:HG12	2:D:841:ARG:N	2.32	0.44
3:H:479:PRO:C	3:H:481:LYS:H	2.25	0.44
1:A:239:TYR:HD2	2:B:804:MET:HE2	1.83	0.44
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.88	0.44
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.99	0.44
2:B:1365:GLU:HA	2:B:1438:ALA:HB2	2.00	0.44
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.33	0.44
1:C:329:SER:HA	1:C:330:PRO:HD3	1.84	0.44
1:C:400:ILE:N	1:C:400:ILE:HD12	2.33	0.44
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.32	0.44
2:D:1236:GLU:HA	2:D:1238:ARG:NH2	2.33	0.44
2:D:1380:ILE:N	2:D:1380:ILE:HD12	2.32	0.44
3:H:705:ARG:C	3:H:707:LYS:H	2.24	0.44
2:B:804:MET:HG2	2:B:805:GLN:H	1.83	0.44
2:B:918:LYS:HE3	2:B:1326:TYR:OH	2.18	0.44
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.52	0.44
3:H:239:ASP:CG	3:H:240:PRO:HD2	2.43	0.44
2:B:1296:LEU:O	2:B:1298:ARG:HG3	2.18	0.43
2:B:1535:ASP:OD1	2:B:1535:ASP:N	2.50	0.43
1:C:111:GLN:O	1:C:125:TYR:HA	2.17	0.43
1:C:129:THR:OG1	1:C:165:GLY:HA2	2.18	0.43
2:D:819:ARG:NH1	2:D:1487:GLU:HG2	2.33	0.43
2:D:1331:LYS:HA	2:D:1332:ASP:CB	2.28	0.43
3:F:222:ALA:N	3:F:223:GLU:CA	2.66	0.43
3:H:106:CYS:SG	3:H:112:LEU:HB2	2.58	0.43
3:H:463:THR:OG1	3:H:464:ASP:N	2.51	0.43
3:H:635:ALA:HB3	3:H:647:ILE:HD11	2.00	0.43
1:A:17:GLU:HG2	1:A:67:THR:OG1	2.18	0.43
2:B:1338:LYS:HD2	2:B:1338:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:LYS:N	1:C:343:LYS:HD2	2.33	0.43
1:C:533:VAL:HG12	1:C:534:LYS:N	2.33	0.43
1:C:577:ASP:CG	2:D:778:THR:HG21	2.43	0.43
2:D:918:LYS:HE3	2:D:1326:TYR:OH	2.19	0.43
2:D:1386:MET:SD	2:D:1473:PRO:HD3	2.57	0.43
3:F:106:CYS:SG	3:F:112:LEU:HB2	2.58	0.43
3:H:380:ILE:O	3:H:384:LEU:HG	2.18	0.43
3:H:513:LYS:HB3	3:H:522:ASP:HB3	1.99	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.32	0.43
2:B:1337:ASN:HB3	2:B:1338:LYS:H	1.63	0.43
1:C:116:ILE:HG12	1:C:205:TYR:CE2	2.53	0.43
2:D:854:ALA:HB2	2:D:860:HIS:HB3	2.00	0.43
3:H:463:THR:O	3:H:466:HIS:HB2	2.17	0.43
1:A:255:ASP:HB2	1:A:300:LYS:HG2	2.00	0.43
1:A:553:PRO:HD2	2:B:802:THR:O	2.19	0.43
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.43
1:C:12:LEU:HG	1:C:99:VAL:HG11	2.00	0.43
1:C:283:LYS:O	1:C:287:ASP:HB2	2.18	0.43
2:D:913:GLY:O	2:D:1331:LYS:HE3	2.18	0.43
3:F:219:GLY:HA2	3:F:455:MET:HE2	1.99	0.43
3:H:240:PRO:HA	3:H:241:SER:HA	1.52	0.43
1:A:283:LYS:O	1:A:287:ASP:HB2	2.18	0.43
2:B:1039:GLN:OE1	2:B:1052:PRO:HG3	2.19	0.43
2:D:833:ARG:HD2	2:D:838:LEU:HD21	2.00	0.43
2:D:1001:ILE:HG13	2:D:1254:PHE:HB2	1.99	0.43
2:D:1039:GLN:OE1	2:D:1052:PRO:HG3	2.19	0.43
3:H:19:ILE:HG13	3:H:71:ALA:C	2.44	0.43
3:H:433:MET:CG	3:H:434:GLU:N	2.82	0.43
3:H:433:MET:CG	3:H:434:GLU:H	2.31	0.43
4:J:202:ARG:HB3	4:J:203:VAL:H	1.62	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.53	0.43
1:A:145:ILE:O	1:A:153:VAL:HG22	2.18	0.43
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.53	0.43
2:D:1498:ILE:HG22	2:D:1499:GLN:HG2	2.00	0.43
3:F:35:TYR:HB2	3:F:43:PRO:HB3	1.99	0.43
3:F:380:ILE:O	3:F:384:LEU:HG	2.18	0.43
3:F:433:MET:CG	3:F:434:GLU:N	2.82	0.43
3:F:433:MET:CG	3:F:434:GLU:H	2.31	0.43
4:I:7:ALA:O	4:I:58:HIS:HE1	2.02	0.43
4:I:30:LEU:O	4:I:107:PRO:HA	2.19	0.43
1:A:269:ILE:HD13	1:A:278:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.18	0.43
2:D:1145:GLY:O	2:D:1149:LYS:HG2	2.19	0.43
2:D:1390:ALA:HA	2:D:1391:PRO:HD3	1.90	0.43
2:D:1536:PHE:H	2:D:1566:ILE:HG12	1.83	0.43
3:F:450:LEU:HD12	3:F:450:LEU:HA	1.93	0.43
3:H:110:TYR:CE1	3:H:135:ASN:HB3	2.54	0.43
4:J:40:ALA:HB2	4:J:90:LEU:O	2.18	0.43
1:A:63:ASN:HB3	5:E:1:NAG:O5	2.18	0.43
1:A:349:ASP:C	1:A:350:LEU:HD12	2.43	0.43
2:B:785:VAL:HG13	2:B:795:VAL:HG12	1.99	0.43
2:B:819:ARG:O	2:B:820:ASN:HB2	2.19	0.43
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.54	0.43
2:B:1631:THR:O	2:B:1635:VAL:HG23	2.19	0.43
1:C:349:ASP:C	1:C:350:LEU:HD12	2.44	0.43
4:I:15:MET:HE2	4:I:127:GLY:HA2	2.00	0.43
1:A:103:LEU:HD22	1:A:103:LEU:N	2.34	0.43
1:A:158:LEU:HD22	1:A:169:LEU:HD11	2.01	0.43
1:C:123:VAL:O	1:C:170:SER:HA	2.19	0.43
1:C:269:ILE:HD13	1:C:278:VAL:HB	2.00	0.43
1:C:552:GLN:HA	1:C:553:PRO:HD3	1.92	0.43
1:C:566:ASP:OD2	2:D:791:LYS:HG3	2.19	0.43
3:F:143:PRO:HG3	3:F:186:TRP:NE1	2.34	0.43
3:H:35:TYR:HB2	3:H:43:PRO:HB3	2.00	0.43
3:H:447:SER:O	4:I:208:LYS:HE2	2.18	0.43
3:H:650:VAL:HG23	3:H:651:VAL:HG23	2.01	0.43
1:A:19:THR:HA	1:A:65:THR:HG22	2.01	0.43
1:A:400:ILE:N	1:A:400:ILE:HD12	2.33	0.43
1:A:495:LEU:HA	1:A:496:PRO:HD3	1.89	0.43
2:B:964:PRO:HB3	2:B:1291:TRP:CZ3	2.54	0.43
2:B:1380:ILE:N	2:B:1380:ILE:HD12	2.34	0.43
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	2.01	0.43
2:D:1115:ASN:O	2:D:1116:GLU:HB2	2.19	0.43
3:F:33:LEU:HD12	3:F:33:LEU:C	2.44	0.43
3:F:219:GLY:HA2	3:F:455:MET:CE	2.49	0.43
3:F:490:VAL:O	3:F:569:PRO:HA	2.19	0.43
3:H:692:ILE:HA	3:H:717:HIS:ND1	2.34	0.43
2:B:839:LYS:O	2:B:895:TYR:HD1	2.02	0.42
2:D:737:GLU:C	2:D:739:ILE:H	2.27	0.42
2:D:1155:GLU:HG3	2:D:1184:LEU:HD21	2.00	0.42
2:D:1338:LYS:N	2:D:1338:LYS:HD2	2.34	0.42
2:D:1490:ARG:HD2	2:D:1590:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:ARG:HA	3:F:81:PRO:HD3	1.94	0.42
1:A:123:VAL:O	1:A:170:SER:HA	2.19	0.42
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.01	0.42
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.92	0.42
2:B:963:THR:HG22	2:B:1318:GLY:HA2	2.01	0.42
2:B:1064:PHE:O	2:B:1068:VAL:HG13	2.19	0.42
2:B:1115:ASN:O	2:B:1116:GLU:HB2	2.19	0.42
2:B:1155:GLU:HG3	2:B:1184:LEU:HD21	2.01	0.42
2:B:1498:ILE:HD12	2:B:1605:TRP:HB2	2.00	0.42
1:C:10:ASN:CB	1:C:635:ARG:HH11	2.33	0.42
1:C:171:TRP:CZ3	1:C:173:ILE:HG12	2.54	0.42
2:D:811:LEU:HG	2:D:813:LEU:HD13	2.01	0.42
2:D:839:LYS:O	2:D:895:TYR:HD1	2.01	0.42
3:F:341:MET:SD	3:F:380:ILE:HG23	2.59	0.42
3:H:80:ARG:HA	3:H:81:PRO:HD3	1.94	0.42
3:H:280:VAL:O	3:H:282:PRO:HD3	2.19	0.42
1:A:241:LYS:HG3	2:B:832:TYR:CE1	2.54	0.42
1:A:533:VAL:HG12	1:A:534:LYS:N	2.34	0.42
2:B:1276:LEU:HD23	2:B:1276:LEU:N	2.34	0.42
2:B:1301:GLU:CD	2:B:1301:GLU:H	2.27	0.42
2:D:959:LEU:HD21	2:D:1297:LEU:CD2	2.49	0.42
2:D:1119:MET:HE1	2:D:1154:LEU:HA	2.02	0.42
2:D:1337:ASN:HB3	2:D:1338:LYS:H	1.63	0.42
3:F:44:TYR:HB3	3:F:72:GLU:O	2.19	0.42
3:F:90:TRP:CD1	3:F:90:TRP:N	2.85	0.42
3:H:113:ARG:NH2	3:H:141:SER:HB2	2.30	0.42
2:B:749:TRP:CE3	2:B:750:LEU:HB2	2.55	0.42
1:C:38:HIS:HD2	1:C:45:LEU:HB3	1.85	0.42
1:C:578:LYS:HD3	2:D:779:THR:HB	2.01	0.42
2:D:1375:ASP:O	2:D:1376:ALA:C	2.63	0.42
2:D:1411:GLU:HG2	2:D:1422:LEU:HD12	2.00	0.42
3:F:44:TYR:CD1	3:F:45:PRO:HA	2.55	0.42
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	2.01	0.42
1:C:145:ILE:O	1:C:153:VAL:HG22	2.19	0.42
1:C:248:PHE:HE2	2:D:1378:MET:HE2	1.84	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
2:D:1387:THR:HG23	2:D:1387:THR:O	2.19	0.42
3:F:113:ARG:NH2	3:F:141:SER:HB2	2.33	0.42
1:A:129:THR:OG1	1:A:165:GLY:HA2	2.20	0.42
1:A:239:TYR:HB2	2:B:804:MET:HE2	1.99	0.42
1:A:414:GLN:HA	1:A:414:GLN:NE2	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:754:GLU:HG3	2:B:769:MET:SD	2.59	0.42
2:B:916:MET:HG3	2:B:1328:ALA:HB3	2.01	0.42
2:B:1253:VAL:O	2:B:1257:LEU:HG	2.20	0.42
2:B:1405:ARG:HE	2:B:1437:LEU:HD22	1.84	0.42
1:C:25:HIS:HA	1:C:26:ASP:HA	1.51	0.42
2:D:977:ARG:HD2	2:D:1240:TYR:CE2	2.55	0.42
2:D:1296:LEU:O	2:D:1298:ARG:HG3	2.18	0.42
3:F:701:LYS:O	3:F:703:GLN:N	2.52	0.42
2:B:1524:LYS:O	2:B:1544:GLU:HB2	2.19	0.42
1:C:459:ARG:HA	1:C:462:GLU:HG2	2.02	0.42
1:C:547:GLN:NE2	1:C:559:MET:HA	2.29	0.42
3:F:497:LEU:HA	3:F:554:LEU:HD23	2.02	0.42
4:I:155:ASN:CG	4:I:162:GLY:HA2	2.45	0.42
4:J:54:LEU:HD21	4:J:67:LYS:HE3	2.01	0.42
2:B:1119:MET:HE1	2:B:1154:LEU:HA	2.01	0.42
1:C:440:ARG:HA	1:C:440:ARG:HD2	1.92	0.42
2:D:1009:THR:HG22	2:D:1261:GLN:HG3	2.01	0.42
2:D:1391:PRO:HB2	2:D:1396:LEU:HD11	2.02	0.42
3:F:280:VAL:O	3:F:282:PRO:HD3	2.20	0.42
3:H:250:LEU:O	3:H:288:THR:HA	2.20	0.42
3:H:490:VAL:O	3:H:569:PRO:HA	2.20	0.42
1:A:541:LEU:HD22	2:B:786:SER:CB	2.49	0.42
1:A:545:SER:HB2	2:B:799:PHE:HZ	1.84	0.42
1:A:606:THR:HA	1:A:607:PRO:HD3	1.94	0.42
2:B:1297:LEU:HD12	2:B:1297:LEU:HA	1.68	0.42
2:B:1500:LYS:HE3	2:B:1500:LYS:HB2	1.93	0.42
1:C:414:GLN:HA	1:C:414:GLN:NE2	2.30	0.42
2:D:1086:ILE:HG23	2:D:1146:SER:HB2	2.00	0.42
2:D:1270:LEU:O	2:D:1290:HIS:HA	2.20	0.42
3:F:32:ALA:HA	3:F:57:TRP:HZ3	1.84	0.42
3:F:650:VAL:HG23	3:F:651:VAL:HG23	2.02	0.42
4:J:64:GLU:HA	4:J:65:PRO:HD3	1.89	0.42
1:A:470:TYR:HA	1:A:510:VAL:O	2.20	0.42
1:A:510:VAL:HG21	1:A:622:LEU:HD12	2.01	0.42
2:B:941:PRO:HA	2:B:942:PRO:HD3	1.90	0.42
2:B:1086:ILE:HG23	2:B:1146:SER:HB2	2.02	0.42
2:D:811:LEU:HG	2:D:813:LEU:CD1	2.50	0.42
2:D:968:MET:O	2:D:969:THR:HB	2.20	0.42
2:D:981:LEU:HB3	2:D:998:PRO:O	2.20	0.42
2:D:1451:GLN:HA	2:D:1452:PRO:HD3	1.95	0.42
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:445:ASP:O	3:F:448:GLN:HG2	2.20	0.42
3:H:546:GLU:HB3	3:H:548:TYR:CE1	2.55	0.42
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.50	0.41
1:C:103:LEU:N	1:C:103:LEU:HD22	2.34	0.41
2:D:1405:ARG:HE	2:D:1437:LEU:HD22	1.85	0.41
3:H:164:TYR:CD1	3:H:191:PRO:HG2	2.55	0.41
4:I:78:HIS:HA	4:I:79:PRO:HD3	1.89	0.41
4:J:7:ALA:O	4:J:58:HIS:HE1	2.03	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.34	0.41
2:B:1342:LYS:HD3	2:B:1342:LYS:N	2.35	0.41
1:C:93:GLN:HE21	1:C:627:SER:HB2	1.84	0.41
1:C:510:VAL:HG21	1:C:622:LEU:HD12	2.02	0.41
3:F:37:CYS:HA	3:F:38:PRO:HD3	1.93	0.41
1:A:112:THR:HB	1:A:117:TYR:OH	2.20	0.41
1:A:220:PHE:CD1	1:A:357:PRO:HG2	2.55	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.56	0.41
1:C:365:VAL:HA	1:C:406:LYS:HE2	2.02	0.41
1:C:459:ARG:HA	1:C:462:GLU:CG	2.50	0.41
2:D:1276:LEU:HD23	2:D:1276:LEU:N	2.36	0.41
2:D:1437:LEU:C	2:D:1437:LEU:HD12	2.45	0.41
3:F:158:LEU:HG	3:F:159:GLU:HG3	2.03	0.41
3:F:299:VAL:H	3:F:340:MET:CE	2.29	0.41
3:H:90:TRP:CD1	3:H:90:TRP:N	2.87	0.41
4:J:30:LEU:O	4:J:107:PRO:HA	2.20	0.41
1:A:31:VAL:CG1	1:A:54:LEU:HB2	2.50	0.41
1:A:236:ARG:HA	1:A:243:VAL:HG23	2.02	0.41
2:B:981:LEU:HB3	2:B:998:PRO:O	2.20	0.41
1:C:143:VAL:O	1:C:155:GLN:HA	2.20	0.41
2:D:819:ARG:O	2:D:820:ASN:HB2	2.21	0.41
2:D:1524:LYS:O	2:D:1544:GLU:HB2	2.20	0.41
3:F:499:ALA:HB2	3:F:675:GLY:HA2	2.02	0.41
3:F:706:GLN:C	3:F:708:GLN:N	2.78	0.41
3:H:44:TYR:CD1	3:H:45:PRO:HA	2.56	0.41
4:I:202:ARG:HB3	4:I:203:VAL:H	1.62	0.41
2:B:1391:PRO:HB2	2:B:1396:LEU:HD11	2.03	0.41
1:C:480:LYS:HG2	1:C:481:ALA:N	2.35	0.41
2:D:1143:LEU:O	2:D:1147:ILE:HG13	2.20	0.41
3:H:497:LEU:HA	3:H:554:LEU:HD23	2.02	0.41
4:J:17:SER:HB3	4:J:54:LEU:HB3	2.02	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.84	0.41
2:B:1060:VAL:HG13	2:B:1064:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.50	0.41
1:C:470:TYR:HA	1:C:510:VAL:O	2.20	0.41
3:F:531:HIS:HA	3:F:532:PRO:HD3	1.98	0.41
4:J:106:ARG:HA	4:J:107:PRO:HD3	1.91	0.41
2:B:1387:THR:HG23	2:B:1387:THR:O	2.21	0.41
1:C:17:GLU:HG2	1:C:67:THR:OG1	2.21	0.41
1:C:112:THR:HB	1:C:117:TYR:OH	2.21	0.41
1:C:233:ILE:HG13	1:C:269:ILE:HD11	2.03	0.41
2:D:983:VAL:O	2:D:985:PRO:HD3	2.20	0.41
3:F:433:MET:C	3:F:435:ASN:N	2.77	0.41
3:H:282:PRO:O	3:H:305:SER:HA	2.21	0.41
3:H:418:ALA:HB3	3:H:427:VAL:HG22	2.02	0.41
3:H:445:ASP:O	3:H:448:GLN:HG2	2.21	0.41
4:I:151:ARG:HB2	9:I:1229:GOL:H12	2.02	0.41
1:A:451:VAL:HB	1:A:495:LEU:HB3	2.03	0.41
2:B:811:LEU:HG	2:B:813:LEU:HD13	2.03	0.41
2:B:1270:LEU:O	2:B:1290:HIS:HA	2.20	0.41
1:C:31:VAL:CG1	1:C:54:LEU:HB2	2.51	0.41
1:C:83:PHE:CD2	1:C:100:LEU:HA	2.55	0.41
3:F:393:PRO:O	3:F:394:ARG:HB2	2.21	0.41
4:I:62:GLN:HA	4:I:63:PRO:HD3	1.85	0.41
4:J:37:LEU:HD11	4:J:90:LEU:HD22	2.02	0.41
2:B:745:PHE:N	2:B:746:PRO:HD3	2.36	0.41
2:B:1005:TYR:CD1	2:B:1258:ALA:HB2	2.53	0.41
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.20	0.41
2:B:1375:ASP:O	2:B:1376:ALA:C	2.64	0.41
2:D:1485:ARG:O	2:D:1486:ASP:HB2	2.20	0.41
2:D:1641:ASN:OXT	3:H:255:SER:HB3	2.20	0.41
3:F:76:ILE:HG23	3:F:197:PHE:CE1	2.55	0.41
3:F:94:PRO:HB2	3:F:95:TYR:CD1	2.56	0.41
3:F:103:SER:HB3	3:F:117:ASN:OD1	2.21	0.41
3:F:196:SER:O	3:F:197:PHE:HB3	2.21	0.41
3:F:452:LEU:HD12	3:F:455:MET:HG3	2.02	0.41
3:F:620:VAL:HG12	3:F:667:PRO:HD2	2.03	0.41
3:H:343:TRP:HE3	3:H:344:PRO:HD2	1.86	0.41
3:H:405:VAL:HG23	3:H:406:GLY:N	2.36	0.41
4:J:15:MET:CE	4:J:127:GLY:HA2	2.51	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
1:C:158:LEU:HD22	1:C:169:LEU:HD11	2.02	0.41
3:F:539:LYS:HG3	3:F:547:PHE:CD1	2.56	0.41
1:A:38:HIS:HD2	1:A:45:LEU:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:HA	1:A:231:VAL:HA	2.02	0.40
2:B:983:VAL:O	2:B:985:PRO:HD3	2.21	0.40
2:B:1022:GLY:O	2:B:1026:LEU:HG	2.21	0.40
2:B:1397:LYS:HZ2	2:B:1412:LEU:HD23	1.87	0.40
2:B:1415:ALA:C	2:B:1417:SER:H	2.30	0.40
2:B:1437:LEU:C	2:B:1437:LEU:HD12	2.47	0.40
2:D:1253:VAL:O	2:D:1257:LEU:HG	2.21	0.40
2:D:1342:LYS:HD3	2:D:1342:LYS:N	2.36	0.40
3:F:190:GLU:HA	3:F:191:PRO:HD3	1.81	0.40
3:H:125:ARG:HH21	3:H:194:GLN:HE22	1.69	0.40
1:A:480:LYS:HG2	1:A:481:ALA:N	2.36	0.40
2:D:1276:LEU:HD23	2:D:1276:LEU:H	1.85	0.40
3:F:318:ASN:HD21	3:F:320:GLU:HG2	1.86	0.40
3:H:219:GLY:HA2	3:H:455:MET:HE1	2.03	0.40
4:I:137:ARG:HA	4:I:138:PRO:HD3	1.90	0.40
1:A:253:ILE:HG12	1:A:302:LEU:CD2	2.52	0.40
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.51	0.40
1:A:459:ARG:HA	1:A:462:GLU:HG2	2.03	0.40
1:A:591:GLN:HE21	1:A:595:TRP:NE1	2.19	0.40
2:B:959:LEU:HD23	2:B:959:LEU:C	2.46	0.40
1:C:410:SER:O	1:C:414:GLN:HG2	2.22	0.40
1:C:474:ASN:ND2	1:C:475:LYS:HG3	2.36	0.40
2:D:1086:ILE:HA	2:D:1090:GLN:NE2	2.37	0.40
3:F:18:GLU:HG2	3:F:70:LYS:HZ1	1.86	0.40
3:F:309:TRP:HZ3	3:F:313:GLN:CG	2.35	0.40
3:H:143:PRO:HB2	3:H:164:TYR:OH	2.20	0.40
3:H:464:ASP:O	3:H:465:TYR:HB2	2.21	0.40
4:I:203:VAL:O	4:I:204:CYS:C	2.64	0.40
4:J:155:ASN:CG	4:J:162:GLY:HA2	2.47	0.40
5:G:2:NAG:HN2	5:G:2:NAG:H5	1.85	0.40
1:C:45:LEU:HA	1:C:46:VAL:HA	1.72	0.40
1:C:249:VAL:HG13	1:C:267:LYS:HB2	2.03	0.40
2:D:1379:SER:C	2:D:1380:ILE:HD12	2.45	0.40
3:F:119:THR:HB	4:I:115:ARG:NH1	2.36	0.40
3:F:254:GLY:HA2	3:F:319:TYR:OH	2.21	0.40
1:A:143:VAL:O	1:A:155:GLN:HA	2.22	0.40
2:B:1143:LEU:O	2:B:1147:ILE:HG13	2.22	0.40
1:C:218:GLU:C	1:C:220:PHE:H	2.30	0.40
2:D:735:ALA:O	2:D:739:ILE:HG13	2.22	0.40
2:D:962:GLY:HA3	2:D:1289:ILE:HG21	2.03	0.40
3:F:408:LEU:HD22	3:F:408:LEU:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:709:VAL:HA	3:F:710:PRO:HD3	1.93	0.40
3:H:408:LEU:HD22	3:H:408:LEU:N	2.36	0.40
3:H:433:MET:C	3:H:435:ASN:N	2.79	0.40
3:H:503:PHE:HB2	3:H:530:PHE:CZ	2.56	0.40
3:H:638:ALA:HA	3:H:639:PRO:HD3	1.97	0.40
4:I:40:ALA:HB2	4:I:90:LEU:O	2.21	0.40
4:I:54:LEU:HD21	4:I:67:LYS:HE3	2.03	0.40
4:I:151:ARG:N	9:I:1229:GOL:H11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/642 (99%)	569 (90%)	59 (9%)	8 (1%)	9	39
1	C	636/642 (99%)	565 (89%)	61 (10%)	10 (2%)	7	36
2	B	895/912 (98%)	802 (90%)	83 (9%)	10 (1%)	11	43
2	D	895/912 (98%)	795 (89%)	92 (10%)	8 (1%)	14	47
3	F	708/732 (97%)	642 (91%)	55 (8%)	11 (2%)	7	36
3	H	705/732 (96%)	637 (90%)	54 (8%)	14 (2%)	6	32
4	I	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	14	47
4	J	226/228 (99%)	199 (88%)	25 (11%)	2 (1%)	14	47
All	All	4927/5028 (98%)	4410 (90%)	452 (9%)	65 (1%)	9	39

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	VAL
1	A	518	ALA

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Mol	Chain	Res	Type
2	B	733	ILE
2	B	965	VAL
2	B	1498	ILE
1	C	289	VAL
1	C	518	ALA
1	C	519	SER
2	D	1498	ILE
3	F	197	PHE
3	F	702	ASN
3	F	706	GLN
3	F	707	LYS
3	H	197	PHE
3	H	702	ASN
3	H	706	GLN
3	H	707	LYS
1	A	290	GLN
1	A	534	LYS
2	B	968	MET
2	B	1377	THR
2	B	1505	VAL
1	C	290	GLN
1	C	534	LYS
2	D	928	GLU
2	D	965	VAL
2	D	1377	THR
2	D	1505	VAL
3	F	199	TYR
3	F	704	LYS
3	F	740	ALA
3	H	199	TYR
3	H	463	THR
3	H	704	LYS
3	H	740	ALA
1	A	519	SER
1	A	549	GLU
2	B	928	GLU
1	C	517	GLY
1	C	549	GLU
2	D	774	LYS
2	D	1534	ASN
3	F	431	LYS
3	F	703	GLN

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Mol	Chain	Res	Type
3	H	431	LYS
3	H	703	GLN
4	I	46	ALA
4	I	47	ALA
4	J	46	ALA
4	J	47	ALA
1	A	574	VAL
2	B	778	THR
2	B	969	THR
1	C	574	VAL
3	F	479	PRO
3	H	433	MET
1	C	27	ALA
3	H	223	GLU
3	H	479	PRO
2	D	1201	PRO
3	H	692	ILE
2	B	1201	PRO
1	C	520	GLY
1	A	520	GLY
3	F	692	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/566 (100%)	556 (99%)	8 (1%)	59	71
1	C	564/566 (100%)	557 (99%)	7 (1%)	63	73
2	B	797/807 (99%)	787 (99%)	10 (1%)	61	72
2	D	797/807 (99%)	790 (99%)	7 (1%)	70	76
3	F	620/635 (98%)	612 (99%)	8 (1%)	61	72
3	H	618/635 (97%)	612 (99%)	6 (1%)	68	75
4	I	181/181 (100%)	179 (99%)	2 (1%)	65	74
4	J	181/181 (100%)	180 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4322/4378 (99%)	4273 (99%)	49 (1%)	65 74

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	VAL
1	A	370	GLN
1	A	414	GLN
1	A	516	ILE
1	A	519	SER
1	A	529	VAL
1	A	630	GLN
1	A	634	GLN
2	B	733	ILE
2	B	898	PHE
2	B	953	GLU
2	B	965	VAL
2	B	1270	LEU
2	B	1276	LEU
2	B	1297	LEU
2	B	1334	LEU
2	B	1342	LYS
2	B	1573	LYS
1	C	249	VAL
1	C	370	GLN
1	C	414	GLN
1	C	516	ILE
1	C	529	VAL
1	C	630	GLN
1	C	634	GLN
2	D	898	PHE
2	D	953	GLU
2	D	1270	LEU
2	D	1276	LEU
2	D	1334	LEU
2	D	1342	LYS
2	D	1573	LYS
3	F	90	TRP
3	F	103	SER
3	F	241	SER
3	F	309	TRP
3	F	468	GLN

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Mol	Chain	Res	Type
3	F	540	LYS
3	F	611	GLU
3	F	705	ARG
3	H	90	TRP
3	H	103	SER
3	H	243	SER
3	H	309	TRP
3	H	468	GLN
3	H	540	LYS
4	I	125	VAL
4	I	198	THR
4	J	125	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	59	ASN
1	A	104	GLN
1	A	132	HIS
1	A	311	HIS
1	A	370	GLN
1	A	414	GLN
1	A	558	GLN
1	A	630	GLN
1	A	634	GLN
2	B	770	ASN
2	B	836	GLN
2	B	860	HIS
2	B	1090	GLN
2	B	1130	GLN
2	B	1176	GLN
2	B	1237	GLN
2	B	1268	GLN
2	B	1443	GLN
2	B	1545	GLN
1	C	38	HIS
1	C	59	ASN
1	C	63	ASN
1	C	93	GLN
1	C	104	GLN
1	C	132	HIS

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Mol	Chain	Res	Type
1	C	225	ASN
1	C	311	HIS
1	C	356	ASN
1	C	370	GLN
1	C	414	GLN
1	C	558	GLN
1	C	630	GLN
1	C	634	GLN
2	D	770	ASN
2	D	836	GLN
2	D	860	HIS
2	D	1090	GLN
2	D	1130	GLN
2	D	1176	GLN
2	D	1237	GLN
2	D	1267	HIS
2	D	1337	ASN
2	D	1499	GLN
2	D	1545	GLN
3	F	63	GLN
3	F	165	HIS
3	F	194	GLN
3	F	357	HIS
3	F	423	ASN
3	F	468	GLN
3	F	591	GLN
3	F	708	GLN
3	F	712	HIS
3	H	63	GLN
3	H	77	HIS
3	H	105	HIS
3	H	165	HIS
3	H	194	GLN
3	H	318	ASN
3	H	357	HIS
3	H	483	HIS
3	H	591	GLN
3	H	708	GLN
3	H	712	HIS
4	I	10	HIS
4	I	19	GLN
4	I	24	HIS

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Mol	Chain	Res	Type
4	I	94	GLN
4	J	10	HIS
4	J	19	GLN
4	J	24	HIS
4	J	94	GLN
4	J	174	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	$\# Z > 2$
5	NAG	E	1	5,1	14,14,15	0.51	0	17,19,21	1.34	2 (11%)
5	NAG	E	2	5	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
5	NAG	G	1	2,5	14,14,15	0.53	0	17,19,21	0.56	0
5	NAG	G	2	5	14,14,15	0.53	0	17,19,21	0.70	0
5	NAG	K	1	5,1	14,14,15	0.56	0	17,19,21	0.62	0
5	NAG	K	2	5	14,14,15	0.56	0	17,19,21	0.62	0
6	NAG	L	1	6,3	14,14,15	0.60	0	17,19,21	1.45	3 (17%)
6	NAG	L	2	6	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
6	BMA	L	3	6	11,11,12	0.27	0	15,15,17	0.52	0
6	NAG	M	1	6,3	14,14,15	0.47	0	17,19,21	1.97	5 (29%)
6	NAG	M	2	6	14,14,15	0.53	0	17,19,21	1.77	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	M	3	6	11,11,12	1.63	2 (18%)	15,15,17	3.36	10 (66%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	3	BMA	C2-C3	3.30	1.57	1.52
6	M	3	BMA	C4-C3	3.04	1.60	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	O5-C5-C6	5.67	118.69	107.66
6	M	3	BMA	O4-C4-C5	4.78	121.09	109.32
6	M	1	NAG	C2-N2-C7	4.72	129.22	122.90
6	M	3	BMA	O3-C3-C4	4.69	121.42	110.38
6	M	3	BMA	O2-C2-C1	4.48	119.47	109.22
6	M	3	BMA	O2-C2-C3	4.41	119.29	110.15
6	M	3	BMA	O3-C3-C2	4.18	118.59	110.05
6	M	1	NAG	C1-O5-C5	3.89	117.40	112.19
5	E	2	NAG	C1-O5-C5	-3.52	107.47	112.19
6	L	1	NAG	C1-O5-C5	3.38	116.71	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	3	BMA	O4-C4-C3	3.34	118.26	110.38
6	L	2	NAG	O5-C1-C2	-3.21	106.32	111.29
5	E	1	NAG	C1-O5-C5	3.20	116.48	112.19
6	L	1	NAG	O5-C1-C2	3.17	116.19	111.29
6	M	1	NAG	C1-C2-N2	-2.87	105.91	110.43
6	M	3	BMA	O6-C6-C5	2.86	121.08	111.33
6	M	2	NAG	O5-C1-C2	-2.85	106.88	111.29
6	M	2	NAG	O3-C3-C2	2.83	115.28	109.40
5	E	1	NAG	O5-C1-C2	2.82	115.66	111.29
6	M	3	BMA	C3-C4-C5	2.68	115.09	110.23
6	M	2	NAG	C2-N2-C7	2.43	126.16	122.90
6	L	2	NAG	C3-C4-C5	2.43	114.64	110.23
6	M	1	NAG	C6-C5-C4	-2.36	107.22	113.02
6	M	2	NAG	C4-C3-C2	-2.31	107.64	111.02
6	M	3	BMA	C1-O5-C5	2.27	115.22	112.19
6	M	2	NAG	C6-C5-C4	-2.25	107.49	113.02
6	L	1	NAG	C2-N2-C7	-2.23	119.91	122.90
6	M	2	NAG	C1-C2-N2	2.19	113.88	110.43
6	M	1	NAG	C8-C7-N2	2.04	119.50	116.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O7-C7-N2-C2
6	M	1	NAG	C8-C7-N2-C2
6	M	1	NAG	O7-C7-N2-C2
6	L	3	BMA	O5-C5-C6-O6

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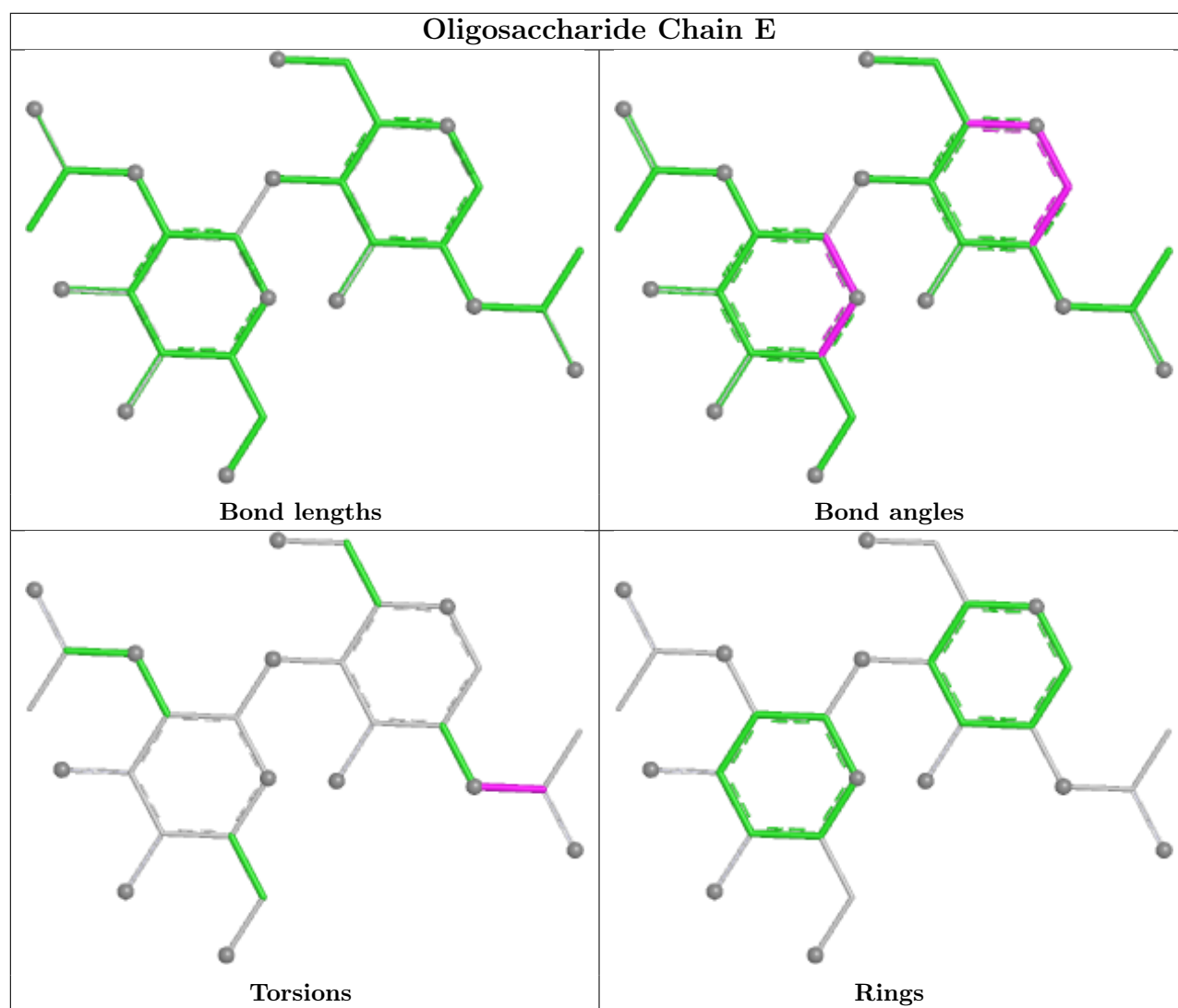
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6

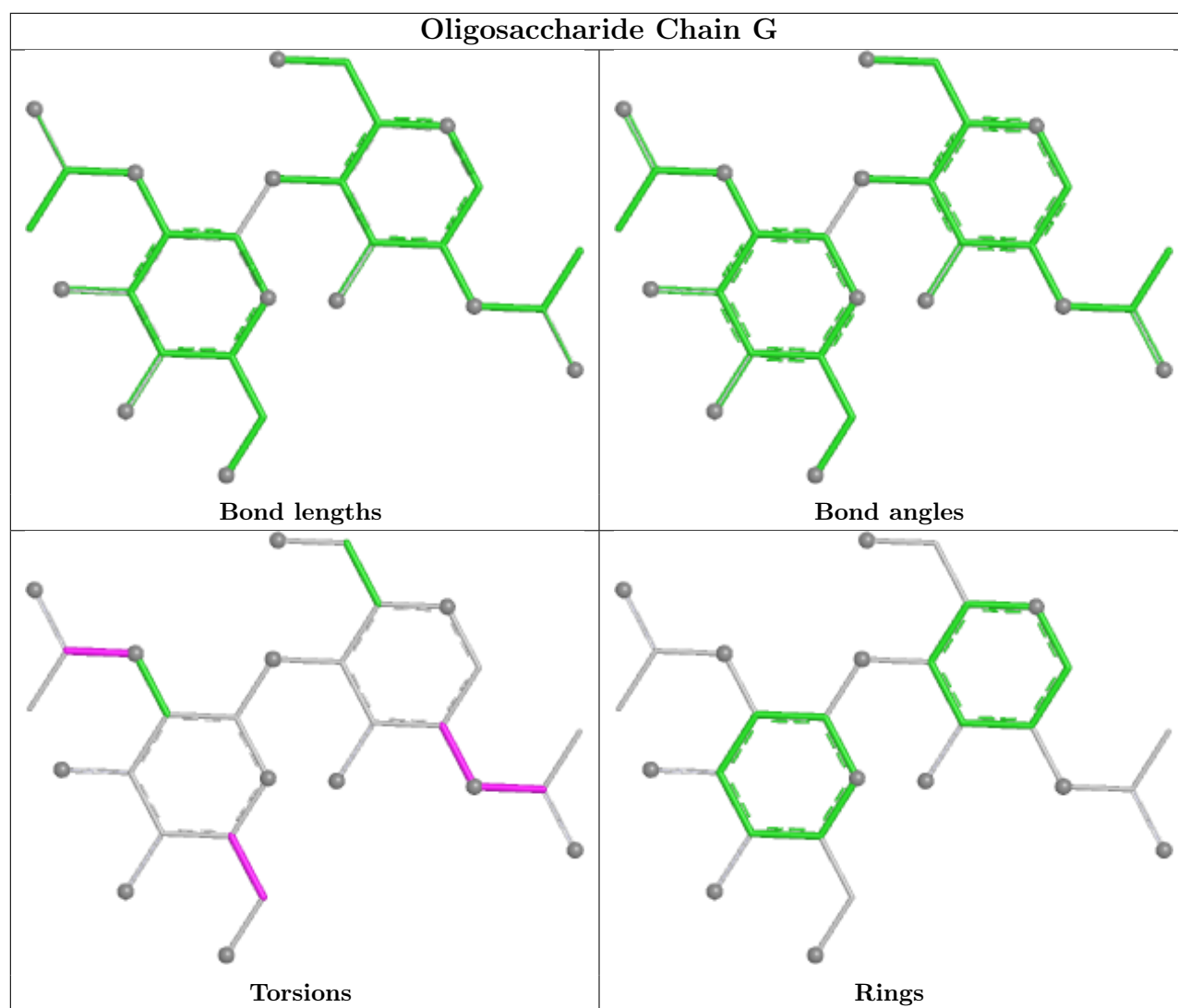
There are no ring outliers.

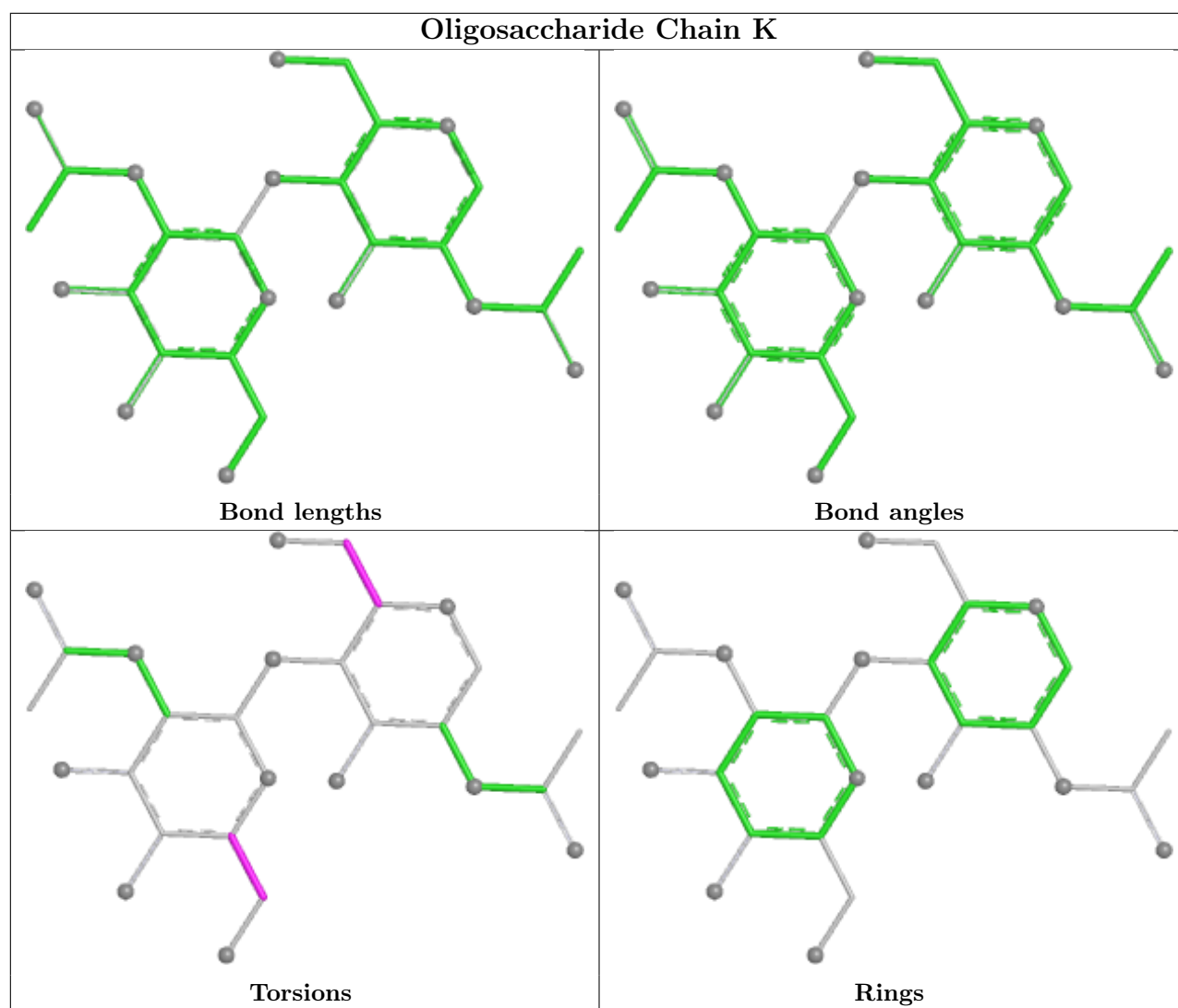
6 monomers are involved in 14 short contacts:

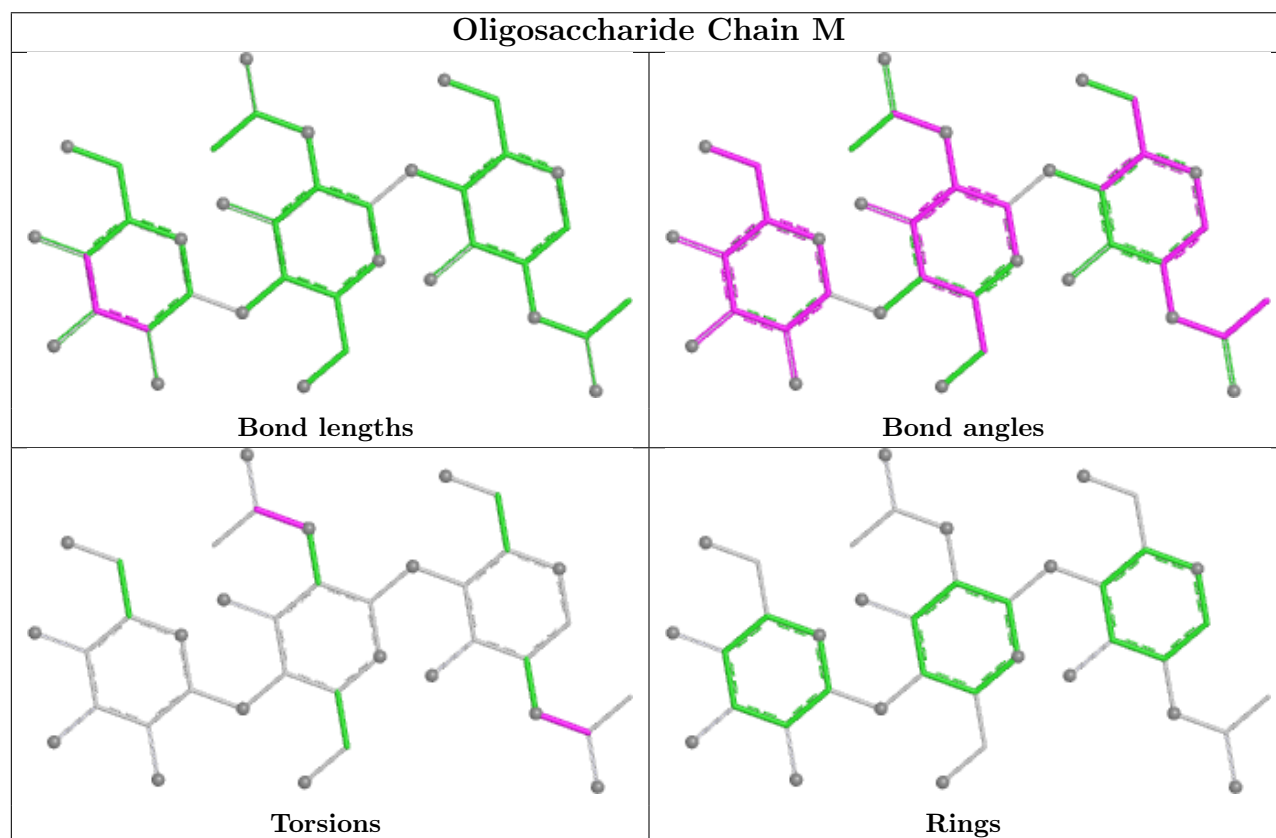
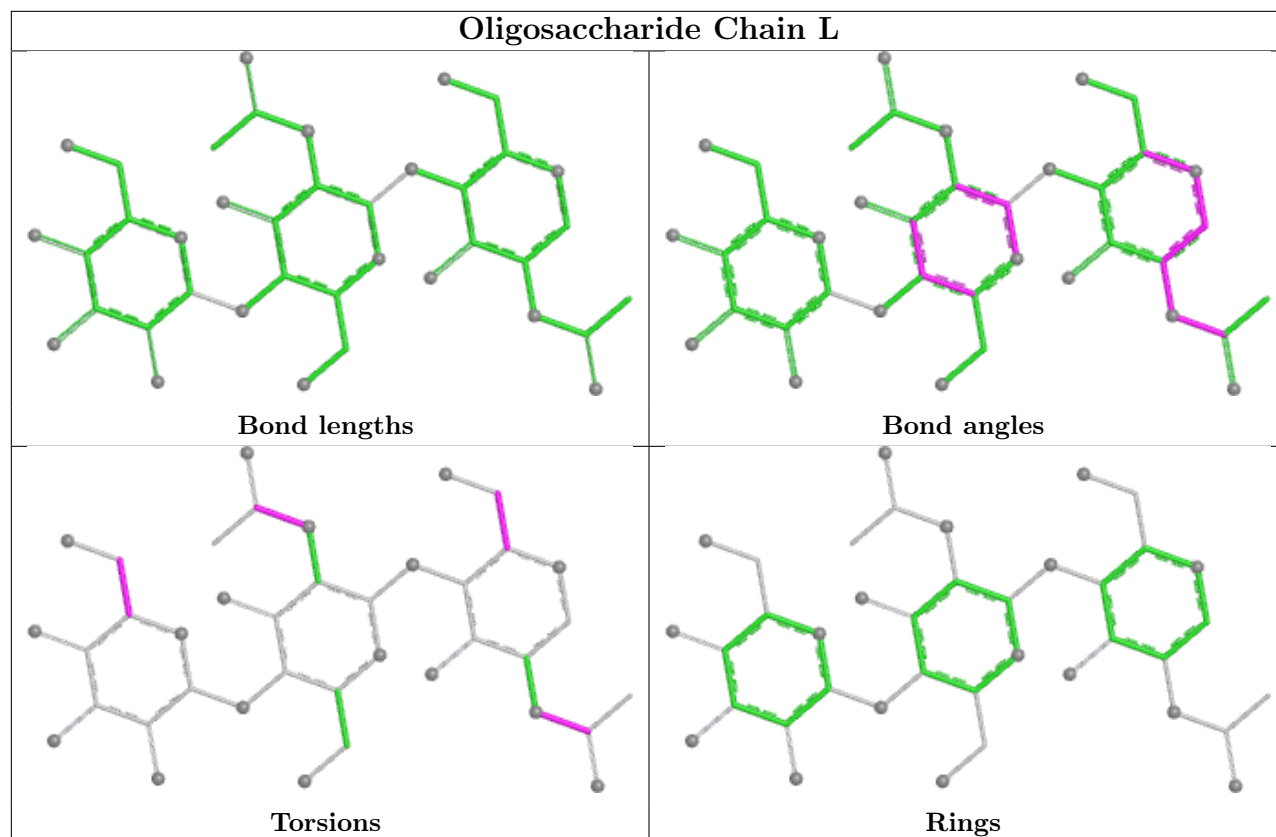
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1	NAG	1	0
5	G	2	NAG	1	0
5	E	1	NAG	2	0
5	K	2	NAG	2	0
5	K	1	NAG	10	0
6	L	2	NAG	1	0

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









5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
8	NAG	F	1743	3	14,14,15	0.53	0	17,19,21	0.56	0
9	GOL	J	1229	-	5,5,5	0.37	0	5,5,5	0.35	0
8	NAG	D	2642	2	14,14,15	0.56	0	17,19,21	0.60	0
9	GOL	I	1229	-	5,5,5	0.38	0	5,5,5	0.19	0
8	NAG	H	1747	3	14,14,15	0.48	0	17,19,21	0.79	0
8	NAG	H	1743	3	14,14,15	0.51	0	17,19,21	0.59	0
8	NAG	F	1747	3	14,14,15	0.58	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	1743	3	-	2/6/23/26	0/1/1/1
9	GOL	J	1229	-	-	2/4/4/4	-
8	NAG	D	2642	2	-	3/6/23/26	0/1/1/1
9	GOL	I	1229	-	-	2/4/4/4	-
8	NAG	H	1747	3	-	1/6/23/26	0/1/1/1
8	NAG	H	1743	3	-	3/6/23/26	0/1/1/1
8	NAG	F	1747	3	1/1/5/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	1747	NAG	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	2642	NAG	C3-C2-N2-C7
8	D	2642	NAG	C8-C7-N2-C2
8	D	2642	NAG	O7-C7-N2-C2
8	F	1743	NAG	C8-C7-N2-C2
8	F	1743	NAG	O7-C7-N2-C2
8	H	1743	NAG	C3-C2-N2-C7
8	H	1743	NAG	C8-C7-N2-C2
8	H	1743	NAG	O7-C7-N2-C2
9	I	1229	GOL	C1-C2-C3-O3
9	J	1229	GOL	C1-C2-C3-O3
9	J	1229	GOL	O2-C2-C3-O3
9	I	1229	GOL	O2-C2-C3-O3
8	F	1747	NAG	O5-C5-C6-O6
8	H	1747	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1743	NAG	1	0
9	J	1229	GOL	4	0
9	I	1229	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	640/642 (99%)	-0.18	3 (0%) 87 68	58, 134, 189, 278	0
1	C	640/642 (99%)	-0.12	5 (0%) 82 60	67, 134, 189, 281	0
2	B	901/912 (98%)	0.09	41 (4%) 37 20	60, 122, 203, 330	0
2	D	901/912 (98%)	-0.05	15 (1%) 69 43	60, 125, 205, 328	0
3	F	714/732 (97%)	-0.41	0 100 100	37, 82, 154, 272	0
3	H	711/732 (97%)	-0.42	3 (0%) 88 72	37, 84, 153, 222	0
4	I	228/228 (100%)	-0.49	0 100 100	46, 79, 125, 218	0
4	J	228/228 (100%)	-0.47	1 (0%) 88 72	42, 79, 125, 220	0
All	All	4963/5028 (98%)	-0.20	68 (1%) 73 48	37, 109, 189, 330	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1154	LEU	6.2
2	B	1158	TYR	4.3
2	B	1125	VAL	4.2
1	C	337	LYS	3.8
2	B	1126	LEU	3.8
2	B	1169	ILE	3.5
2	B	1151	GLY	3.4
2	D	1151	GLY	3.4
2	B	1119	MET	3.3
3	H	344	PRO	3.2
2	B	1129	LEU	3.1
2	B	1188	PHE	3.0
2	B	1092	PRO	3.0
3	H	396	ASP	3.0
2	B	1078	LEU	2.9
1	C	40	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	1118	ASP	2.9
2	B	1132	ALA	2.9
2	B	1056	LEU	2.9
2	B	1170	ALA	2.8
1	C	166	VAL	2.8
2	B	1189	LEU	2.7
2	B	1150	ALA	2.7
2	B	1204	GLN	2.6
2	D	1154	LEU	2.5
2	B	1253	VAL	2.5
1	C	46	VAL	2.5
2	D	1186	ASN	2.5
2	B	1198	TRP	2.5
1	C	634	GLN	2.5
2	B	1122	THR	2.4
2	D	1016	GLY	2.4
2	D	1093	ASP	2.4
2	B	1153	PHE	2.4
1	A	257	GLU	2.4
2	B	1096	PHE	2.3
2	B	1254	PHE	2.3
2	B	1081	ALA	2.3
2	B	786	SER	2.3
2	B	1057	THR	2.3
2	B	1317	GLN	2.2
2	D	1107	MET	2.2
2	B	1146	SER	2.2
1	A	412	ALA	2.2
2	B	1212	SER	2.2
2	D	1230	VAL	2.1
2	B	1085	LEU	2.1
2	B	1174	LEU	2.1
2	B	1203	LYS	2.1
2	B	1159	MET	2.1
2	B	1499	GLN	2.1
2	B	1101	PRO	2.1
2	B	1251	PHE	2.1
2	D	973	VAL	2.1
2	B	1077	VAL	2.1
1	A	497	LEU	2.1
2	B	1136	CYS	2.1
4	J	200	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	1183	PRO	2.1
2	D	1160	ASN	2.1
2	D	1129	LEU	2.1
2	B	1173	ALA	2.1
2	B	1172	TYR	2.0
2	B	1128	SER	2.0
2	D	1156	ALA	2.0
3	H	463	THR	2.0
2	D	763	GLY	2.0
2	D	1500	LYS	2.0

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](#)

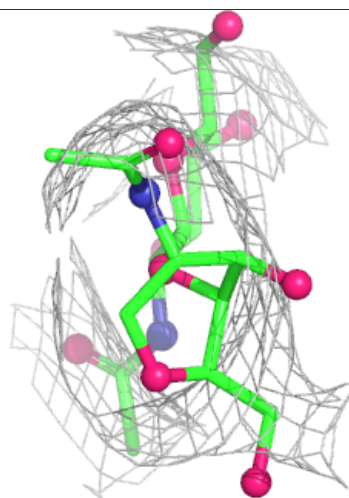
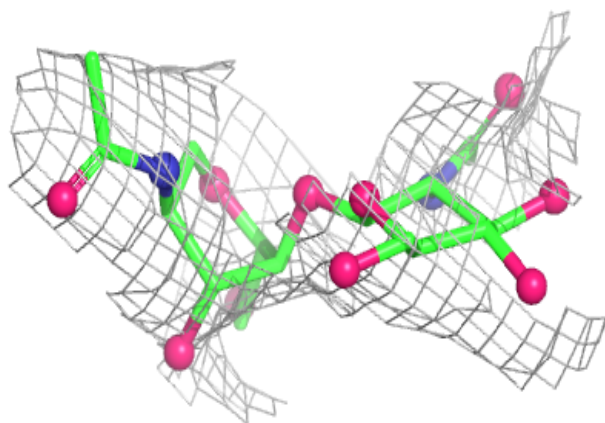
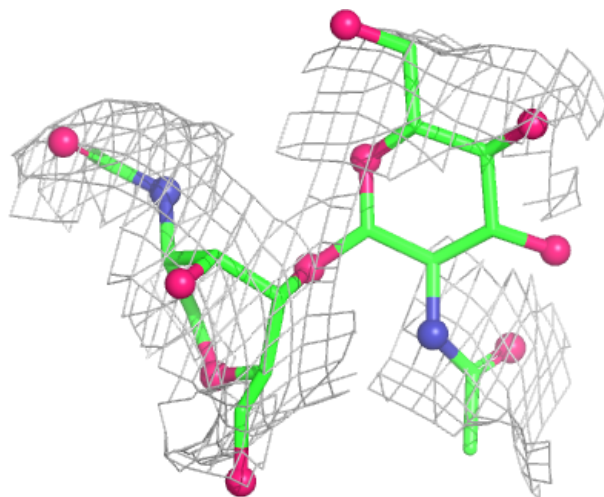
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	E	1	14/15	-	-	129,188,212,214	0
5	NAG	E	2	14/15	-	-	160,201,217,223	0
5	NAG	G	1	14/15	-	-	102,141,165,192	0
5	NAG	G	2	14/15	-	-	114,185,200,200	0
5	NAG	K	2	14/15	0.32	0.13	155,202,219,222	0
5	NAG	K	1	14/15	0.45	0.11	123,187,212,212	0
6	BMA	L	3	11/12	0.45	0.12	128,162,204,271	0
6	BMA	M	3	11/12	0.45	0.10	132,155,186,196	0
6	NAG	M	2	14/15	0.63	0.11	160,172,206,213	0
6	NAG	L	2	14/15	0.72	0.09	118,138,166,168	0
6	NAG	L	1	14/15	0.81	0.13	91,116,131,137	0
6	NAG	M	1	14/15	0.85	0.11	96,122,150,154	0

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

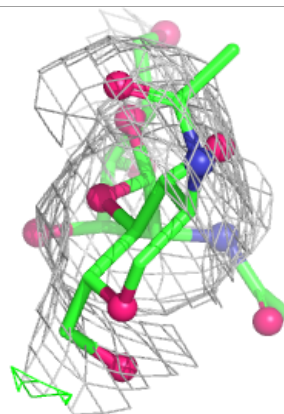
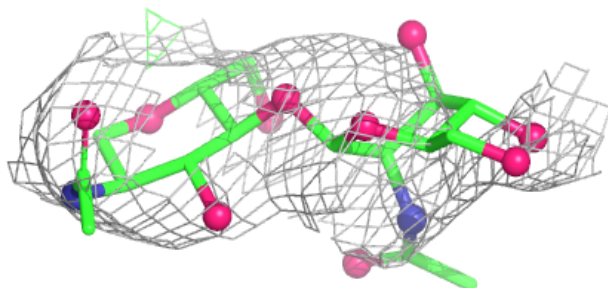
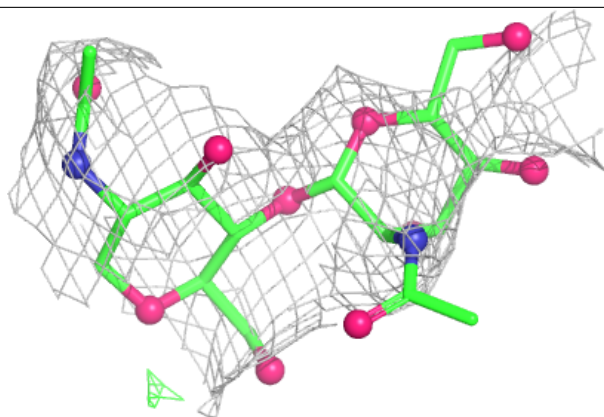
Electron density around Chain E:

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



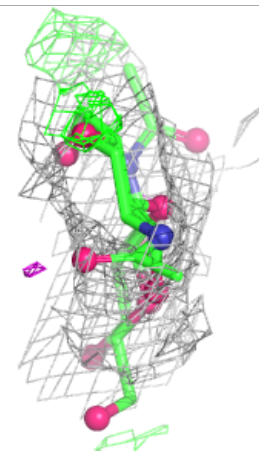
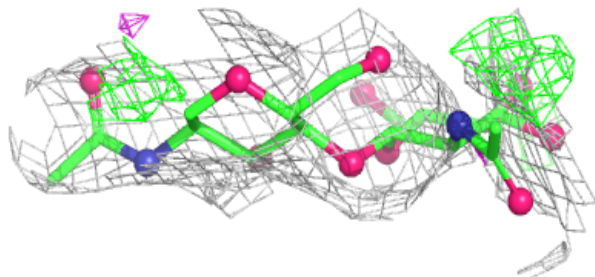
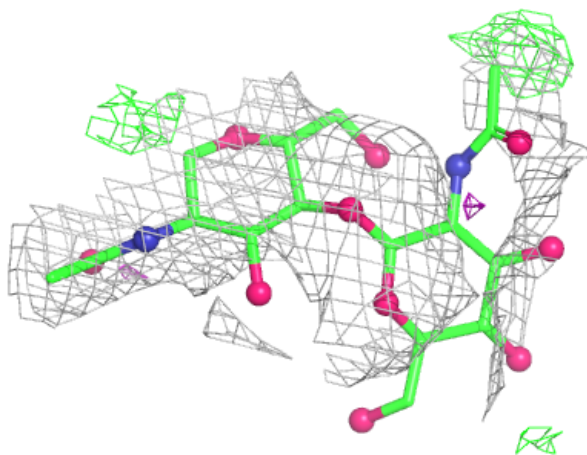
Electron density around Chain G:

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



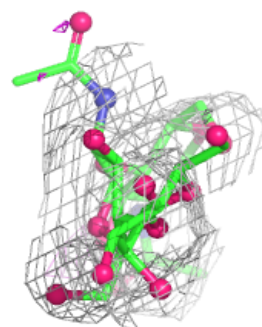
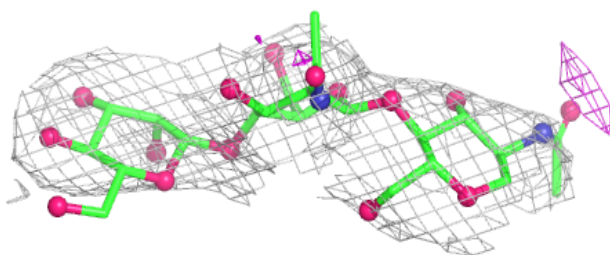
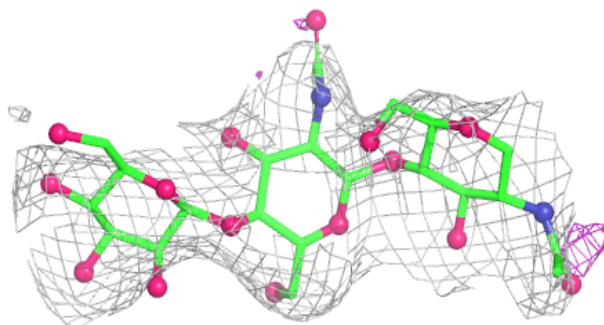
Electron density around Chain K:

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

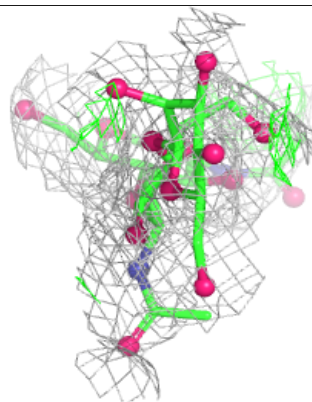
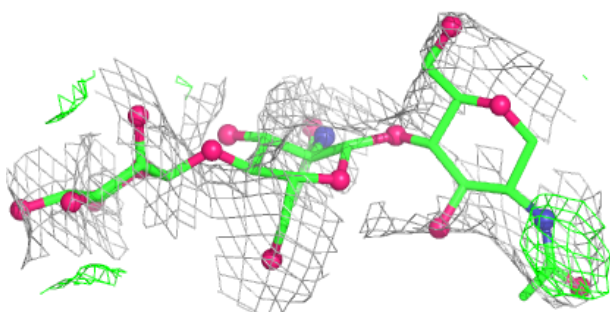
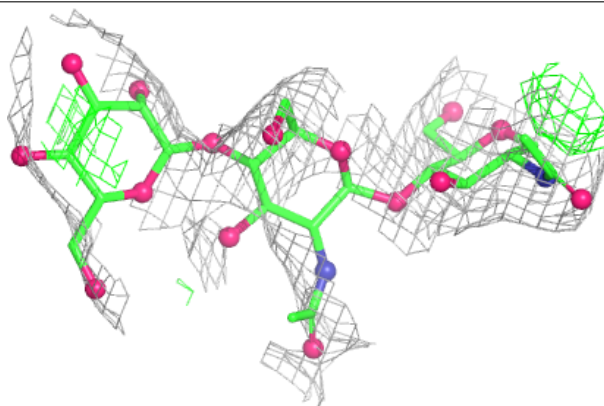


Electron density around Chain L:

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

**Electron density around Chain M:**

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



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($\text{\AA}^2$)	Q<0.9
8	NAG	H	1747	14/15	0.61	0.12	118,163,182,198	0
8	NAG	F	1743	14/15	0.68	0.16	97,143,202,215	0
8	NAG	F	1747	14/15	0.82	0.13	135,154,184,195	0
8	NAG	H	1743	14/15	0.83	0.12	117,167,189,193	0
8	NAG	D	2642	14/15	0.86	0.11	104,146,166,179	0
9	GOL	I	1229	6/6	0.95	0.13	73,107,124,127	0
7	MG	A	1645	1/1	0.96	0.07	108,108,108,108	0
7	MG	C	1645	1/1	0.97	0.04	127,127,127,127	0
9	GOL	J	1229	6/6	0.97	0.08	58,74,87,95	0
7	MG	H	1742	1/1	0.98	0.16	140,140,140,140	0
7	MG	F	1742	1/1	0.99	0.08	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.