



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:53 AM UTC

PDB ID : 9C22 / pdb_00009c22
Title : Crystal structure of chimeric hemagglutinin cH11/1 in complex with broad protective antibody 3E1
Authors : Nguyen, T.K.Y.; Wilson, I.A.
Deposited on : 2024-05-30
Resolution : 4.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

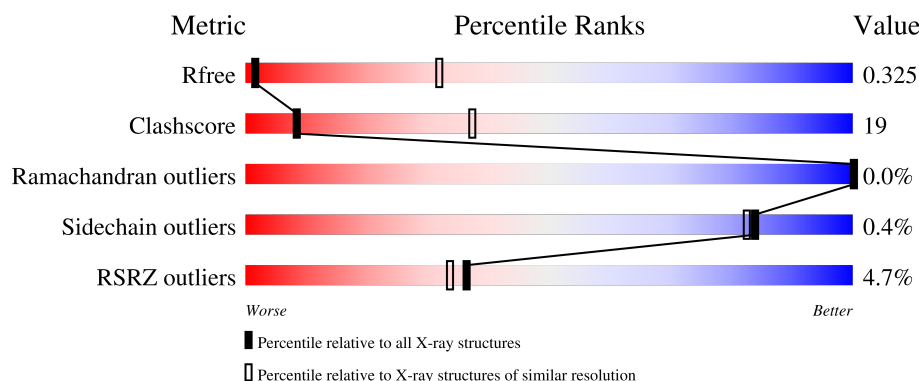
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.60 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.



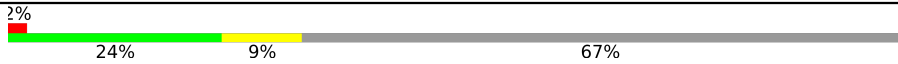
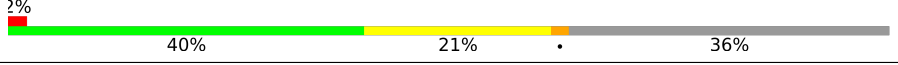
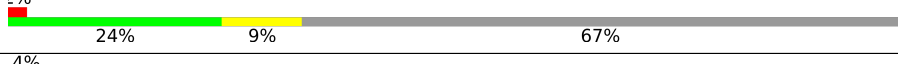
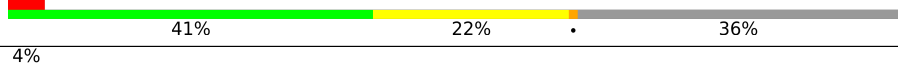
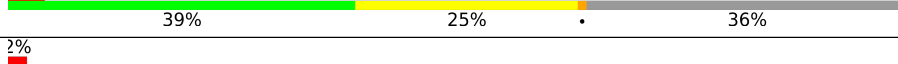
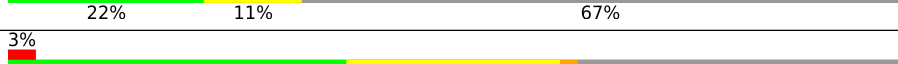
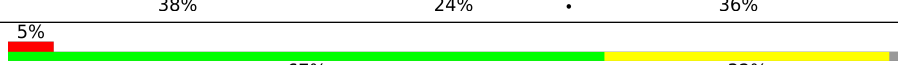
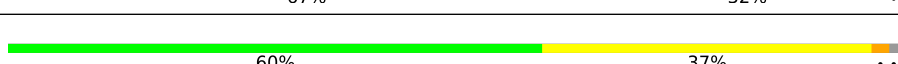
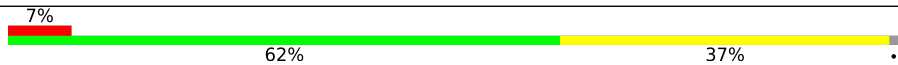
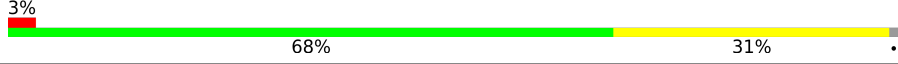
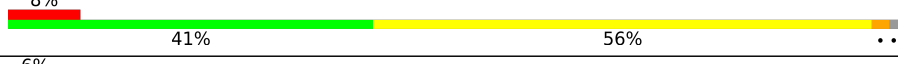
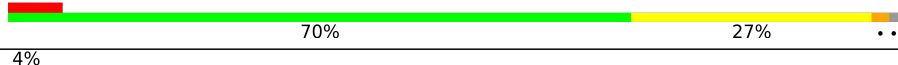
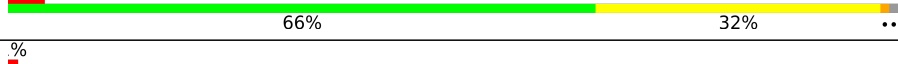
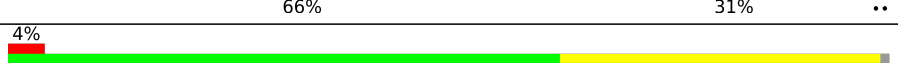
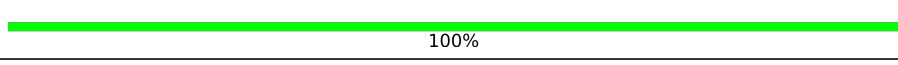
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1007 (5.28-3.92)
Clashscore	190562	1022 (5.26-3.94)
Ramachandran outliers	187476	1069 (5.30-3.90)
Sidechain outliers	187428	1051 (5.30-3.90)
RSRZ outliers	180081	1002 (5.28-3.92)

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	B	504	
1	C	504	
1	H	504	
1	I	504	
1	L	504	

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Mol	Chain	Length	Quality of chain
1	P	504	
1	Q	504	
1	U	504	
1	V	504	
1	Y	504	
1	a	504	
1	b	504	
2	D	214	
2	J	214	
2	M	214	
2	R	214	
2	W	214	
2	c	214	
3	E	224	
3	K	224	
3	N	224	
3	S	224	
3	X	224	
3	d	224	
4	A	2	
4	Z	2	
5	F	3	
5	G	3	
5	O	3	
5	T	3	

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Mol	Chain	Length	Quality of chain
5	e	3	 67% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43211 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	C	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	H	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	I	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	L	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	P	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	Q	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	U	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	V	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	Y	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			
1	a	168	Total	C	N	O	S	0	0	0
			1360	850	231	273	6			
1	b	323	Total	C	N	O	S	0	0	0
			2505	1585	432	475	13			

- Molecule 2 is a protein called Antibody 3E1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	J	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			

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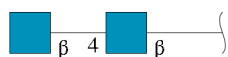
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	R	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			
2	W	211	Total	C	N	O	S	0	0	0
			1628	1025	272	326	5			
2	c	212	Total	C	N	O	S	0	0	0
			1636	1029	273	329	5			

- Molecule 3 is a protein called Antibody 3E1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	K	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	N	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	S	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	X	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			
3	d	221	Total	C	N	O	S	0	0	0
			1658	1050	278	325	5			

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



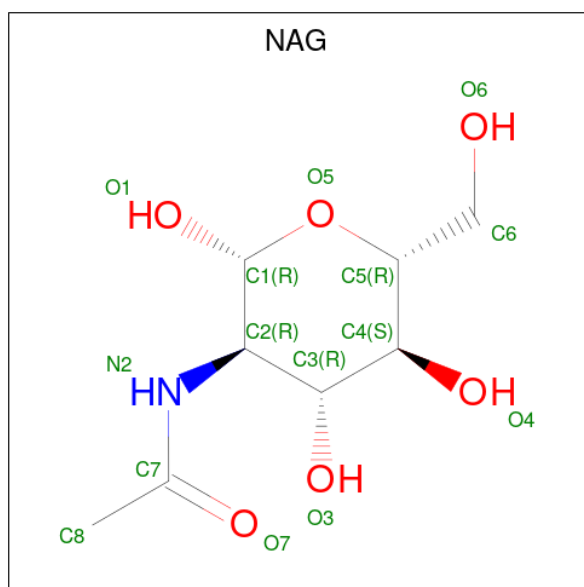
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.

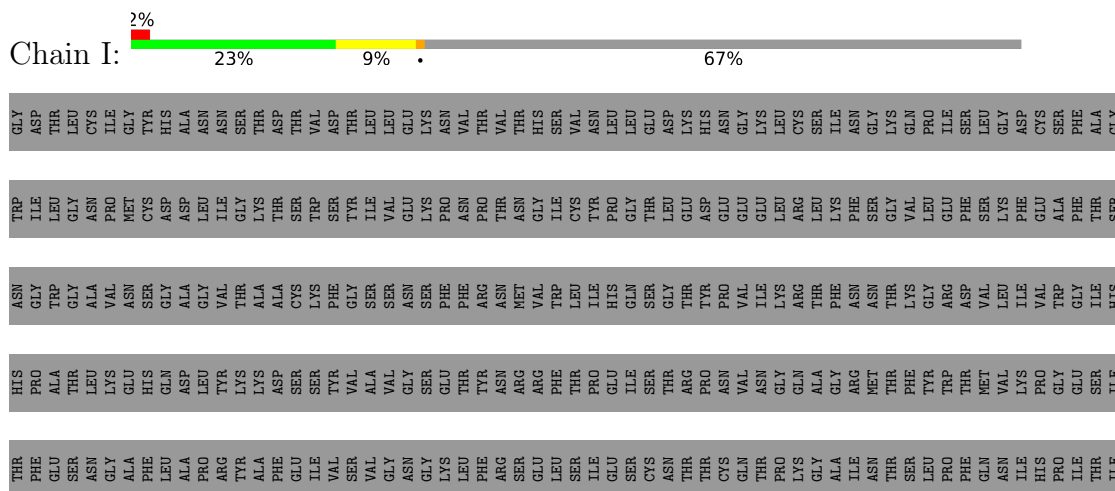


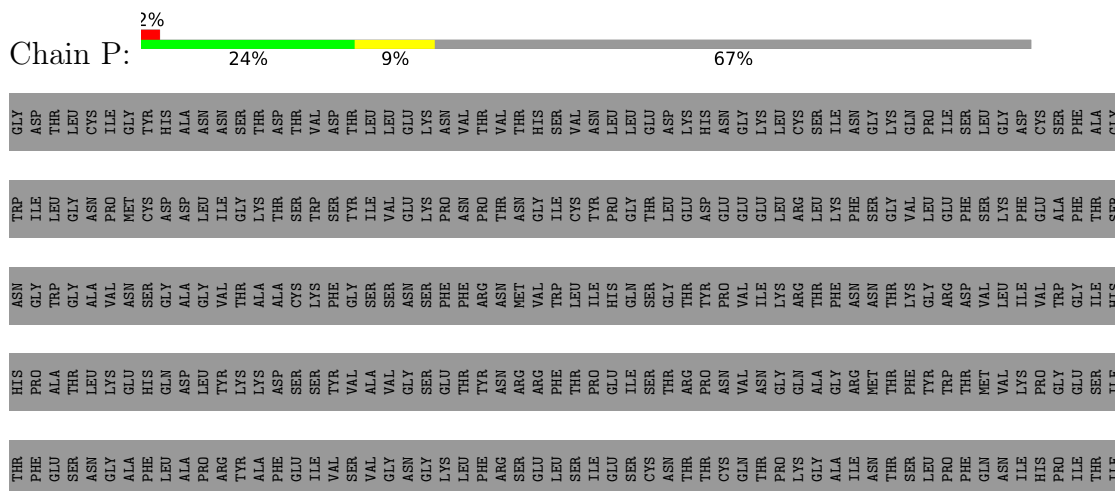
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	T	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

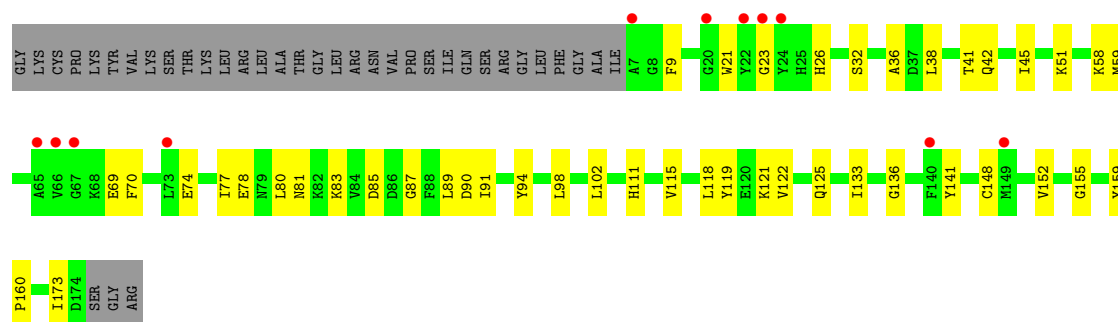
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



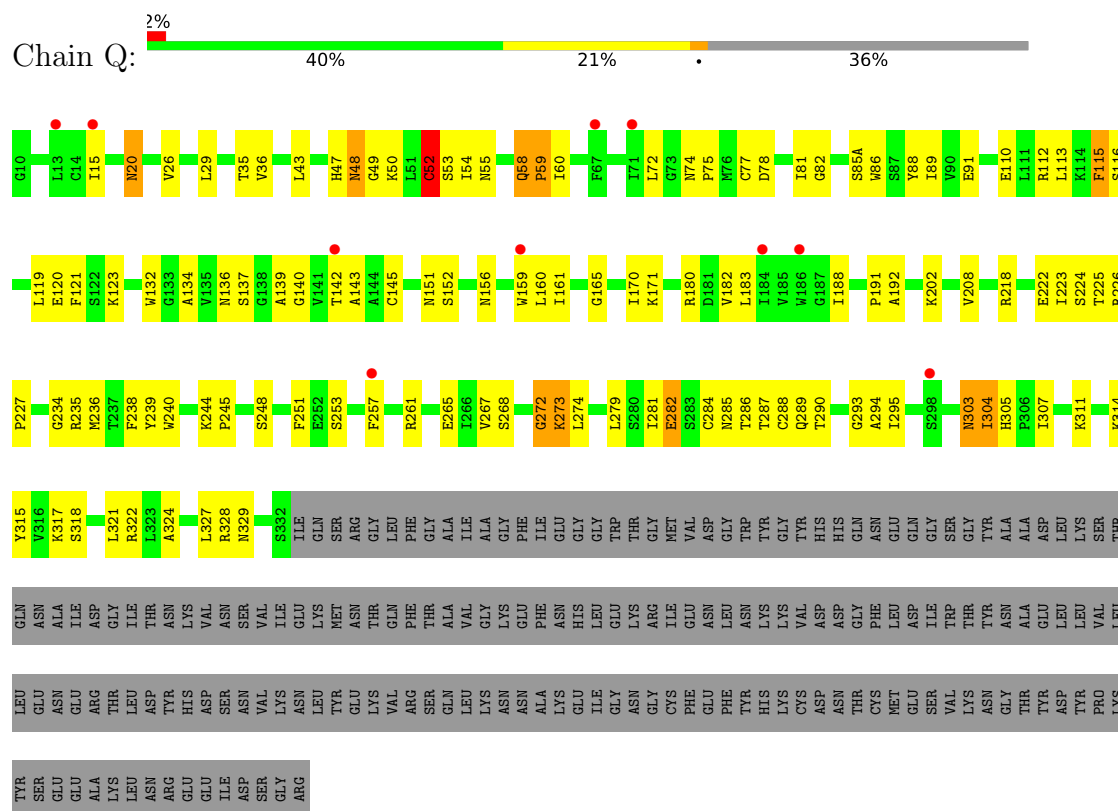
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	V	1	Total	C	N	O	0	0
			14	8	1	5		





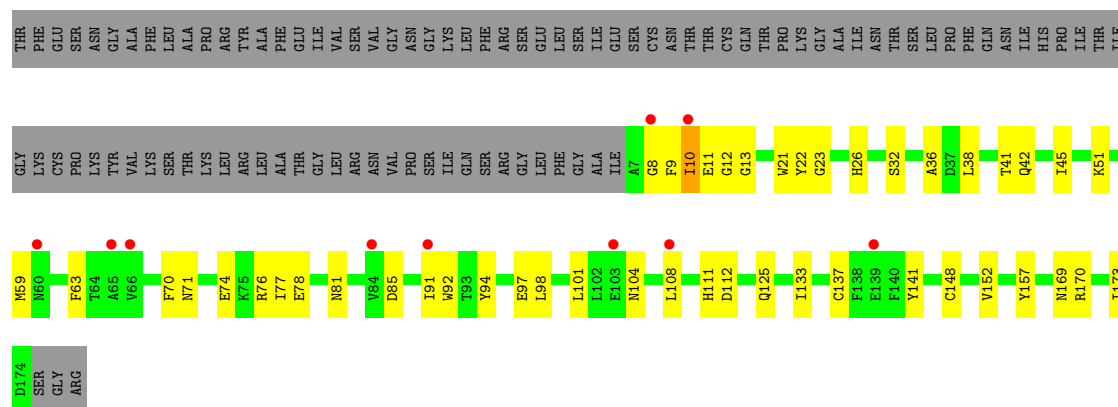


- Molecule 1: Hemagglutinin

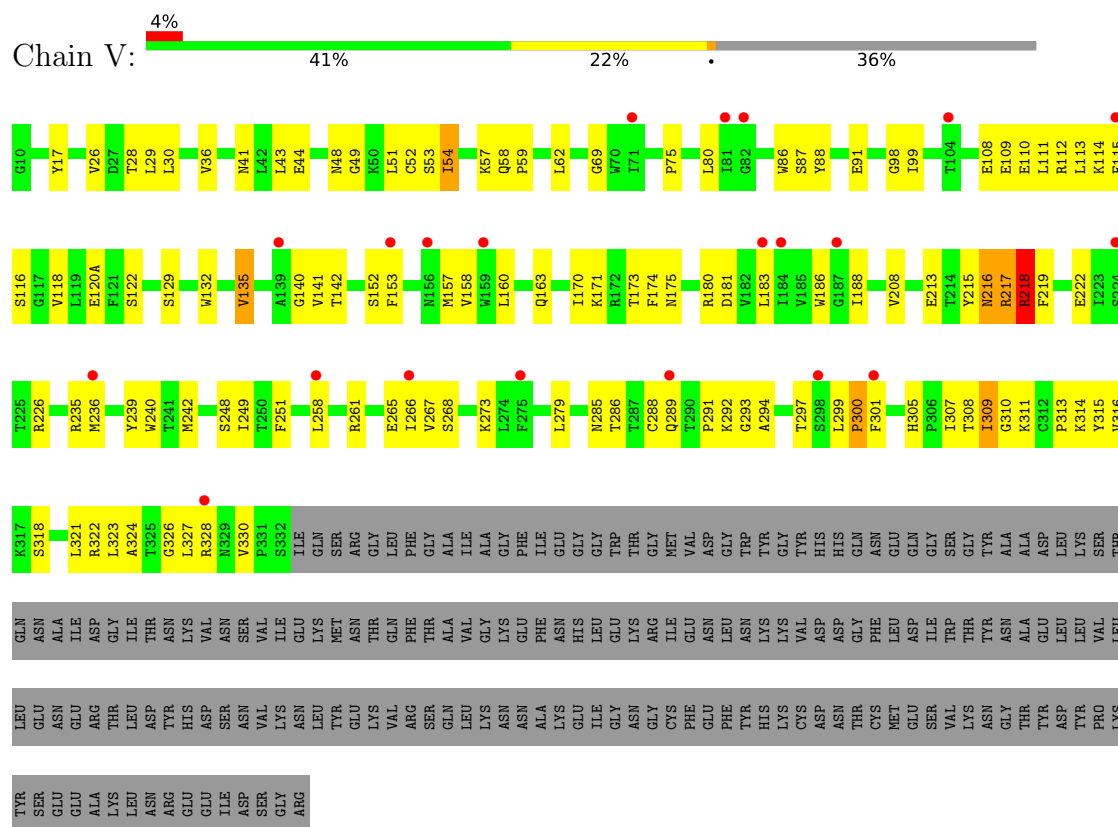


- Molecule 1: Hemagglutinin

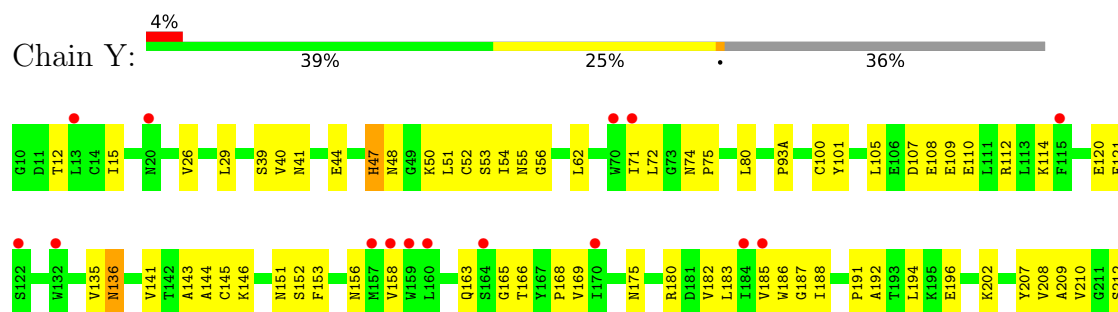


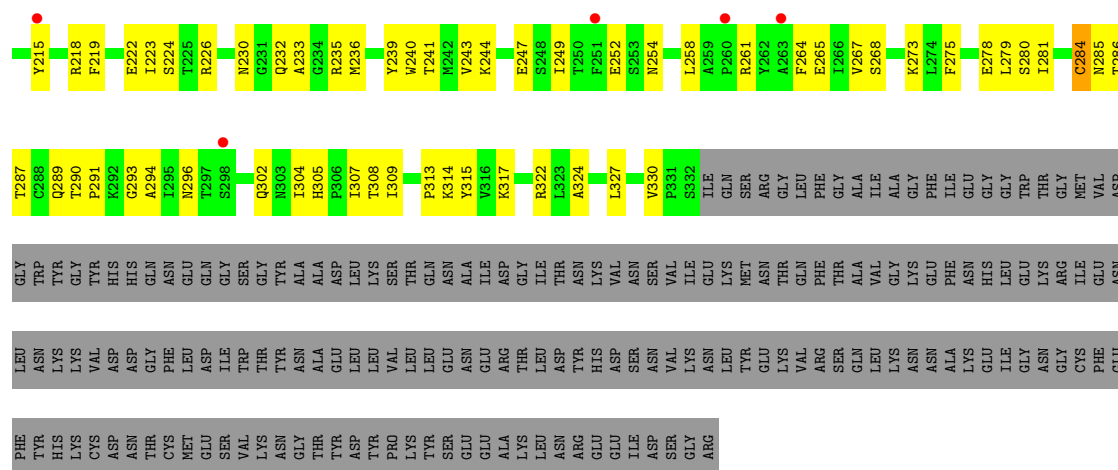


• Molecule 1: Hemagglutinin

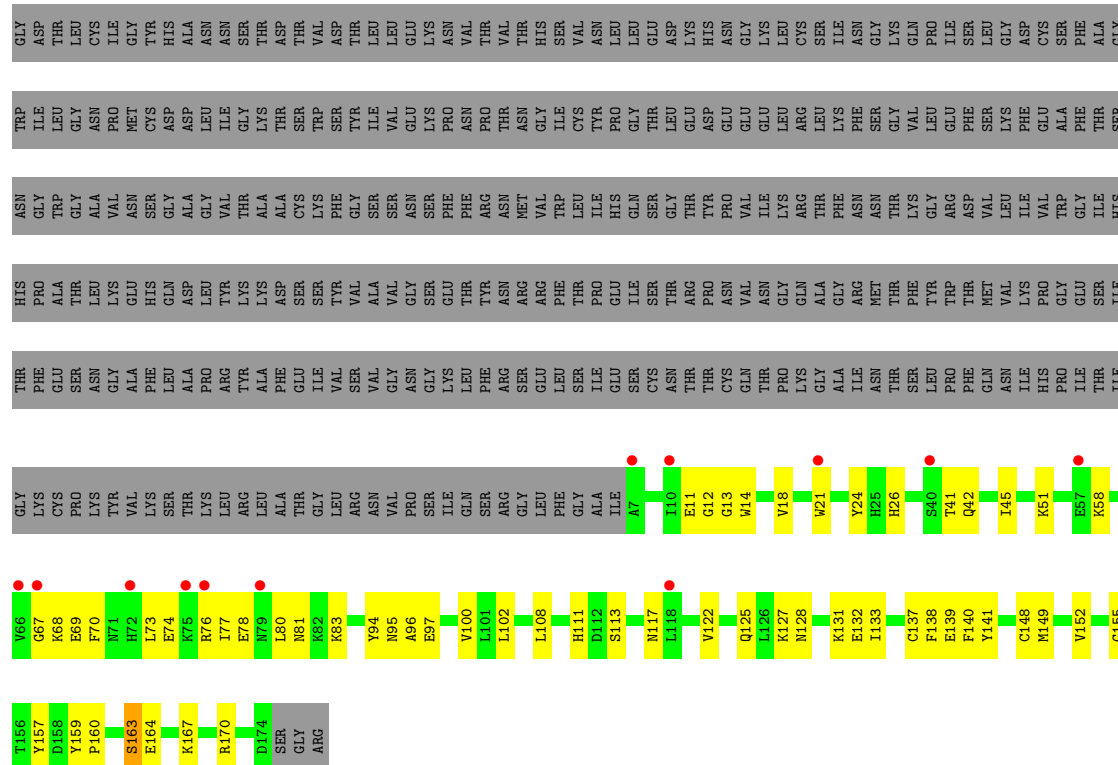


• Molecule 1: Hemagglutinin

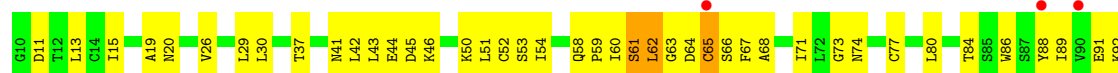


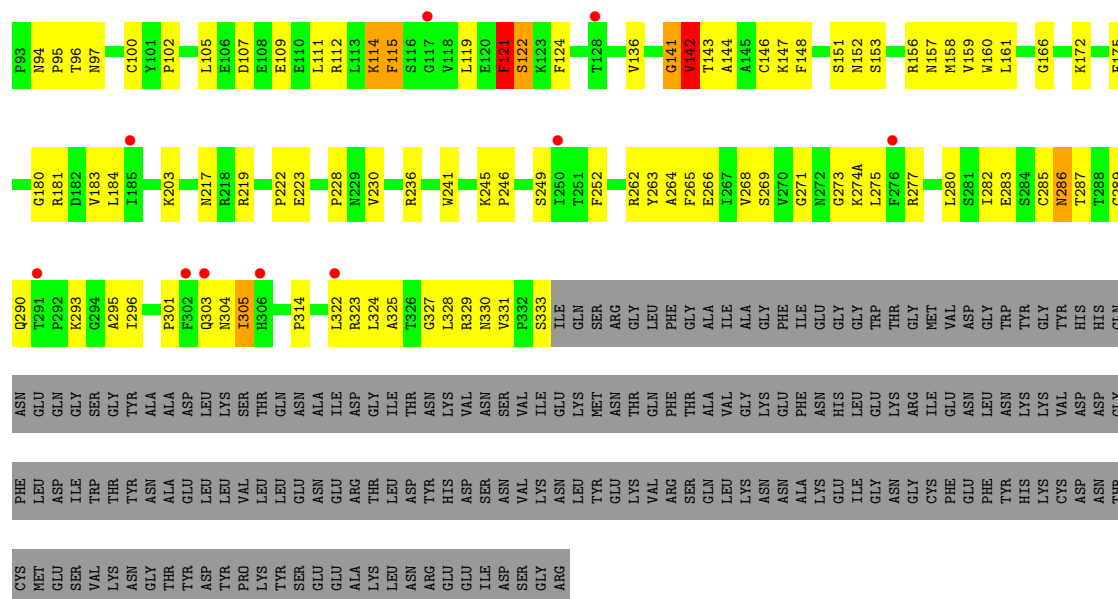


• Molecule 1: Hemagglutinin

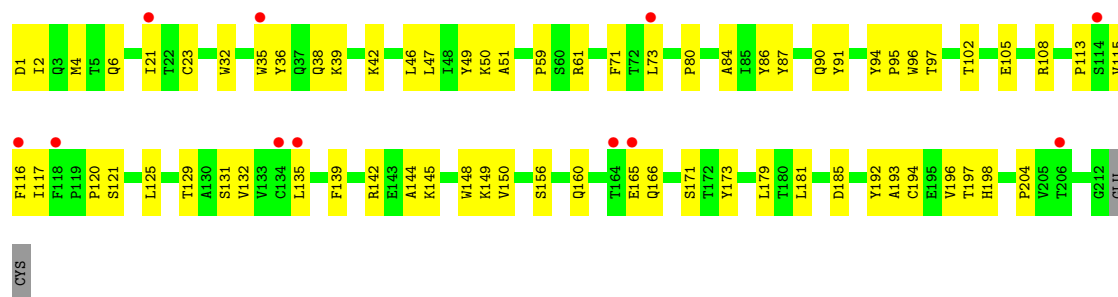


• Molecule 1: Hemagglutinin

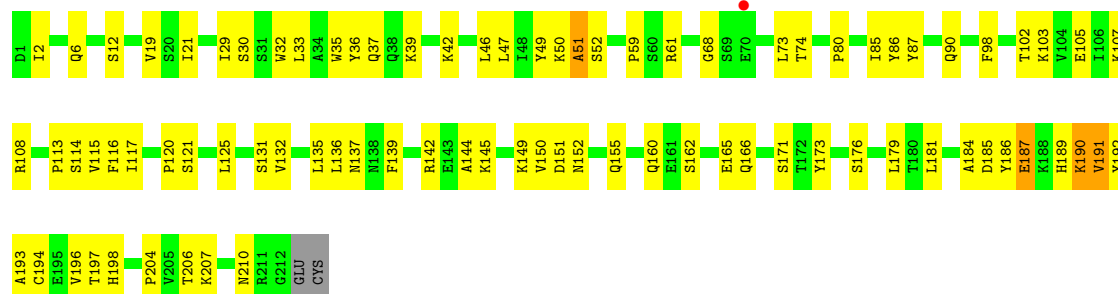




• Molecule 2: Antibody 3E1 Fab light chain

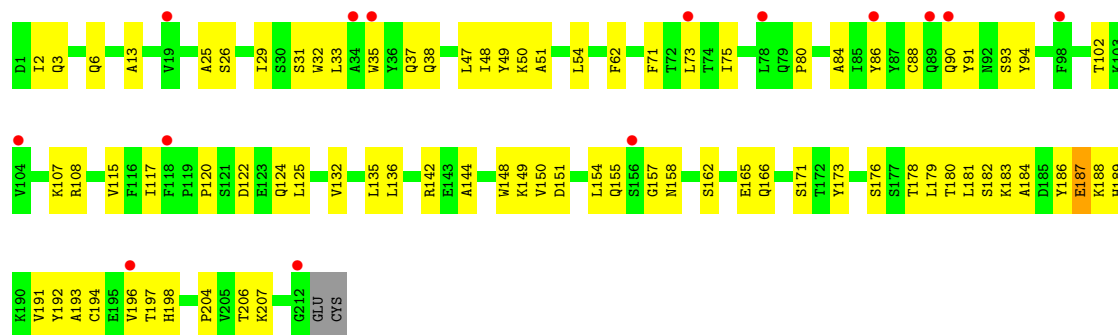


• Molecule 2: Antibody 3E1 Fab light chain

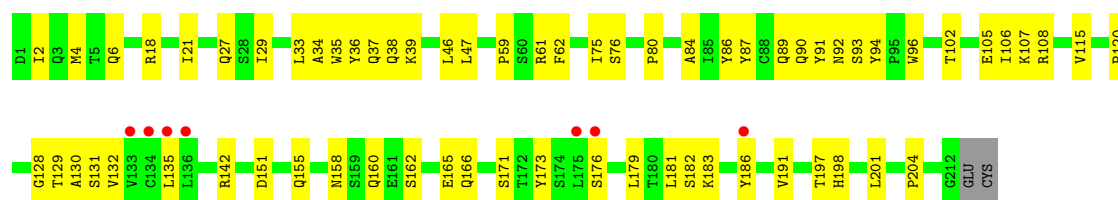


• Molecule 2: Antibody 3E1 Fab light chain

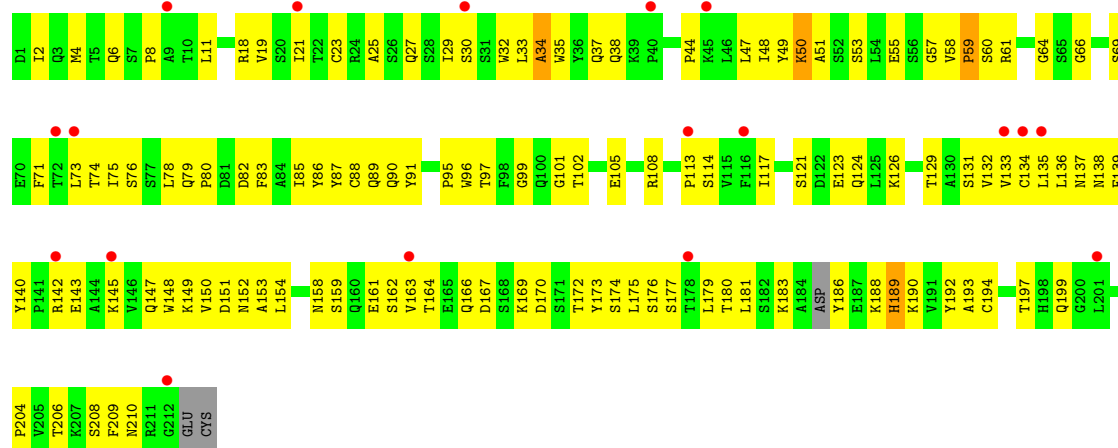




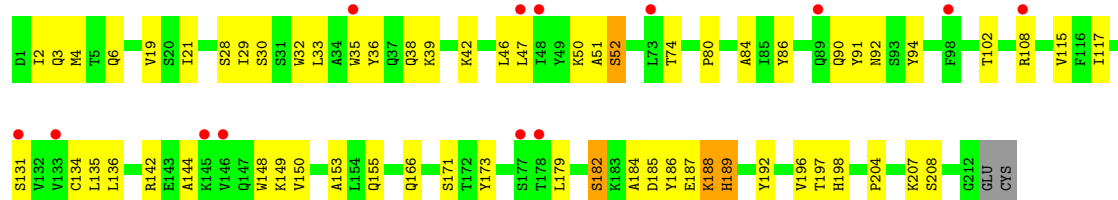
• Molecule 2: Antibody 3E1 Fab light chain



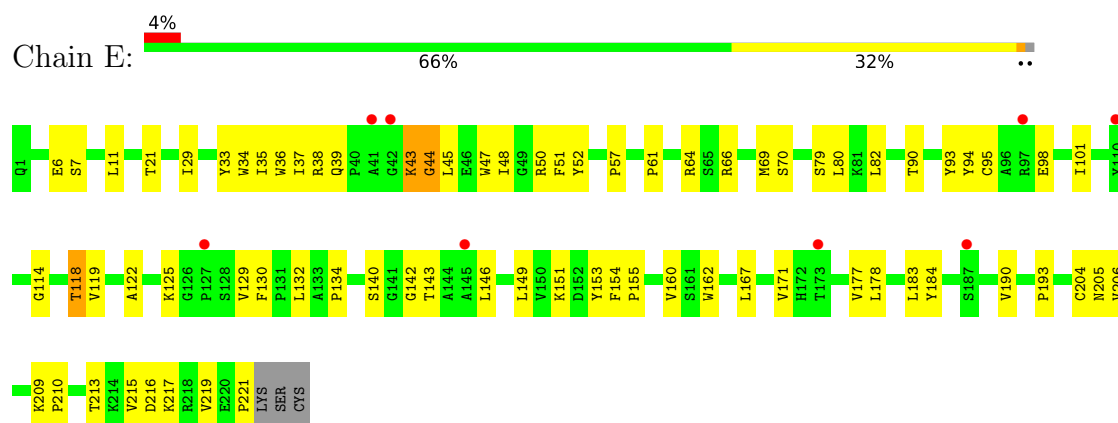
• Molecule 2: Antibody 3E1 Fab light chain



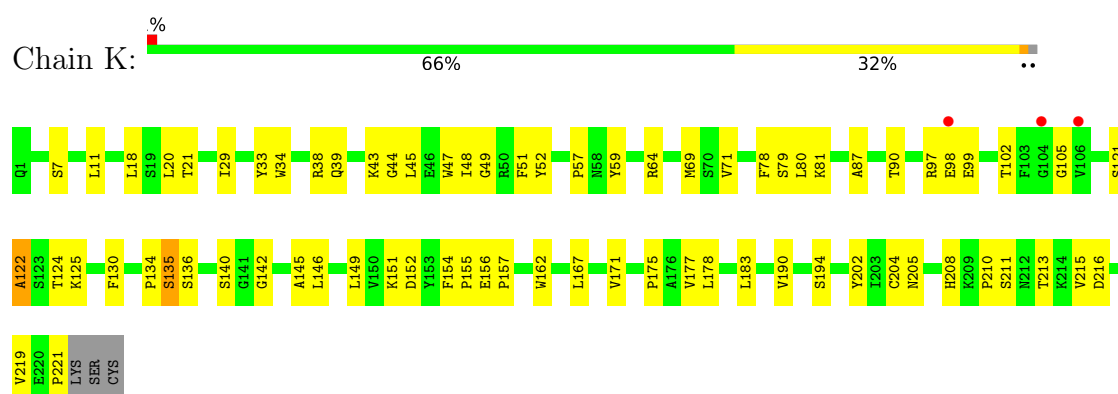
• Molecule 2: Antibody 3E1 Fab light chain



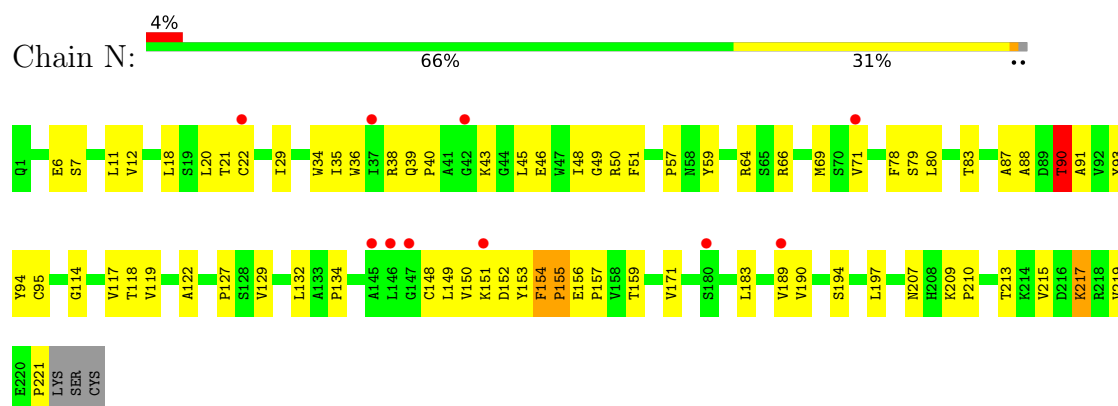
- Molecule 3: Antibody 3E1 Fab heavy chain



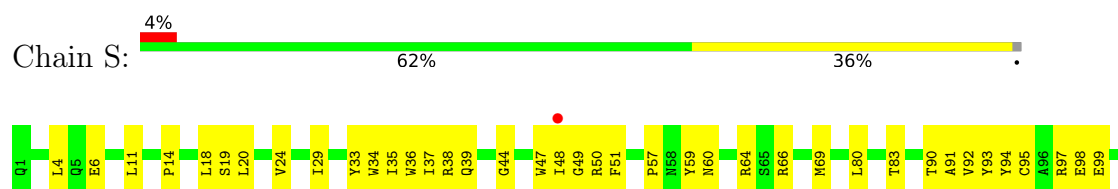
- Molecule 3: Antibody 3E1 Fab heavy chain

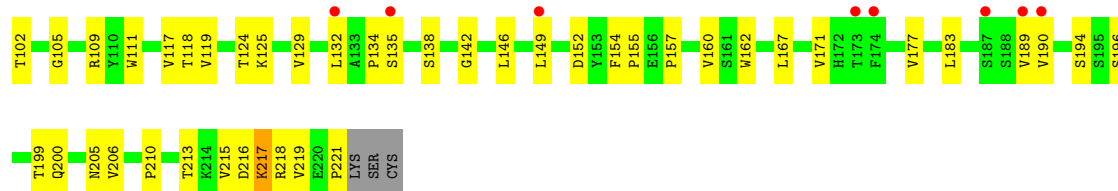


- Molecule 3: Antibody 3E1 Fab heavy chain

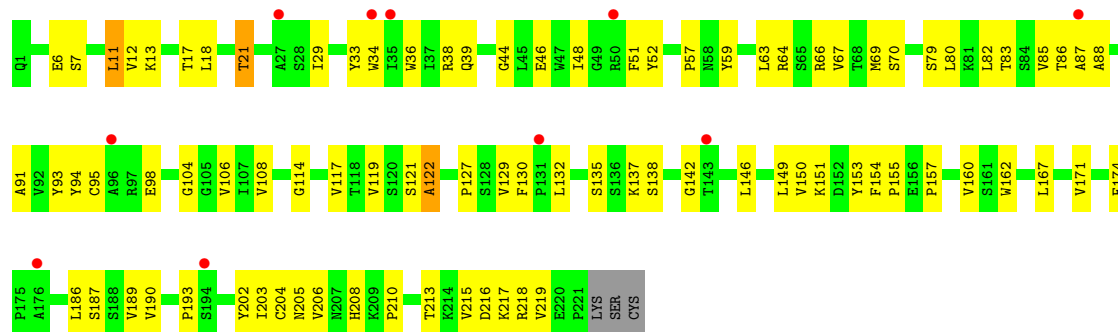


- Molecule 3: Antibody 3E1 Fab heavy chain

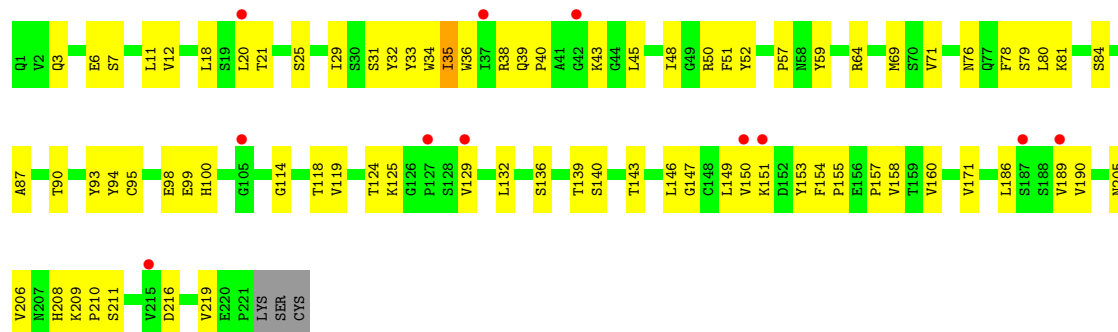




• Molecule 3: Antibody 3E1 Fab heavy chain



• Molecule 3: Antibody 3E1 Fab heavy chain



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



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



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

Chain F:  33% 67%

MAG1
MAG2
BMA3

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

Chain G:  33% 67%

MAG1
MAG2
BMA3

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

Chain O:  33% 67%

MAG1
MAG2
BMA3

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

Chain T:  67% 33%

MAG1
MAG2
BMA3

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

Chain e:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.43Å 194.50Å 214.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 4.60 48.05 – 4.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.05-4.60) 99.4 (48.05-4.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 4.64Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.293 , 0.325 0.301 , 0.325	Depositor DCC
R_{free} test set	2050 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	133.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 423.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	43211	wwPDB-VP
Average B, all atoms (Å ²)	208.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	B	0.22	0/1387	0.57	4/1869 (0.2%)
1	C	0.30	1/2566 (0.0%)	0.61	7/3482 (0.2%)
1	H	0.23	0/1387	0.57	2/1869 (0.1%)
1	I	0.32	1/1387 (0.1%)	0.60	4/1869 (0.2%)
1	L	0.37	2/2566 (0.1%)	0.77	10/3482 (0.3%)
1	P	0.17	0/1387	0.37	0/1869
1	Q	0.42	1/2566 (0.0%)	1.04	20/3482 (0.6%)
1	U	0.20	0/1387	0.47	1/1869 (0.1%)
1	V	0.33	0/2566	0.64	4/3482 (0.1%)
1	Y	0.27	0/2566	0.64	8/3482 (0.2%)
1	a	0.23	0/1387	0.54	2/1869 (0.1%)
1	b	0.38	1/2566 (0.0%)	0.97	16/3482 (0.5%)
2	D	0.20	0/1674	0.53	2/2273 (0.1%)
2	J	0.28	0/1674	0.72	8/2273 (0.4%)
2	M	0.25	0/1674	0.52	1/2273 (0.0%)
2	R	0.24	0/1674	0.50	0/2273
2	W	0.47	0/1665	0.82	4/2259 (0.2%)
2	c	0.26	0/1674	0.66	6/2273 (0.3%)
3	E	0.26	0/1700	0.61	4/2323 (0.2%)
3	K	0.24	0/1700	0.63	5/2323 (0.2%)
3	N	0.31	0/1700	0.72	8/2323 (0.3%)
3	S	0.25	0/1700	0.57	3/2323 (0.1%)
3	X	0.28	1/1700 (0.1%)	0.59	4/2323 (0.2%)
3	d	0.30	0/1700	0.60	1/2323 (0.0%)
All	All	0.30	7/43953 (0.0%)	0.68	124/59668 (0.2%)

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	C	0	1
1	I	0	1
1	Q	0	1
1	V	0	1
1	b	0	1
2	W	0	1
3	E	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	59	PRO	N-CD	9.64	1.61	1.47
1	I	77	ILE	CA-C	7.95	1.62	1.52
1	L	54	ILE	N-CA	7.89	1.56	1.46
1	b	121	PHE	C-N	-7.03	1.24	1.33
1	L	55	ASN	N-CA	6.32	1.54	1.45
3	X	85	VAL	N-CA	5.95	1.53	1.46
1	C	306	PRO	N-CD	-5.79	1.39	1.47

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	54	ILE	N-CA-C	31.70	143.19	110.23
1	b	62	LEU	N-CA-C	-24.22	74.68	110.52
1	L	139	ALA	N-CA-C	-20.65	80.06	107.73
1	Q	55	ASN	N-CA-C	-18.13	89.06	113.18
1	b	114	LYS	N-CA-C	-13.15	94.09	111.71
2	W	60	SER	N-CA-C	-13.06	97.31	113.38
1	b	142	VAL	N-CA-C	-13.06	91.30	108.93
1	L	137	SER	N-CA-C	-13.06	97.48	113.41
1	a	163	SER	N-CA-C	12.61	124.76	111.14
1	b	62	LEU	CB-CA-C	12.46	131.64	109.83
3	E	44	GLY	N-CA-C	12.40	128.13	112.14
1	H	62	GLN	N-CA-C	12.34	128.74	110.48
1	Q	287	THR	N-CA-C	12.25	127.66	112.23
1	Q	54	ILE	CB-CA-C	-11.87	96.51	111.70
2	J	190	LYS	N-CA-C	11.84	127.81	112.41
3	K	136	SER	N-CA-C	-11.39	99.51	113.41
1	Y	47	HIS	N-CA-C	-10.84	93.81	109.96
3	N	155	PRO	N-CA-C	-10.70	92.33	112.01
1	b	141	GLY	N-CA-C	-10.49	88.31	113.18
1	b	121	PHE	N-CA-C	10.08	125.15	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	122	SER	N-CA-CB	-9.62	95.65	110.65
1	Y	136	ASN	N-CA-C	-9.39	96.21	110.30
1	L	55	ASN	N-CA-C	-9.16	101.39	114.12
1	Q	281	ILE	N-CA-C	-8.96	97.28	109.37
1	Q	59	PRO	N-CA-C	-8.95	95.10	111.03
3	N	154	PHE	N-CA-C	8.88	129.44	109.81
1	Y	47	HIS	CB-CA-C	8.74	122.74	110.16
2	c	182	SER	N-CA-C	-8.70	98.58	110.68
1	I	78	GLU	N-CA-C	8.70	121.63	111.02
1	a	163	SER	CB-CA-C	-8.49	97.48	110.90
1	B	135	ASN	N-CA-C	-8.45	104.01	112.97
1	C	129	SER	N-CA-C	-8.33	102.28	111.36
1	Q	286	THR	CB-CA-C	-8.31	95.58	110.36
1	Q	287	THR	N-CA-CB	-8.23	97.63	110.30
2	J	187	GLU	N-CA-C	-8.22	100.29	110.65
3	X	86	THR	N-CA-C	8.16	123.69	111.04
2	J	191	VAL	N-CA-CB	-8.15	101.67	111.21
2	c	189	HIS	N-CA-C	8.13	122.15	109.96
3	X	21	THR	N-CA-C	8.04	122.21	107.99
1	b	122	SER	N-CA-C	7.94	121.36	108.41
1	L	57	LYS	N-CA-C	-7.91	98.43	110.70
1	H	62	GLN	N-CA-CB	-7.89	98.30	110.29
1	Q	272	GLY	N-CA-C	-7.66	95.04	113.18
2	J	190	LYS	N-CA-CB	-7.61	98.64	111.20
1	b	115	PHE	N-CA-C	-7.53	102.77	110.97
1	V	135	VAL	N-CA-C	-7.51	98.43	108.35
1	Q	273	LYS	N-CA-C	-7.45	98.59	110.14
1	C	126	ALA	N-CA-CB	-7.41	97.97	110.49
1	I	76	ARG	N-CA-C	-7.35	103.20	111.14
1	I	12	GLY	N-CA-C	7.22	123.64	112.60
3	N	90	THR	N-CA-C	-7.21	95.06	107.61
2	J	191	VAL	N-CA-C	7.12	118.39	107.99
1	Y	136	ASN	CB-CA-C	7.12	119.95	110.06
3	K	122	ALA	N-CA-C	6.96	118.82	110.19
1	Q	59	PRO	N-CA-CB	6.95	110.78	102.72
3	E	43	LYS	CB-CA-C	-6.91	102.25	113.37
3	N	90	THR	N-CA-CB	6.89	121.25	110.71
1	b	142	VAL	N-CA-CB	-6.88	102.58	110.49
2	c	182	SER	CB-CA-C	-6.88	102.18	111.88
1	C	125	GLU	CB-CA-C	-6.88	95.67	110.45
1	V	217	ARG	N-CA-C	-6.80	100.10	110.30
1	Q	20	ASN	CB-CA-C	-6.72	98.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	122	ALA	N-CA-C	-6.72	101.86	110.53
1	C	304	ILE	N-CA-C	6.71	116.72	110.42
1	V	135	VAL	N-CA-CB	6.70	122.35	111.36
2	W	34	ALA	N-CA-CB	-6.69	99.18	110.49
1	C	114	LYS	N-CA-C	6.65	119.53	111.82
1	L	99	ILE	N-CA-C	-6.64	100.60	109.30
1	b	65	CYS	N-CA-C	-6.64	104.81	113.17
1	B	65	ALA	N-CA-C	-6.60	100.12	109.96
1	B	66	VAL	N-CA-C	-6.59	104.75	110.74
1	Q	281	ILE	CB-CA-C	6.58	122.31	111.59
1	L	100	CYS	N-CA-C	-6.58	101.02	111.02
1	b	61	SER	N-CA-C	-6.52	100.39	110.10
3	E	43	LYS	N-CA-C	-6.51	98.73	109.80
3	X	87	ALA	N-CA-CB	6.47	121.32	110.77
1	L	295	ILE	N-CA-CB	6.45	121.87	111.23
1	L	136	ASN	N-CA-C	-6.45	98.32	108.63
1	b	121	PHE	O-C-N	-6.44	114.94	122.86
3	d	35	ILE	N-CA-C	6.41	117.14	108.17
1	Q	48	ASN	N-CA-C	-6.39	100.71	110.30
1	Q	136	ASN	N-CA-C	-6.31	100.56	109.96
1	b	305	ILE	N-CA-C	6.28	117.64	111.67
2	W	170	ASP	CB-CA-C	6.18	121.60	112.09
1	Y	281	ILE	N-CA-CB	6.17	117.44	110.72
3	N	219	VAL	N-CA-CB	6.07	120.23	112.34
1	Q	20	ASN	N-CA-C	6.05	116.55	108.38
1	Q	282	GLU	N-CA-C	-6.03	97.49	108.65
1	Q	115	PHE	N-CA-C	-6.01	105.44	112.89
3	S	19	SER	N-CA-CB	-5.83	100.89	110.68
1	B	78	GLU	N-CA-C	5.82	117.62	111.28
1	b	305	ILE	CB-CA-C	-5.81	104.94	111.80
1	L	59	PRO	N-CA-CB	-5.74	98.02	103.19
2	M	187	GLU	N-CA-C	-5.71	106.48	113.50
2	c	188	LYS	CB-CA-C	5.71	120.21	110.74
3	N	154	PHE	CB-CA-C	-5.69	98.95	110.17
1	C	305	HIS	N-CA-CB	5.67	120.47	110.37
3	K	121	SER	N-CA-C	5.62	119.76	113.01
2	W	59	PRO	N-CA-C	-5.61	100.91	112.47
3	S	217	LYS	N-CA-C	5.59	117.90	109.23
1	Y	280	SER	N-CA-C	5.57	117.26	110.41
1	b	114	LYS	N-CA-CB	5.53	120.29	111.66
1	L	294	ALA	CB-CA-C	5.52	119.79	109.86
3	N	88	ALA	N-CA-C	5.50	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ARG	N-CA-C	-5.49	105.38	111.36
2	D	156	SER	N-CA-C	5.40	117.17	111.28
3	K	135	SER	N-CA-C	-5.38	103.20	110.68
1	Q	59	PRO	CA-N-CD	-5.35	104.51	112.00
2	J	51	ALA	CB-CA-C	5.31	121.00	110.42
1	U	10	ILE	N-CA-C	5.30	120.36	109.34
2	c	52	SER	CB-CA-C	-5.29	101.28	109.80
3	N	217	LYS	N-CA-C	5.27	117.40	109.23
3	E	118	THR	N-CA-C	5.24	117.79	109.24
3	K	135	SER	CB-CA-C	-5.21	104.54	111.88
2	D	156	SER	N-CA-CB	-5.19	102.49	110.12
1	Y	281	ILE	N-CA-C	-5.17	101.14	108.58
1	I	11	GLU	N-CA-C	-5.11	101.01	108.07
2	J	184	ALA	N-CA-C	-5.08	99.97	110.80
2	c	52	SER	N-CA-CB	-5.08	103.08	111.01
1	V	218	ARG	N-CA-C	-5.07	101.60	109.72
1	Y	48	ASN	N-CA-C	-5.06	102.02	110.17
2	J	187	GLU	N-CA-CB	5.06	116.17	110.35
3	S	218	ARG	N-CA-C	5.06	117.38	110.55
1	Q	136	ASN	CB-CA-C	5.04	117.42	110.16

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	115	PHE	Peptide
3	E	38	ARG	Sidechain
1	I	76	ARG	Sidechain
1	Q	52	CYS	Mainchain
1	V	218	ARG	Sidechain
2	W	27	GLN	Peptide
1	b	121	PHE	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1360	0	1276	37	0
1	C	2505	0	2455	110	0
1	H	1360	0	1276	55	0
1	I	1360	0	1276	63	0
1	L	2505	0	2453	117	0
1	P	1360	0	1276	45	0
1	Q	2505	0	2455	108	0
1	U	1360	0	1276	60	0
1	V	2505	0	2455	116	0
1	Y	2505	0	2453	135	0
1	a	1360	0	1276	59	0
1	b	2505	0	2459	133	0
2	D	1636	0	1591	58	0
2	J	1636	0	1591	69	0
2	M	1636	0	1591	62	1
2	R	1636	0	1591	59	0
2	W	1628	0	1586	136	0
2	c	1636	0	1591	57	2
3	E	1658	0	1642	61	0
3	K	1658	0	1642	55	0
3	N	1658	0	1642	53	0
3	S	1658	0	1642	78	2
3	X	1658	0	1642	76	0
3	d	1658	0	1640	63	1
4	A	28	0	25	0	0
4	Z	28	0	25	0	0
5	F	39	0	34	1	0
5	G	39	0	34	1	0
5	O	39	0	34	2	0
5	T	39	0	34	0	0
5	e	39	0	34	0	0
6	V	14	0	13	0	0
All	All	43211	0	42010	1628	3

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 19.

All (1628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:6:GLN:CD	2:W:99:GLY:HA3	1.54	1.31
2:R:166:GLN:HE21	2:R:171:SER:CB	1.44	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:166:GLN:NE2	2:R:171:SER:HB3	1.49	1.24
1:C:304:ILE:O	1:C:305:HIS:CD2	1.98	1.17
1:b:54:ILE:HG23	1:b:285:CYS:O	1.48	1.14
2:W:6:GLN:NE2	2:W:88:CYS:SG	2.24	1.10
2:W:21:ILE:HD11	2:W:73:LEU:CD1	1.81	1.09
3:S:35:ILE:CD1	3:S:98:GLU:HB2	1.83	1.08
2:W:21:ILE:CD1	2:W:73:LEU:HD12	1.82	1.08
1:V:41:ASN:HA	1:V:322:ARG:HA	1.34	1.08
3:S:35:ILE:HD11	3:S:98:GLU:HB2	1.09	1.07
1:Y:51:LEU:HD22	1:Y:279:LEU:CD1	1.87	1.03
1:Q:116:SER:HA	1:Q:272:GLY:O	1.59	1.01
1:Y:51:LEU:CD2	1:Y:279:LEU:HD13	1.91	1.00
1:Y:146:LYS:HG2	1:Y:151:ASN:HA	1.41	1.00
1:b:273:GLY:O	1:b:274(A):LYS:HG3	1.61	0.99
1:Y:44:GLU:HB3	1:Y:302:GLN:HE22	1.25	0.98
2:W:6:GLN:HE22	2:W:88:CYS:H	1.08	0.97
3:d:35:ILE:CD1	3:d:50:ARG:HG2	1.96	0.96
2:W:61:ARG:O	2:W:75:ILE:HA	1.68	0.94
1:L:216:ASN:HA	1:L:218:ARG:HH22	1.33	0.94
1:C:109:GLU:HB2	1:I:76:ARG:NH1	1.83	0.93
2:W:166:GLN:O	2:W:167:ASP:OD1	1.87	0.92
2:W:6:GLN:NE2	2:W:99:GLY:HA3	1.84	0.92
1:Y:51:LEU:HD22	1:Y:279:LEU:HD13	0.96	0.91
1:b:54:ILE:CG2	1:b:285:CYS:O	2.18	0.90
2:c:29:ILE:HA	2:c:92:ASN:HD22	1.36	0.89
1:C:109:GLU:HB2	1:I:76:ARG:HH12	1.38	0.89
2:W:38:GLN:HE22	3:X:39:GLN:HE22	1.18	0.88
3:S:38:ARG:HD2	3:S:91:ALA:HB3	1.54	0.88
2:W:21:ILE:HD11	2:W:73:LEU:HD12	0.91	0.86
3:S:18:LEU:HD13	3:S:20:LEU:HD13	1.57	0.86
1:C:302:GLN:HB2	1:C:304:ILE:HD12	1.59	0.85
2:W:6:GLN:CD	2:W:99:GLY:CA	2.46	0.85
1:B:77:ILE:HG21	1:I:77:ILE:HG12	1.59	0.84
1:U:21:TRP:CH2	1:V:326:GLY:HA3	2.12	0.84
3:X:13:LYS:HD3	3:X:121:SER:HA	1.57	0.84
1:b:41:ASN:HA	1:b:323:ARG:HA	1.60	0.84
1:Y:143:ALA:H	1:Y:151:ASN:HD22	1.25	0.84
1:V:291:PRO:HD3	1:V:307:ILE:HG21	1.59	0.83
1:Y:175:ASN:ND2	5:O:1:NAG:O3	2.10	0.83
1:Y:302:GLN:HG2	1:Y:313:PRO:HB2	1.58	0.83
3:E:39:GLN:OE1	3:E:43:LYS:O	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:166:GLN:HE21	2:R:171:SER:HB3	0.69	0.83
1:Q:113:LEU:O	1:Q:116:SER:HB2	1.79	0.82
1:L:58:GLN:O	1:L:86:TRP:HA	1.80	0.82
1:C:60:ILE:HG23	1:C:86:TRP:HB3	1.62	0.82
2:W:6:GLN:NE2	2:W:88:CYS:H	1.78	0.81
3:d:35:ILE:HD13	3:d:50:ARG:HG2	1.62	0.81
3:S:4:LEU:HD12	3:S:111:TRP:HB3	1.62	0.81
1:L:59:PRO:HD3	1:L:87:SER:HB2	1.60	0.81
1:Y:44:GLU:HB3	1:Y:302:GLN:NE2	1.95	0.81
3:E:36:TRP:HD1	3:E:69:MET:SD	2.04	0.81
1:Q:121:PHE:HE2	1:Q:123:LYS:HG3	1.46	0.80
3:d:40:PRO:HG2	3:d:43:LYS:HB2	1.64	0.80
1:Q:116:SER:CA	1:Q:272:GLY:O	2.29	0.80
1:C:109:GLU:CB	1:I:76:ARG:NH1	2.45	0.80
3:K:155:PRO:HB2	3:K:210:PRO:HG2	1.63	0.80
1:V:307:ILE:HG23	1:V:307:ILE:O	1.80	0.80
1:L:26:VAL:HG21	1:L:324:ALA:HB2	1.63	0.80
1:b:91:GLU:HB3	1:b:277:ARG:HG2	1.62	0.79
1:b:273:GLY:O	1:b:274(A):LYS:CG	2.31	0.79
1:H:21:TRP:HB2	1:H:41:THR:HG22	1.65	0.79
1:U:9:PHE:CG	1:U:10:ILE:N	2.51	0.79
1:L:86:TRP:CZ2	1:L:118:VAL:HG12	2.18	0.78
2:M:120:PRO:HD3	2:M:132:VAL:HG22	1.65	0.78
2:R:4:MET:SD	2:R:90:GLN:NE2	2.56	0.78
1:Q:288:CYS:SG	1:Q:311:LYS:O	2.42	0.77
1:V:226:ARG:HE	1:b:217:ASN:ND2	1.83	0.77
1:V:226:ARG:HE	1:b:217:ASN:HD22	1.30	0.77
3:S:35:ILE:HG13	3:S:50:ARG:HG2	1.67	0.76
1:V:41:ASN:OD1	1:V:41:ASN:O	2.03	0.76
1:L:89:ILE:HB	1:L:274:LEU:HD23	1.67	0.76
1:C:305:HIS:HB3	1:C:306:PRO:HD2	1.67	0.76
1:V:51:LEU:HD23	1:V:293:GLY:HA2	1.67	0.76
2:W:34:ALA:HB2	2:W:51:ALA:HA	1.67	0.75
2:W:38:GLN:HG2	2:W:85:ILE:HD12	1.67	0.75
1:V:291:PRO:HD3	1:V:307:ILE:CG2	2.15	0.75
1:C:117:GLY:HA2	1:C:271:ASN:HA	1.69	0.75
2:W:6:GLN:HE22	2:W:88:CYS:N	1.82	0.75
3:E:36:TRP:HB3	3:E:48:ILE:HD12	1.69	0.74
1:b:121:PHE:HB2	1:b:268:VAL:HB	1.69	0.74
3:E:36:TRP:HD1	3:E:69:MET:CE	2.00	0.74
1:I:21:TRP:HD1	1:I:41:THR:HG23	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:29:LEU:HD13	1:a:51:LYS:HD2	1.70	0.74
2:J:186:TYR:O	2:J:186:TYR:CD1	2.41	0.74
1:Q:43:LEU:HD21	1:Q:303:ASN:HD21	1.51	0.74
1:V:57:LYS:NZ	1:V:120(A):GLU:OE2	2.18	0.74
1:Q:116:SER:C	1:Q:272:GLY:O	2.31	0.73
1:a:163:SER:O	1:a:167:LYS:HG3	1.89	0.73
1:C:304:ILE:O	1:C:305:HIS:HD2	1.69	0.73
1:Q:116:SER:O	1:Q:272:GLY:O	2.06	0.73
1:Y:146:LYS:HG2	1:Y:151:ASN:CA	2.16	0.73
3:E:35:ILE:HG12	3:E:50:ARG:HG2	1.71	0.73
1:b:53:SER:HB3	1:b:290:GLN:NE2	2.03	0.73
3:E:36:TRP:CD1	3:E:69:MET:SD	2.81	0.73
1:b:115:PHE:HB2	1:b:274(A):LYS:HA	1.72	0.72
1:V:26:VAL:HG21	1:V:324:ALA:HB2	1.70	0.72
2:W:38:GLN:NE2	3:X:39:GLN:HE22	1.88	0.71
1:Q:235:ARG:HH21	1:V:213:GLU:HA	1.54	0.71
1:U:22:TYR:H	1:U:41:THR:CG2	2.03	0.71
1:Y:75:PRO:HG2	1:Y:145:CYS:HB3	1.72	0.71
1:H:10:ILE:CG2	1:L:17:TYR:HE2	2.03	0.71
1:P:70:PHE:HB2	1:P:78:GLU:HB2	1.70	0.71
1:U:21:TRP:HZ3	1:V:327:LEU:H	1.36	0.71
2:D:131:SER:HA	2:D:179:LEU:O	1.91	0.71
1:U:42:GLN:HE22	2:W:32:TRP:CD1	2.07	0.71
2:W:38:GLN:HE22	3:X:39:GLN:NE2	1.88	0.71
1:Y:51:LEU:HD12	1:Y:51:LEU:O	1.90	0.71
1:L:86:TRP:HZ2	1:L:118:VAL:CG1	2.03	0.71
3:E:7:SER:OG	3:E:21:THR:OG1	2.07	0.71
1:b:58:GLN:HB2	1:b:282:ILE:HD11	1.72	0.71
1:B:127:LYS:NZ	1:I:132:GLU:O	2.23	0.71
1:B:133:ILE:HD11	1:B:139:GLU:HG3	1.73	0.70
1:H:133:ILE:HD12	1:H:137:CYS:HB2	1.73	0.70
1:Y:100:CYS:O	1:Y:230:ASN:ND2	2.23	0.70
3:N:35:ILE:HG12	3:N:50:ARG:HG2	1.73	0.70
1:L:51:LEU:HD13	1:L:90:VAL:HG21	1.74	0.70
1:L:216:ASN:C	1:L:218:ARG:NH2	2.50	0.70
2:W:18:ARG:HA	2:W:75:ILE:O	1.91	0.70
1:V:41:ASN:HD22	1:V:322:ARG:NH2	1.90	0.70
1:C:222:GLU:HB3	1:L:218:ARG:HG3	1.74	0.70
2:R:6:GLN:NE2	2:R:86:TYR:O	2.25	0.69
1:U:92:TRP:CD1	1:V:314:LYS:HZ3	2.10	0.69
2:W:21:ILE:CG1	2:W:73:LEU:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:7:SER:HB3	3:X:21:THR:HB	1.72	0.69
1:C:308:THR:OG1	1:C:312:CYS:SG	2.49	0.69
1:Y:41:ASN:HB2	1:Y:322:ARG:CZ	2.22	0.69
1:I:54:SER:HB2	1:L:29:LEU:HD12	1.73	0.69
1:V:292:LYS:HG2	1:V:305:HIS:CD2	2.28	0.69
3:S:47:TRP:CH2	3:S:49:GLY:HA2	2.27	0.69
2:W:21:ILE:HG12	2:W:73:LEU:HB2	1.74	0.69
1:Y:143:ALA:H	1:Y:151:ASN:ND2	1.91	0.69
3:S:38:ARG:HD3	3:S:93:TYR:CE1	2.28	0.69
1:C:60:ILE:O	1:C:60:ILE:HG13	1.93	0.68
1:Y:290:THR:HG22	1:Y:308:THR:HG22	1.75	0.68
1:C:117:GLY:N	1:C:272:GLY:O	2.27	0.68
1:I:167:LYS:HG2	1:I:170:ARG:HH12	1.59	0.68
3:S:37:ILE:CD1	3:S:47:TRP:HA	2.22	0.68
1:Y:224:SER:OG	1:Y:226:ARG:NH1	2.26	0.68
1:L:22:SER:O	1:L:329:ASN:ND2	2.27	0.68
2:J:155:GLN:HE22	2:J:179:LEU:HD13	1.58	0.68
1:C:288:CYS:SG	1:C:308:THR:OG1	2.52	0.68
3:E:160:VAL:HG22	3:E:206:VAL:HG22	1.76	0.67
1:U:92:TRP:HD1	1:V:314:LYS:NZ	1.92	0.67
2:W:6:GLN:NE2	2:W:88:CYS:N	2.41	0.67
2:W:131:SER:O	3:X:151:LYS:NZ	2.27	0.67
1:H:22:TYR:H	1:H:41:THR:CG2	2.08	0.67
3:X:149:LEU:HD13	3:X:151:LYS:HE3	1.75	0.67
1:B:21:TRP:HD1	1:B:41:THR:HG23	1.59	0.67
2:J:32:TRP:HZ3	2:J:50:LYS:HG3	1.59	0.67
3:N:7:SER:OG	3:N:21:THR:OG1	2.13	0.67
1:Q:85(A):SER:HA	1:Q:120:GLU:HG2	1.77	0.67
2:D:144:ALA:HB2	2:D:198:HIS:HD2	1.60	0.67
2:R:181:LEU:HD13	2:R:183:LYS:HE3	1.77	0.67
3:S:38:ARG:HG3	3:S:92:VAL:O	1.94	0.67
2:c:6:GLN:NE2	2:c:86:TYR:O	2.27	0.67
1:I:133:ILE:HB	1:I:137:CYS:HB2	1.75	0.67
3:K:33:TYR:HB2	3:K:98:GLU:HB3	1.76	0.67
1:P:21:TRP:HD1	1:P:41:THR:HG23	1.58	0.67
2:W:33:LEU:HD22	2:W:91:TYR:HE2	1.59	0.67
2:c:166:GLN:HE21	2:c:171:SER:HB3	1.60	0.67
1:B:59:MET:HE1	1:B:92:TRP:CE3	2.30	0.66
1:L:216:ASN:CA	1:L:218:ARG:HH22	2.07	0.66
1:b:92:LYS:HB3	1:b:95:PRO:HD2	1.76	0.66
2:R:166:GLN:NE2	2:R:171:SER:CB	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:TRP:CH2	1:L:326:GLY:HA2	2.30	0.66
3:N:40:PRO:HG2	3:N:43:LYS:HB2	1.76	0.66
3:S:135:SER:HB2	3:S:138:SER:HB2	1.76	0.66
2:M:94:TYR:OH	3:N:50:ARG:NH1	2.28	0.66
1:L:57:LYS:HG3	1:L:57:LYS:O	1.94	0.66
1:U:92:TRP:CD1	1:V:314:LYS:NZ	2.64	0.66
1:C:302:GLN:HB2	1:C:304:ILE:CD1	2.25	0.66
1:L:86:TRP:CZ2	1:L:118:VAL:CG1	2.79	0.66
1:Q:82:GLY:H	1:Q:123:LYS:HZ1	1.42	0.66
2:R:37:GLN:HB2	2:R:47:LEU:HD11	1.78	0.66
1:b:91:GLU:CB	1:b:277:ARG:HG2	2.25	0.66
1:C:211:GLY:HA3	1:Y:226:ARG:HG2	1.78	0.65
2:D:166:GLN:HE21	2:D:171:SER:HB3	1.60	0.65
2:M:166:GLN:HE21	2:M:171:SER:HB3	1.61	0.65
2:c:29:ILE:HG23	2:c:92:ASN:HB2	1.77	0.65
3:d:7:SER:OG	3:d:21:THR:OG1	2.13	0.65
2:R:39:LYS:HD2	2:R:84:ALA:HB2	1.77	0.65
2:W:33:LEU:HA	2:W:50:LYS:H	1.61	0.65
1:b:59:PRO:HD2	1:b:89:ILE:HG12	1.79	0.65
1:b:157:ASN:HA	1:b:263:TYR:HD2	1.61	0.65
2:c:186:TYR:HD2	2:c:189:HIS:HD2	1.45	0.65
2:D:115:VAL:HA	2:D:135:LEU:O	1.95	0.65
1:b:43:LEU:HB2	1:b:322:LEU:HB2	1.78	0.65
1:b:51:LEU:HD22	1:b:280:LEU:HB2	1.77	0.65
1:b:91:GLU:HB3	1:b:277:ARG:HA	1.77	0.65
2:c:144:ALA:HB2	2:c:198:HIS:HD2	1.62	0.65
1:V:48:ASN:OD1	1:V:49:GLY:N	2.30	0.65
1:V:215:TYR:OH	1:V:249:ILE:HD12	1.97	0.65
2:W:150:VAL:HG22	2:W:190:LYS:HG2	1.78	0.65
1:Y:108:GLU:HG2	1:Y:109:GLU:HG3	1.78	0.65
1:B:76:ARG:NH1	1:H:74:GLU:OE1	2.27	0.65
3:E:36:TRP:CD1	3:E:69:MET:CE	2.80	0.65
3:E:61:PRO:HA	3:E:64:ARG:HE	1.62	0.65
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.78	0.65
3:S:160:VAL:HG22	3:S:206:VAL:HG22	1.79	0.65
1:C:26:VAL:HG21	1:C:324:ALA:HB2	1.78	0.64
3:K:29:ILE:HG23	3:K:34:TRP:NE1	2.12	0.64
3:S:37:ILE:HD12	3:S:47:TRP:HA	1.79	0.64
2:W:6:GLN:CG	2:W:99:GLY:HA3	2.26	0.64
3:X:160:VAL:HG22	3:X:206:VAL:HG22	1.79	0.64
2:M:108:ARG:HE	2:M:171:SER:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:144:ALA:HB2	2:M:198:HIS:HD2	1.60	0.64
3:K:155:PRO:HG2	3:K:208:HIS:CE1	2.32	0.64
1:P:85:ASP:OD1	1:a:83:LYS:NZ	2.25	0.64
2:W:166:GLN:O	2:W:167:ASP:CG	2.41	0.64
3:S:129:VAL:O	3:S:217:LYS:NZ	2.23	0.64
1:U:21:TRP:HB2	1:U:41:THR:HG22	1.80	0.64
1:U:108:LEU:HD13	1:V:328:ARG:HE	1.63	0.64
2:c:6:GLN:HE21	2:c:102:THR:HG23	1.62	0.64
1:C:53:SER:OG	1:C:87:SER:OG	2.11	0.64
2:J:30:SER:O	2:J:68:GLY:N	2.27	0.64
1:L:86:TRP:HZ2	1:L:118:VAL:HG12	1.60	0.64
3:S:18:LEU:HD13	3:S:20:LEU:CD1	2.28	0.64
1:C:226:ARG:HG2	1:L:211:GLY:HA3	1.80	0.64
1:V:113:LEU:O	1:V:116:SER:OG	2.11	0.64
2:W:6:GLN:OE1	2:W:101:GLY:N	2.23	0.64
2:W:159:SER:HB2	2:W:179:LEU:HD12	1.80	0.64
2:R:108:ARG:NE	2:R:171:SER:HB2	2.12	0.63
1:U:9:PHE:CD2	1:U:10:ILE:N	2.66	0.63
1:C:113:LEU:HD21	1:I:75:LYS:HG3	1.79	0.63
3:K:7:SER:OG	3:K:21:THR:OG1	2.16	0.63
2:W:50:LYS:HD2	3:X:104:GLY:HA2	1.80	0.63
1:Y:183:LEU:HD11	1:Y:240:TRP:HB2	1.80	0.63
1:C:56:GLY:HA3	1:C:284:CYS:HB3	1.80	0.63
1:Y:158:VAL:HG23	1:Y:261:ARG:HB2	1.81	0.63
3:X:203:ILE:HG12	3:X:218:ARG:HG2	1.81	0.63
1:Y:93(A):PRO:HD2	1:Y:278:GLU:OE2	1.98	0.63
1:b:115:PHE:HD2	1:b:274(A):LYS:HG2	1.63	0.63
1:C:216:ASN:OD1	1:Y:226:ARG:NH1	2.31	0.63
1:b:183:VAL:HG22	1:b:266:GLU:HG2	1.81	0.63
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.80	0.63
2:D:131:SER:OG	3:E:151:LYS:NZ	2.31	0.63
1:Q:91:GLU:O	1:Q:91:GLU:HG2	1.96	0.63
3:X:171:VAL:HG22	3:X:190:VAL:HG22	1.81	0.63
1:H:139:GLU:HG2	1:L:12:THR:HG22	1.81	0.63
1:V:53:SER:O	1:V:285:ASN:HA	1.98	0.63
1:a:21:TRP:HD1	1:a:41:THR:HG23	1.64	0.63
1:I:55:VAL:HG23	1:L:29:LEU:HD11	1.80	0.63
2:M:29:ILE:HG22	2:M:32:TRP:H	1.64	0.63
3:N:152:ASP:HB3	3:N:183:LEU:HD13	1.81	0.63
3:N:194:SER:HA	3:N:197:LEU:HG	1.81	0.63
1:C:41:ASN:HB2	1:C:322:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:51:LEU:HD12	1:V:279:LEU:HB2	1.81	0.62
2:W:85:ILE:HA	2:W:102:THR:O	1.99	0.62
1:b:119:LEU:HB2	1:b:271:GLY:N	2.14	0.62
1:L:58:GLN:N	1:L:59:PRO:HD2	2.14	0.62
2:M:6:GLN:NE2	2:M:86:TYR:O	2.30	0.62
1:C:56:GLY:HA3	1:C:284:CYS:CB	2.29	0.62
2:R:108:ARG:HE	2:R:171:SER:HB2	1.64	0.62
2:R:120:PRO:HD3	2:R:132:VAL:HG22	1.80	0.62
1:b:91:GLU:HB3	1:b:277:ARG:CG	2.29	0.62
3:d:87:ALA:O	3:d:90:THR:HG22	1.98	0.62
3:d:129:VAL:HA	3:d:149:LEU:O	1.99	0.62
2:J:131:SER:HA	2:J:179:LEU:O	1.99	0.62
2:W:162:SER:OG	2:W:176:SER:OG	2.17	0.62
1:Y:143:ALA:N	1:Y:151:ASN:HD22	1.95	0.62
2:c:28:SER:O	2:c:29:ILE:HD13	2.00	0.62
3:d:140:SER:O	3:d:143:THR:OG1	2.15	0.62
3:K:102:THR:OG1	3:K:105:GLY:O	2.16	0.62
2:D:90:GLN:HG2	2:D:97:THR:O	2.00	0.62
1:H:10:ILE:HG21	1:L:17:TYR:HE2	1.65	0.62
3:K:125:LYS:HD2	3:K:183:LEU:HD21	1.82	0.62
1:b:290:GLN:HA	1:b:295:ALA:HA	1.81	0.62
2:J:166:GLN:HE21	2:J:171:SER:HB3	1.64	0.62
3:N:29:ILE:HG23	3:N:34:TRP:NE1	2.15	0.62
1:Y:273:LYS:HB2	1:Y:309:ILE:HD11	1.81	0.62
2:M:108:ARG:NE	2:M:171:SER:HB2	2.15	0.61
3:X:129:VAL:O	3:X:217:LYS:NZ	2.21	0.61
1:Y:182:VAL:HA	1:Y:264:PHE:O	2.00	0.61
3:K:38:ARG:HB2	3:K:48:ILE:HD11	1.81	0.61
2:M:124:GLN:OE1	3:N:151:LYS:NZ	2.33	0.61
1:Q:116:SER:O	1:Q:272:GLY:N	2.27	0.61
1:Q:156:ASN:O	1:Q:261:ARG:HB3	2.00	0.61
3:d:51:PHE:HD1	3:d:57:PRO:HB3	1.63	0.61
2:R:155:GLN:HE22	2:R:179:LEU:HD13	1.65	0.61
2:M:181:LEU:HD22	2:M:183:LYS:HE3	1.82	0.61
1:Q:191:PRO:HG2	1:Q:223:ILE:HG12	1.81	0.61
2:W:38:GLN:CB	2:W:85:ILE:HB	2.30	0.61
2:D:6:GLN:NE2	2:D:86:TYR:O	2.33	0.61
1:H:10:ILE:HG13	1:H:11:GLU:H	1.64	0.61
1:H:10:ILE:HG13	1:H:11:GLU:N	2.15	0.61
3:N:39:GLN:HB2	3:N:45:LEU:HD23	1.82	0.61
3:N:90:THR:HG23	3:N:118:THR:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:GLU:HB3	1:L:302:GLN:HG2	1.83	0.61
1:H:74:GLU:HB3	1:H:77:ILE:HD11	1.83	0.61
1:V:226:ARG:NE	1:b:217:ASN:ND2	2.48	0.61
3:E:154:PHE:HB3	3:E:155:PRO:HD3	1.83	0.61
1:L:80:LEU:HA	1:L:83:LYS:HD2	1.81	0.61
1:P:74:GLU:HB3	1:P:77:ILE:HD11	1.82	0.61
3:S:134:PRO:HD2	3:S:221:PRO:HA	1.83	0.61
1:b:74:ASN:HB3	1:b:77:CYS:SG	2.40	0.61
3:d:98:GLU:OE2	3:d:99:GLU:O	2.19	0.61
2:R:166:GLN:HG2	2:R:171:SER:HA	1.83	0.60
3:X:29:ILE:HG23	3:X:34:TRP:NE1	2.16	0.60
2:D:6:GLN:HE21	2:D:102:THR:HG23	1.66	0.60
1:U:12:GLY:O	1:V:17:TYR:CE2	2.53	0.60
1:U:70:PHE:HB2	1:U:78:GLU:HB2	1.81	0.60
1:U:76:ARG:HD2	1:a:69:GLU:O	2.01	0.60
2:J:142:ARG:HG3	2:J:173:TYR:CD2	2.36	0.60
1:L:223:ILE:H	1:Y:218:ARG:NH1	1.99	0.60
1:b:54:ILE:HD13	1:b:286:ASN:HA	1.83	0.60
2:M:6:GLN:HE21	2:M:102:THR:HG23	1.66	0.60
3:d:29:ILE:HG23	3:d:34:TRP:NE1	2.17	0.60
1:B:51:LYS:HG3	1:Y:29:LEU:HD13	1.83	0.60
1:L:216:ASN:HA	1:L:218:ARG:NH2	2.12	0.60
3:N:93:TYR:O	3:N:114:GLY:HA2	2.01	0.60
3:X:63:LEU:HD13	3:X:67:VAL:HG21	1.82	0.60
1:Y:188:ILE:HG12	1:Y:208:VAL:HG21	1.82	0.60
3:d:90:THR:OG1	3:d:118:THR:HA	2.01	0.60
1:Q:284:CYS:SG	1:Q:285:ASN:N	2.74	0.60
3:S:33:TYR:HB2	3:S:98:GLU:HB3	1.84	0.60
3:K:59:TYR:HB2	3:K:64:ARG:HD3	1.83	0.60
1:U:74:GLU:HB3	1:U:77:ILE:HD11	1.83	0.60
1:b:89:ILE:HB	1:b:275:LEU:HD22	1.84	0.60
1:C:218:ARG:HD2	1:Y:223:ILE:N	2.15	0.60
1:L:101:TYR:CE2	1:L:236:MET:HG3	2.36	0.60
2:M:2:ILE:HD11	2:M:93:SER:HB2	1.82	0.60
1:Q:20:ASN:C	1:Q:20:ASN:OD1	2.44	0.60
2:W:6:GLN:HE21	2:W:88:CYS:CB	2.15	0.60
1:C:122:SER:HB2	1:C:264:PHE:HB3	1.83	0.60
1:L:48:ASN:CG	1:L:294:ALA:O	2.45	0.60
1:I:111:HIS:HB3	1:Y:327:LEU:HD22	1.84	0.60
3:K:39:GLN:HB2	3:K:45:LEU:HD23	1.84	0.60
2:R:197:THR:HG22	2:R:204:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:26:HIS:HB2	1:a:149:MET:HE3	1.83	0.60
3:K:51:PHE:HD1	3:K:57:PRO:HB3	1.67	0.59
1:Q:35:THR:HG22	1:Q:329:ASN:HB3	1.84	0.59
1:Q:78:ASP:HA	1:Q:81:ILE:HG13	1.84	0.59
1:V:108:GLU:HG2	1:V:109:GLU:HG3	1.84	0.59
2:c:142:ARG:HG3	2:c:173:TYR:CD2	2.37	0.59
1:Y:210:VAL:HB	1:Y:215:TYR:HE2	1.66	0.59
2:D:116:PHE:HB2	2:D:135:LEU:HD23	1.84	0.59
1:H:70:PHE:HB2	1:H:78:GLU:HB2	1.84	0.59
1:Q:60:ILE:HB	1:Q:89:ILE:HG12	1.84	0.59
3:d:160:VAL:HG22	3:d:206:VAL:HG22	1.83	0.59
1:H:76:ARG:NH1	1:Y:109:GLU:HB3	2.17	0.59
3:K:135:SER:O	3:K:135:SER:OG	2.18	0.59
1:b:180:GLY:O	1:b:181:ARG:HG3	2.02	0.59
1:V:180:ARG:NH1	1:V:267:VAL:HG13	2.18	0.59
1:V:309:ILE:HD12	1:V:309:ILE:H	1.67	0.59
1:C:120:GLU:HB2	1:C:267:VAL:H	1.66	0.59
2:M:48:ILE:HG12	2:M:54:LEU:HA	1.84	0.59
1:Y:74:ASN:OD1	1:Y:75:PRO:HD2	2.02	0.59
1:H:76:ARG:HH22	1:I:69:GLU:H	1.49	0.59
2:M:142:ARG:HG3	2:M:173:TYR:CD2	2.37	0.59
1:V:307:ILE:O	1:V:307:ILE:CG2	2.51	0.59
1:a:74:GLU:HB3	1:a:77:ILE:HD11	1.85	0.59
1:a:163:SER:O	1:a:167:LYS:CG	2.51	0.59
3:N:51:PHE:HD1	3:N:57:PRO:HB3	1.68	0.59
2:R:151:ASP:HA	2:R:191:VAL:HB	1.85	0.59
1:B:38:LEU:O	1:B:42:GLN:HB2	2.03	0.59
2:D:142:ARG:HG3	2:D:173:TYR:CD2	2.38	0.59
1:I:133:ILE:HD11	1:I:139:GLU:HB2	1.84	0.59
1:Y:146:LYS:CG	1:Y:151:ASN:HA	2.26	0.59
1:V:180:ARG:HH12	1:V:267:VAL:HG13	1.67	0.59
1:b:136:VAL:HG11	1:b:161:LEU:HB3	1.85	0.59
3:K:162:TRP:HB3	3:K:167:LEU:HB2	1.85	0.58
1:Q:218:ARG:NH1	1:b:223:GLU:HA	2.18	0.58
2:R:6:GLN:HE21	2:R:102:THR:HG23	1.68	0.58
2:W:137:ASN:HA	2:W:174:SER:HB2	1.84	0.58
1:b:44:GLU:HG2	1:b:296:ILE:HG21	1.85	0.58
1:b:59:PRO:HD3	1:b:86:TRP:HB2	1.85	0.58
2:M:32:TRP:HZ3	2:M:50:LYS:HG3	1.69	0.58
1:P:51:LYS:HB2	1:b:30:LEU:HD23	1.84	0.58
3:S:109:ARG:H	3:S:111:TRP:NE1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:25:ALA:HB2	2:M:90:GLN:HE22	1.67	0.58
3:S:47:TRP:CZ2	3:S:49:GLY:HA2	2.39	0.58
2:W:32:TRP:CZ3	3:X:106:VAL:HB	2.38	0.58
2:M:149:LYS:HB2	2:M:193:ALA:HB3	1.85	0.58
1:P:38:LEU:O	1:P:42:GLN:HB2	2.04	0.58
1:B:50:ASN:ND2	1:Y:29:LEU:O	2.34	0.58
3:N:59:TYR:HB2	3:N:64:ARG:HD3	1.85	0.58
1:Y:74:ASN:ND2	1:Y:100:CYS:SG	2.77	0.58
1:a:11:GLU:HG2	1:a:12:GLY:H	1.67	0.58
1:b:121:PHE:CB	1:b:268:VAL:HB	2.34	0.58
3:d:125:LYS:HD2	3:d:154:PHE:HB2	1.86	0.58
1:B:106:ARG:HH22	1:I:105:GLU:HG2	1.68	0.58
1:C:52:CYS:HB3	1:C:283:SER:O	2.04	0.58
2:R:106:ILE:HB	2:R:166:GLN:HE22	1.68	0.58
2:W:210:ASN:H	3:X:137:LYS:HD2	1.68	0.58
2:D:35:TRP:O	2:D:47:LEU:N	2.35	0.57
1:H:133:ILE:HD11	1:H:139:GLU:HG3	1.86	0.57
2:J:155:GLN:NE2	2:J:179:LEU:HD13	2.18	0.57
1:P:111:HIS:HB3	1:Q:327:LEU:HD21	1.85	0.57
1:Y:101:TYR:CD1	1:Y:236:MET:HG2	2.38	0.57
2:c:184:ALA:C	2:c:186:TYR:H	2.12	0.57
3:N:69:MET:HE2	3:N:80:LEU:HD21	1.85	0.57
1:H:76:ARG:NH1	1:I:69:GLU:O	2.34	0.57
2:M:115:VAL:HA	2:M:135:LEU:O	2.04	0.57
1:Q:47:HIS:CE1	1:Q:49:GLY:HA2	2.40	0.57
1:I:51:LYS:HB2	1:L:30:LEU:HD23	1.87	0.57
1:L:291:PRO:HD2	1:L:305:HIS:CD2	2.39	0.57
3:S:35:ILE:CG1	3:S:50:ARG:HG2	2.33	0.57
1:V:273:LYS:HZ3	1:V:307:ILE:HG13	1.68	0.57
1:Y:100:CYS:HB2	1:Y:145:CYS:SG	2.44	0.57
3:X:6:GLU:OE2	3:X:95:CYS:N	2.34	0.57
1:a:128:ASN:H	1:a:159:TYR:HE2	1.51	0.57
3:E:29:ILE:HG23	3:E:34:TRP:NE1	2.20	0.57
3:S:102:THR:OG1	3:S:105:GLY:O	2.20	0.57
2:W:83:PHE:HD1	2:W:105:GLU:HA	1.70	0.57
2:c:153:ALA:O	2:c:155:GLN:NE2	2.38	0.57
1:L:53:SER:HA	1:L:59:PRO:HG2	1.87	0.57
2:M:186:TYR:O	2:M:186:TYR:CD1	2.57	0.57
1:V:111:LEU:HG	1:V:115:PHE:HE2	1.69	0.57
3:d:155:PRO:HG2	3:d:208:HIS:CE1	2.39	0.57
3:E:51:PHE:HD1	3:E:57:PRO:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:GLY:C	1:L:58:GLN:H	2.13	0.57
1:Q:132:TRP:HB3	1:Q:170:ILE:HD12	1.86	0.57
1:U:77:ILE:HG23	1:a:70:PHE:HE1	1.70	0.57
2:W:57:GLY:O	2:W:59:PRO:O	2.22	0.57
2:W:86:TYR:O	2:W:101:GLY:HA2	2.04	0.57
2:W:197:THR:HG22	2:W:204:PRO:HB3	1.86	0.57
1:b:91:GLU:OE2	1:b:92:LYS:O	2.21	0.57
2:c:117:ILE:HG12	2:c:134:CYS:SG	2.45	0.57
1:C:113:LEU:HD23	1:I:75:LYS:HB3	1.87	0.56
1:I:111:HIS:HB2	1:Y:327:LEU:HD13	1.87	0.56
3:K:69:MET:HE2	3:K:80:LEU:HD21	1.87	0.56
2:M:188:LYS:HG2	2:M:189:HIS:CE1	2.40	0.56
3:S:47:TRP:HZ2	3:S:50:ARG:HD3	1.70	0.56
2:D:149:LYS:HB2	2:D:193:ALA:HB3	1.87	0.56
2:D:160:GLN:NE2	3:E:178:LEU:O	2.38	0.56
2:J:6:GLN:HG2	2:J:102:THR:HG23	1.87	0.56
1:L:135:VAL:HG11	1:L:160:LEU:HB3	1.87	0.56
2:R:115:VAL:HA	2:R:135:LEU:O	2.04	0.56
3:S:109:ARG:HB2	3:S:111:TRP:CZ2	2.40	0.56
1:V:288:CYS:HB3	1:V:309:ILE:HD13	1.86	0.56
3:E:129:VAL:O	3:E:217:LYS:NZ	2.20	0.56
1:H:21:TRP:HZ3	1:L:327:LEU:H	1.54	0.56
1:Q:139:ALA:HB1	1:Q:161:ILE:HD12	1.88	0.56
2:W:6:GLN:OE1	2:W:99:GLY:C	2.49	0.56
3:X:70:SER:OG	3:X:79:SER:OG	2.24	0.56
1:b:73:GLY:HA3	1:b:156:ARG:H	1.71	0.56
2:c:115:VAL:HA	2:c:135:LEU:O	2.05	0.56
2:M:115:VAL:O	2:M:207:LYS:NZ	2.23	0.56
1:Q:121:PHE:CE2	1:Q:123:LYS:HG3	2.36	0.56
1:Q:304:ILE:HG22	1:Q:305:HIS:H	1.71	0.56
2:W:89:GLN:OE1	2:W:91:TYR:OH	2.23	0.56
1:b:105:LEU:HD11	1:b:241:TRP:HD1	1.69	0.56
3:d:59:TYR:HB2	3:d:64:ARG:HD3	1.87	0.56
1:I:148:CYS:O	1:I:152:VAL:HG23	2.06	0.56
2:R:142:ARG:HG3	2:R:173:TYR:CD2	2.39	0.56
3:d:98:GLU:OE1	3:d:98:GLU:O	2.23	0.56
1:Q:236:MET:HB3	1:Q:238:PHE:CE1	2.41	0.56
1:U:125:GLN:HG2	1:U:157:TYR:HB3	1.88	0.56
1:b:26:VAL:HG21	1:b:325:ALA:HB2	1.87	0.56
1:b:115:PHE:HA	1:b:275:LEU:HG	1.88	0.56
1:b:303:GLN:HG3	1:b:314:PRO:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:CYS:O	1:C:230:ASN:ND2	2.33	0.56
1:L:92:LYS:HG2	1:L:278:GLU:HG2	1.86	0.56
1:C:56:GLY:CA	1:C:284:CYS:HA	2.36	0.56
2:D:150:VAL:HG22	2:D:192:TYR:HD1	1.71	0.56
1:Y:44:GLU:CB	1:Y:302:GLN:HE22	2.10	0.56
1:B:81:ASN:HB2	1:I:80:LEU:HD22	1.88	0.56
1:H:21:TRP:CH2	1:L:326:GLY:CA	2.88	0.56
1:I:70:PHE:HB2	1:I:78:GLU:HB2	1.87	0.56
1:P:148:CYS:O	1:P:152:VAL:HG23	2.06	0.56
2:c:108:ARG:NE	2:c:171:SER:HB2	2.21	0.56
3:d:33:TYR:HB2	3:d:98:GLU:HB3	1.88	0.56
1:Q:72:LEU:HD13	1:Q:238:PHE:CD2	2.41	0.55
1:Q:180:ARG:HH12	1:Q:267:VAL:HG13	1.71	0.55
1:Y:244:LYS:HB2	1:Y:247:GLU:OE2	2.05	0.55
1:P:81:ASN:HB2	1:a:80:LEU:HD22	1.87	0.55
1:a:148:CYS:O	1:a:152:VAL:HG23	2.07	0.55
1:C:56:GLY:HA3	1:C:284:CYS:CA	2.36	0.55
1:H:13:GLY:H	1:L:332:SER:HA	1.71	0.55
1:L:100:CYS:O	1:L:230:ASN:ND2	2.39	0.55
1:U:148:CYS:O	1:U:152:VAL:HG23	2.06	0.55
1:V:215:TYR:HB2	1:V:217:ARG:HG3	1.87	0.55
1:Y:226:ARG:HE	1:Y:235:ARG:HG2	1.71	0.55
1:b:115:PHE:CD2	1:b:274(A):LYS:HG2	2.41	0.55
1:C:52:CYS:HB2	1:C:286:THR:OG1	2.05	0.55
1:I:163:SER:O	1:I:167:LYS:HG3	2.07	0.55
1:U:141:TYR:CZ	1:U:170:ARG:HG3	2.41	0.55
1:U:76:ARG:HH11	1:b:109:GLU:HB2	1.70	0.55
1:b:166:GLY:C	1:b:203:LYS:HG3	2.31	0.55
1:C:48:ASN:HD21	1:C:294:ALA:HB3	1.69	0.55
1:C:304:ILE:O	1:C:305:HIS:CG	2.58	0.55
2:c:33:LEU:HD22	2:c:90:GLN:HG2	1.87	0.55
3:d:69:MET:HE2	3:d:80:LEU:HD21	1.87	0.55
1:L:236:MET:SD	1:L:258:LEU:HD11	2.47	0.55
1:Q:52:CYS:HB3	1:Q:294:ALA:HB2	1.89	0.55
3:X:69:MET:HE2	3:X:80:LEU:HD21	1.89	0.55
1:Y:287:THR:HG22	1:Y:296:ASN:HA	1.88	0.55
3:d:93:TYR:O	3:d:114:GLY:HA2	2.06	0.55
1:L:215:TYR:CZ	1:L:241:THR:HB	2.41	0.55
1:Q:188:ILE:HG12	1:Q:208:VAL:HG21	1.87	0.55
3:S:51:PHE:HD1	3:S:57:PRO:HB3	1.72	0.55
1:V:181:ASP:HB3	1:V:242:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:88:ALA:HB2	3:X:119:VAL:HG23	1.87	0.55
1:Y:26:VAL:HG21	1:Y:324:ALA:HB2	1.89	0.55
1:Y:302:GLN:HE21	1:Y:313:PRO:HG2	1.72	0.55
1:I:7:ALA:HA	1:I:10:ILE:HB	1.88	0.55
2:M:124:GLN:CD	3:N:151:LYS:NZ	2.65	0.55
1:Q:171:LYS:HA	1:Q:251:PHE:O	2.07	0.55
3:S:146:LEU:HD22	3:S:219:VAL:HG12	1.88	0.55
1:V:226:ARG:NE	1:b:217:ASN:HD22	2.01	0.55
3:X:51:PHE:HD1	3:X:57:PRO:HB3	1.72	0.55
1:Y:166:THR:HA	1:Y:202:LYS:HD2	1.89	0.55
1:I:51:LYS:HG3	1:L:29:LEU:CD2	2.36	0.54
2:J:85:ILE:HG12	2:J:103:LYS:HG2	1.88	0.54
3:K:90:THR:HG23	3:K:90:THR:O	2.07	0.54
2:M:31:SER:HA	2:M:71:PHE:HE2	1.73	0.54
1:Q:52:CYS:SG	1:Q:53:SER:N	2.80	0.54
1:Q:235:ARG:HG3	1:V:216:ASN:HD21	1.72	0.54
3:S:36:TRP:O	3:S:37:ILE:HD13	2.06	0.54
2:W:6:GLN:NE2	2:W:99:GLY:CA	2.63	0.54
2:W:123:GLU:OE1	3:X:217:LYS:NZ	2.34	0.54
1:L:223:ILE:H	1:Y:218:ARG:HH11	1.54	0.54
2:W:124:GLN:HE22	3:X:151:LYS:HZ3	1.55	0.54
1:b:141:GLY:H	1:b:160:TRP:HB3	1.71	0.54
2:D:108:ARG:NE	2:D:171:SER:HB2	2.23	0.54
3:E:47:TRP:HE1	3:E:50:ARG:HG3	1.72	0.54
1:H:111:HIS:HB3	1:L:327:LEU:HD21	1.90	0.54
1:P:77:ILE:HD12	1:a:77:ILE:HG21	1.90	0.54
1:Q:304:ILE:O	1:Q:315:TYR:CE1	2.60	0.54
1:a:113:SER:O	1:a:117:ASN:ND2	2.40	0.54
1:C:29:LEU:HD13	1:H:51:LYS:HG3	1.90	0.54
1:Q:218:ARG:NH1	1:b:222:PRO:O	2.39	0.54
1:a:24:TYR:HB3	1:b:13:LEU:HD11	1.89	0.54
2:D:90:GLN:HG3	2:D:90:GLN:O	2.07	0.54
2:J:160:GLN:HB3	3:K:177:VAL:HG11	1.89	0.54
2:J:160:GLN:NE2	3:K:178:LEU:O	2.41	0.54
1:L:289:GLN:HA	1:L:294:ALA:HB2	1.90	0.54
3:S:59:TYR:HB2	3:S:64:ARG:HD3	1.90	0.54
2:W:34:ALA:HB3	2:W:48:ILE:O	2.07	0.54
3:d:132:LEU:HD12	3:d:147:GLY:HA3	1.90	0.54
3:E:39:GLN:HB2	3:E:45:LEU:HD23	1.90	0.54
2:M:32:TRP:CZ3	2:M:50:LYS:HG3	2.43	0.54
1:Q:29:LEU:HD21	1:U:51:LYS:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:183:LEU:HD11	1:Q:240:TRP:HB2	1.88	0.54
2:R:131:SER:HA	2:R:179:LEU:O	2.07	0.54
1:I:21:TRP:CD1	1:I:41:THR:HG23	2.38	0.54
3:K:167:LEU:HD11	3:K:202:TYR:HD1	1.71	0.54
1:P:59:MET:C	1:Q:314:LYS:HZ2	2.16	0.54
2:W:87:TYR:HE2	3:X:44:GLY:HA2	1.73	0.54
1:I:89:LEU:HD11	1:Y:317:LYS:HG2	1.88	0.54
1:L:52:CYS:SG	1:L:284:CYS:HB2	2.47	0.54
1:C:59:PRO:HG2	1:C:281:ILE:HG22	1.90	0.54
1:L:58:GLN:H	1:L:59:PRO:HD2	1.72	0.54
1:V:132:TRP:H	1:V:132:TRP:HE3	1.54	0.54
3:X:213:THR:HG22	3:X:215:VAL:HG23	1.88	0.54
1:Y:146:LYS:HE2	1:Y:151:ASN:HB3	1.89	0.54
1:C:56:GLY:HA3	1:C:284:CYS:HA	1.89	0.54
3:E:93:TYR:O	3:E:114:GLY:HA2	2.08	0.54
3:K:149:LEU:HB3	3:K:151:LYS:HE3	1.88	0.54
3:S:97:ARG:HB3	3:S:111:TRP:CE2	2.43	0.54
1:V:288:CYS:C	1:V:294:ALA:HA	2.33	0.54
3:K:135:SER:HB3	3:K:145:ALA:HB3	1.91	0.53
3:S:99:GLU:OE2	3:S:111:TRP:HZ2	1.91	0.53
1:U:21:TRP:HH2	1:V:326:GLY:HA3	1.66	0.53
1:C:54:ILE:HG13	1:C:55:ASN:H	1.73	0.53
1:b:68:ALA:HB1	1:b:71:ILE:HD13	1.89	0.53
1:P:77:ILE:HG21	1:U:77:ILE:HD12	1.89	0.53
2:R:108:ARG:HE	2:R:171:SER:CB	2.21	0.53
3:S:29:ILE:HG23	3:S:34:TRP:NE1	2.24	0.53
1:Y:62:LEU:HD22	1:Y:80:LEU:HD13	1.89	0.53
2:M:166:GLN:HG2	2:M:171:SER:HA	1.91	0.53
1:V:188:ILE:HG12	1:V:208:VAL:HG21	1.90	0.53
1:V:314:LYS:HG2	1:V:315:TYR:H	1.72	0.53
1:Y:146:LYS:HG2	1:Y:151:ASN:CB	2.38	0.53
2:c:50:LYS:C	2:c:52:SER:H	2.16	0.53
3:N:134:PRO:HD2	3:N:221:PRO:HA	1.90	0.53
1:P:118:LEU:HA	1:P:121:LYS:HE2	1.90	0.53
1:Q:244:LYS:HB3	1:Q:245:PRO:HD2	1.90	0.53
3:S:154:PHE:HB2	3:S:155:PRO:HD3	1.91	0.53
2:W:34:ALA:HB2	2:W:51:ALA:CA	2.36	0.53
1:Y:41:ASN:HA	1:Y:322:ARG:HA	1.89	0.53
1:Y:71:ILE:O	1:Y:156:ASN:ND2	2.41	0.53
1:a:111:HIS:HB3	1:b:328:LEU:HD21	1.89	0.53
1:C:100:CYS:HB2	1:C:145:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:151:ASP:HA	2:M:191:VAL:HB	1.91	0.53
1:Q:52:CYS:O	1:Q:88:TYR:OH	2.22	0.53
1:b:122:SER:HB2	1:b:265:PHE:HB3	1.90	0.53
1:C:107:ASP:OD2	1:I:73:LEU:HD22	2.09	0.53
2:J:187:GLU:OE1	2:J:187:GLU:O	2.26	0.53
3:X:13:LYS:CD	3:X:121:SER:HA	2.32	0.53
1:a:100:VAL:HG13	1:b:324:LEU:HD23	1.90	0.53
1:Y:39:SER:OG	1:Y:322:ARG:HD3	2.09	0.53
1:a:70:PHE:HB2	1:a:78:GLU:HB2	1.91	0.53
2:J:33:LEU:HD22	2:J:90:GLN:HG2	1.91	0.53
1:V:171:LYS:HA	1:V:251:PHE:O	2.09	0.53
1:b:91:GLU:CG	1:b:277:ARG:HG2	2.38	0.53
1:b:112:ARG:NH2	1:b:277:ARG:HD3	2.24	0.53
2:D:139:PHE:HE1	2:D:142:ARG:HA	1.74	0.53
3:E:61:PRO:HB3	3:E:64:ARG:HH21	1.74	0.53
3:E:146:LEU:HD22	3:E:219:VAL:HG12	1.90	0.53
2:J:115:VAL:HA	2:J:135:LEU:O	2.09	0.53
1:V:69:GLY:HA3	1:V:98:GLY:HA2	1.90	0.53
1:V:316:VAL:HG12	1:V:318:SER:H	1.74	0.53
1:b:64:ASP:HA	1:b:97:ASN:O	2.09	0.53
3:N:6:GLU:OE2	3:N:95:CYS:N	2.38	0.52
2:W:2:ILE:HG22	2:W:4:MET:SD	2.50	0.52
1:b:54:ILE:HG21	1:b:286:ASN:HA	1.90	0.52
2:c:94:TYR:OH	3:d:50:ARG:NH1	2.42	0.52
3:d:71:VAL:HG22	3:d:78:PHE:HB3	1.90	0.52
1:Q:142:THR:N	1:Q:152:SER:O	2.42	0.52
1:U:97:GLU:OE1	1:a:58:LYS:NZ	2.31	0.52
1:a:42:GLN:OE1	2:c:32:TRP:NE1	2.43	0.52
1:H:76:ARG:NH2	1:I:69:GLU:H	2.06	0.52
2:J:108:ARG:NE	2:J:171:SER:HB2	2.24	0.52
3:N:38:ARG:HB3	3:N:48:ILE:HD11	1.91	0.52
1:Q:251:PHE:HB3	1:Q:257:PHE:HZ	1.74	0.52
1:V:59:PRO:HB3	1:V:88:TYR:CD1	2.44	0.52
2:W:149:LYS:HB3	2:W:193:ALA:HB3	1.92	0.52
2:c:187:GLU:O	2:c:188:LYS:C	2.51	0.52
2:D:145:LYS:HB2	2:D:197:THR:OG1	2.10	0.52
2:J:144:ALA:HB2	2:J:198:HIS:HD2	1.74	0.52
2:W:50:LYS:HA	2:W:50:LYS:HE3	1.90	0.52
2:W:172:THR:O	2:W:173:TYR:C	2.50	0.52
1:Y:180:ARG:HD2	1:Y:265:GLU:OE2	2.09	0.52
2:c:29:ILE:HA	2:c:92:ASN:ND2	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:32:TRP:HZ3	2:c:50:LYS:HE2	1.73	0.52
2:D:108:ARG:HE	2:D:171:SER:HB2	1.75	0.52
1:V:288:CYS:O	1:V:294:ALA:HA	2.10	0.52
1:V:289:GLN:HG3	1:V:294:ALA:HB2	1.92	0.52
2:W:183:LYS:HG3	2:W:183:LYS:O	2.09	0.52
2:c:35:TRP:O	2:c:47:LEU:N	2.36	0.52
3:E:70:SER:OG	3:E:79:SER:OG	2.28	0.52
1:L:53:SER:HB2	1:L:56:GLY:O	2.10	0.52
1:P:77:ILE:CG2	1:U:77:ILE:HD12	2.40	0.52
3:X:59:TYR:HB2	3:X:64:ARG:HD3	1.91	0.52
1:b:102:PRO:HB3	1:b:230:VAL:HB	1.91	0.52
3:d:150:VAL:HG11	3:d:158:VAL:HG21	1.91	0.52
2:D:91:TYR:HA	2:D:96:TRP:CD1	2.45	0.52
2:M:155:GLN:HE22	2:M:179:LEU:HD13	1.75	0.52
2:R:80:PRO:HG3	2:R:108:ARG:HH22	1.74	0.52
2:M:144:ALA:HB2	2:M:198:HIS:CD2	2.43	0.52
3:S:97:ARG:H	3:S:111:TRP:CD1	2.28	0.52
2:W:58:VAL:O	2:W:59:PRO:C	2.53	0.52
1:C:120:GLU:HB3	1:C:266:ILE:HG23	1.91	0.52
2:D:113:PRO:HB3	2:D:139:PHE:HB3	1.92	0.52
3:E:90:THR:HG22	3:E:119:VAL:H	1.74	0.52
1:Q:303:ASN:ND2	1:Q:318:SER:O	2.43	0.52
1:B:21:TRP:CH2	1:C:326:GLY:HA3	2.44	0.52
1:L:44:GLU:CD	1:L:295:ILE:HD11	2.35	0.52
2:M:13:ALA:HA	2:M:107:LYS:HE2	1.91	0.52
2:M:186:TYR:HD1	2:M:192:TYR:OH	1.92	0.52
1:V:314:LYS:HG2	1:V:315:TYR:N	2.24	0.52
1:Y:273:LYS:NZ	1:Y:308:THR:H	2.08	0.52
1:C:29:LEU:HD12	1:C:30:LEU:N	2.25	0.51
3:S:213:THR:HG22	3:S:215:VAL:HG23	1.91	0.51
2:W:21:ILE:HD12	2:W:35:TRP:CZ3	2.45	0.51
2:W:34:ALA:HB1	2:W:35:TRP:HD1	1.75	0.51
2:W:208:SER:O	3:X:138:SER:OG	2.27	0.51
1:Y:144:ALA:O	1:Y:146:LYS:HG3	2.08	0.51
1:b:62:LEU:HG	1:b:80:LEU:HD21	1.92	0.51
1:C:180:ARG:NH1	1:C:267:VAL:HG13	2.25	0.51
1:C:244:LYS:HB3	1:C:245:PRO:HD2	1.91	0.51
1:L:244:LYS:HB3	1:L:245:PRO:HD2	1.91	0.51
1:Q:53:SER:HB2	1:Q:59:PRO:HD3	1.91	0.51
2:R:96:TRP:HB2	3:S:47:TRP:CD1	2.44	0.51
2:W:32:TRP:CB	2:W:91:TYR:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LYS:NZ	1:C:282:GLU:HB3	2.25	0.51
1:L:222:GLU:HB3	1:Y:218:ARG:HD3	1.91	0.51
1:Q:112:ARG:HG2	1:Q:112:ARG:HH11	1.75	0.51
1:V:222:GLU:HB3	1:b:219:ARG:HD3	1.93	0.51
2:W:6:GLN:OE1	2:W:99:GLY:HA3	2.03	0.51
3:d:171:VAL:HG22	3:d:190:VAL:HG22	1.93	0.51
2:D:166:GLN:HG2	2:D:171:SER:HA	1.92	0.51
1:I:11:GLU:HG2	1:I:12:GLY:H	1.75	0.51
1:I:54:SER:HB2	1:L:29:LEU:CD1	2.39	0.51
2:J:36:TYR:CZ	2:J:46:LEU:HD13	2.45	0.51
2:M:35:TRP:CE2	2:M:73:LEU:HB2	2.45	0.51
2:M:80:PRO:HG3	2:M:108:ARG:HH22	1.76	0.51
3:N:155:PRO:HG3	3:N:210:PRO:HG2	1.92	0.51
1:P:102:LEU:HD21	1:Q:29:LEU:HD22	1.93	0.51
3:S:6:GLU:OE2	3:S:95:CYS:N	2.41	0.51
1:a:108:LEU:HD13	1:b:329:ARG:HE	1.75	0.51
1:B:148:CYS:O	1:B:152:VAL:HG23	2.09	0.51
3:E:69:MET:HE2	3:E:80:LEU:HD13	1.91	0.51
1:Q:36:VAL:HA	1:Q:328:ARG:HA	1.92	0.51
1:Q:235:ARG:NH2	1:V:213:GLU:HA	2.24	0.51
1:b:91:GLU:OE1	1:b:277:ARG:HB3	2.10	0.51
1:C:119:LEU:O	1:C:268:SER:HB2	2.11	0.51
3:E:171:VAL:HG22	3:E:190:VAL:HG22	1.93	0.51
2:J:142:ARG:HH21	2:J:165:GLU:HA	1.76	0.51
1:L:102:PRO:HG3	1:L:229:VAL:HB	1.92	0.51
1:P:90:ASP:OD1	1:Q:317:LYS:NZ	2.32	0.51
1:V:226:ARG:HD2	1:V:235:ARG:HG2	1.93	0.51
1:H:41:THR:O	1:H:45:ILE:HG13	2.11	0.51
2:J:185:ASP:O	2:J:186:TYR:C	2.54	0.51
2:J:197:THR:HG22	2:J:204:PRO:HB3	1.92	0.51
2:R:166:GLN:CG	2:R:171:SER:HA	2.40	0.51
1:Y:141:VAL:HG11	1:Y:152:SER:HA	1.92	0.51
1:C:115:PHE:HA	1:C:118:VAL:HG12	1.91	0.51
1:Q:227:PRO:HG2	1:V:248:SER:O	2.10	0.51
1:Q:290:THR:OG1	1:Q:293:GLY:O	2.24	0.51
2:D:2:ILE:HB	2:D:90:GLN:HE22	1.75	0.51
1:V:188:ILE:HD13	1:V:219:PHE:HB2	1.92	0.51
1:Y:110:GLU:O	1:Y:114:LYS:HG2	2.11	0.51
2:D:160:GLN:HB3	3:E:177:VAL:HG11	1.92	0.51
1:L:51:LEU:HB2	1:L:280:SER:O	2.10	0.51
3:N:66:ARG:HD2	3:N:83:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:47:TRP:O	3:S:60:ASN:HB2	2.11	0.51
2:J:6:GLN:HG2	2:J:102:THR:CG2	2.41	0.50
3:K:213:THR:HG22	3:K:215:VAL:HG23	1.92	0.50
2:M:117:ILE:HG12	2:M:194:CYS:SG	2.52	0.50
1:b:144:ALA:HB1	1:b:147:LYS:HE3	1.93	0.50
1:L:302:GLN:HG3	1:L:313:PRO:HB2	1.93	0.50
1:P:83:LYS:NZ	1:U:85:ASP:OD1	2.38	0.50
1:P:91:ILE:HD13	1:U:91:ILE:HD13	1.92	0.50
1:Q:86:TRP:CZ2	1:Q:115:PHE:CE1	2.99	0.50
3:S:38:ARG:CD	3:S:91:ALA:HB3	2.35	0.50
1:L:188:ILE:HD13	1:L:219:PHE:HB2	1.94	0.50
1:H:148:CYS:O	1:H:152:VAL:HG23	2.12	0.50
1:P:58:LYS:NZ	1:a:97:GLU:OE1	2.40	0.50
1:V:41:ASN:ND2	1:V:322:ARG:NH2	2.60	0.50
1:V:273:LYS:NZ	1:V:308:THR:O	2.37	0.50
2:W:136:LEU:HB2	2:W:175:LEU:O	2.10	0.50
2:W:159:SER:HA	2:W:180:THR:H	1.76	0.50
1:a:102:LEU:HA	1:b:29:LEU:HD23	1.93	0.50
1:B:7:ALA:N	1:H:113:SER:HB2	2.26	0.50
2:D:49:TYR:C	2:D:51:ALA:N	2.69	0.50
1:L:101:TYR:HE2	1:L:236:MET:HG3	1.75	0.50
2:M:124:GLN:CD	3:N:151:LYS:HZ3	2.19	0.50
1:P:23:GLY:HA3	1:P:36:ALA:HA	1.94	0.50
1:Q:192:ALA:HB1	1:Q:225:THR:HA	1.94	0.50
2:R:142:ARG:HH21	2:R:165:GLU:HA	1.77	0.50
1:V:48:ASN:ND2	1:V:52:CYS:SG	2.84	0.50
2:W:210:ASN:HB2	3:X:137:LYS:NZ	2.27	0.50
1:a:68:LYS:HB2	1:a:70:PHE:CE2	2.46	0.50
3:E:149:LEU:HD13	3:E:151:LYS:NZ	2.27	0.50
1:L:44:GLU:HG2	1:L:297:THR:HG21	1.94	0.50
1:L:60:ILE:HD13	1:L:83:LYS:HB3	1.94	0.50
2:M:3:GLN:HB2	2:M:26:SER:HB3	1.93	0.50
1:Q:180:ARG:NH1	1:Q:267:VAL:HG13	2.26	0.50
1:Q:289:GLN:NE2	1:Q:290:THR:O	2.45	0.50
2:W:38:GLN:HB3	2:W:85:ILE:HB	1.92	0.50
1:b:181:ARG:NH1	1:b:268:VAL:HG13	2.27	0.50
2:D:80:PRO:HG3	2:D:108:ARG:HH22	1.76	0.50
3:K:171:VAL:HG22	3:K:190:VAL:HG22	1.93	0.50
1:L:56:GLY:C	1:L:58:GLN:N	2.69	0.50
2:M:38:GLN:O	2:M:84:ALA:HB1	2.11	0.50
3:N:11:LEU:HG	3:N:155:PRO:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD11	1:C:317:LYS:HG2	1.94	0.50
2:J:189:HIS:CG	2:J:190:LYS:H	2.30	0.50
2:M:115:VAL:HB	2:M:207:LYS:HE3	1.94	0.50
1:Q:43:LEU:HB2	1:Q:321:LEU:HB2	1.94	0.50
1:V:44:GLU:OE1	1:V:297:THR:HG21	2.11	0.50
2:W:29:ILE:O	2:W:90:GLN:NE2	2.45	0.50
2:W:164:THR:HG23	3:X:174:PHE:CD1	2.47	0.50
2:c:108:ARG:HE	2:c:171:SER:HB2	1.76	0.50
1:C:71:ILE:O	1:C:156:ASN:ND2	2.43	0.50
1:L:84:THR:O	1:L:86:TRP:CZ3	2.65	0.50
1:L:137:SER:HA	1:L:160:LEU:HD23	1.92	0.50
1:Y:40:VAL:C	1:Y:322:ARG:HG3	2.37	0.50
1:Y:182:VAL:HB	1:Y:243:VAL:CG1	2.42	0.50
1:b:115:PHE:HB2	1:b:274(A):LYS:CA	2.40	0.50
1:C:53:SER:OG	1:C:57:LYS:O	2.30	0.49
3:E:39:GLN:CD	3:E:43:LYS:O	2.55	0.49
2:W:158:ASN:ND2	2:W:180:THR:O	2.45	0.49
1:B:111:HIS:HB3	1:C:327:LEU:HD21	1.94	0.49
1:C:79:ASP:OD1	1:C:79:ASP:N	2.45	0.49
2:M:135:LEU:HD22	3:N:189:VAL:HG11	1.94	0.49
2:M:162:SER:OG	2:M:176:SER:OG	2.29	0.49
2:R:155:GLN:NE2	2:R:179:LEU:HD13	2.26	0.49
2:W:48:ILE:HG13	2:W:53:SER:O	2.13	0.49
1:C:86:TRP:O	1:C:119:LEU:HD11	2.13	0.49
1:C:287:THR:OG1	1:C:296:ASN:HA	2.12	0.49
1:H:21:TRP:HH2	1:L:326:GLY:CA	2.25	0.49
1:H:92:TRP:CG	1:L:314:LYS:HZ1	2.29	0.49
1:Q:74:ASN:OD1	1:Q:75:PRO:HD2	2.13	0.49
3:S:162:TRP:HB3	3:S:167:LEU:HB2	1.93	0.49
1:b:41:ASN:N	1:b:323:ARG:HG3	2.27	0.49
3:d:11:LEU:HD23	3:d:118:THR:HB	1.93	0.49
1:I:61:THR:HG21	1:Y:314:LYS:NZ	2.27	0.49
2:J:50:LYS:C	2:J:52:SER:H	2.19	0.49
1:L:62:LEU:HD22	1:L:80:LEU:HD13	1.93	0.49
2:M:33:LEU:HD12	2:M:90:GLN:HG2	1.94	0.49
2:R:96:TRP:O	3:S:47:TRP:HB2	2.12	0.49
1:V:129:SER:HB3	1:V:158:VAL:HG21	1.93	0.49
3:X:162:TRP:CE2	3:X:190:VAL:HG23	2.48	0.49
2:c:80:PRO:HG3	2:c:108:ARG:HH22	1.78	0.49
3:d:38:ARG:HB2	3:d:48:ILE:HD11	1.95	0.49
1:C:89:ILE:HB	1:C:274:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PHE:H	1:C:267:VAL:HB	1.78	0.49
1:C:161:ILE:HG22	1:C:162:HIS:CD2	2.48	0.49
1:C:218:ARG:HD3	1:Y:222:GLU:HA	1.94	0.49
3:E:213:THR:HG22	3:E:215:VAL:HG23	1.94	0.49
3:N:71:VAL:HG22	3:N:78:PHE:HB3	1.95	0.49
3:S:111:TRP:HA	3:S:111:TRP:CE3	2.47	0.49
1:U:42:GLN:HE22	2:W:32:TRP:HD1	1.60	0.49
1:V:292:LYS:HG2	1:V:305:HIS:NE2	2.27	0.49
2:D:4:MET:HE1	2:D:23:CYS:SG	2.53	0.49
1:I:13:GLY:N	1:Y:330:VAL:HG23	2.28	0.49
2:M:35:TRP:CZ3	2:M:88:CYS:HB3	2.48	0.49
1:P:70:PHE:HE1	1:a:77:ILE:HG23	1.77	0.49
1:Q:137:SER:HA	1:Q:160:LEU:HD23	1.93	0.49
1:Q:142:THR:HG22	1:Q:145:CYS:H	1.78	0.49
2:R:38:GLN:O	2:R:84:ALA:HB1	2.12	0.49
1:b:119:LEU:HB3	1:b:269:SER:C	2.38	0.49
3:d:6:GLU:OE2	3:d:95:CYS:N	2.43	0.49
3:d:39:GLN:HB2	3:d:45:LEU:HD23	1.95	0.49
1:L:216:ASN:CA	1:L:218:ARG:NH2	2.72	0.49
1:Q:82:GLY:H	1:Q:123:LYS:NZ	2.09	0.49
1:Q:226:ARG:HH21	1:Q:235:ARG:N	2.11	0.49
2:R:36:TYR:CZ	2:R:46:LEU:HD13	2.48	0.49
3:S:47:TRP:CZ3	3:S:49:GLY:HA2	2.47	0.49
3:S:171:VAL:HG22	3:S:190:VAL:HG22	1.94	0.49
1:U:22:TYR:H	1:U:41:THR:HG22	1.75	0.49
1:V:109:GLU:HG2	1:V:112:ARG:NH2	2.28	0.49
2:W:34:ALA:CB	2:W:51:ALA:HA	2.40	0.49
2:c:36:TYR:CZ	2:c:46:LEU:HD13	2.48	0.49
1:C:157:MET:CE	1:C:186:TRP:HA	2.43	0.49
1:L:41:ASN:HA	1:L:322:ARG:HG2	1.95	0.49
3:S:155:PRO:HB2	3:S:210:PRO:HG2	1.95	0.49
2:W:58:VAL:N	2:W:59:PRO:HD2	2.28	0.49
1:Y:47:HIS:HB3	1:Y:304:ILE:HG23	1.94	0.49
1:Y:54:ILE:HG23	1:Y:55:ASN:H	1.78	0.49
3:d:12:VAL:HG21	3:d:18:LEU:HD13	1.95	0.49
1:B:77:ILE:CG2	1:I:77:ILE:HG12	2.36	0.49
3:N:127:PRO:HA	3:N:152:ASP:O	2.13	0.49
3:N:213:THR:HG22	3:N:215:VAL:HG23	1.95	0.49
3:K:33:TYR:CD2	3:K:52:TYR:HB2	2.48	0.49
1:L:86:TRP:HZ2	1:L:118:VAL:HG11	1.77	0.49
2:R:34:ALA:HB3	2:R:89:GLN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:59:MET:SD	1:V:301:PHE:HZ	2.36	0.49
1:V:173:THR:HA	1:V:249:ILE:O	2.13	0.49
1:I:51:LYS:HG3	1:L:29:LEU:HD21	1.94	0.48
1:b:102:PRO:HB2	1:b:236:ARG:HD3	1.95	0.48
1:B:52:VAL:HG22	1:C:323:LEU:HD21	1.95	0.48
1:C:209:ALA:HB1	1:Y:224:SER:HB3	1.94	0.48
2:J:39:LYS:HB2	2:J:42:LYS:HD3	1.95	0.48
1:L:86:TRP:O	1:L:119:LEU:HD12	2.13	0.48
1:Q:226:ARG:HE	1:Q:235:ARG:HG2	1.78	0.48
1:V:44:GLU:OE2	1:V:297:THR:OG1	2.30	0.48
2:W:64:GLY:HA2	2:W:73:LEU:HA	1.94	0.48
2:W:89:GLN:OE1	2:W:91:TYR:CZ	2.65	0.48
3:X:48:ILE:HA	3:X:63:LEU:HD21	1.95	0.48
1:Y:135:VAL:O	1:Y:136:ASN:C	2.54	0.48
2:D:96:TRP:CZ2	3:E:50:ARG:NH1	2.81	0.48
2:J:80:PRO:HG3	2:J:108:ARG:HH22	1.78	0.48
1:U:38:LEU:O	1:U:42:GLN:HB2	2.13	0.48
1:Y:236:MET:HE2	1:Y:258:LEU:HD11	1.95	0.48
2:c:33:LEU:HB2	2:c:51:ALA:HB2	1.93	0.48
2:J:108:ARG:HE	2:J:171:SER:HB2	1.78	0.48
1:L:210:VAL:N	1:L:218:ARG:NH1	2.58	0.48
1:V:188:ILE:HD12	1:V:239:TYR:CE2	2.49	0.48
1:H:25:HIS:HB3	1:L:14:CYS:HB2	1.95	0.48
1:H:76:ARG:CZ	1:Y:109:GLU:HB3	2.42	0.48
1:L:123:LYS:HE2	1:L:264:PHE:HE1	1.79	0.48
1:L:141:VAL:HG12	1:L:152:SER:HA	1.95	0.48
1:Q:288:CYS:HB2	1:Q:295:ILE:O	2.14	0.48
2:W:192:TYR:HB2	2:W:209:PHE:O	2.14	0.48
1:Y:121:PHE:HA	1:Y:267:VAL:H	1.77	0.48
1:Y:121:PHE:CE2	1:Y:264:PHE:HD1	2.31	0.48
1:a:164:GLU:HA	1:a:167:LYS:HB2	1.96	0.48
1:b:84:THR:O	1:b:121:PHE:N	2.35	0.48
1:L:75:PRO:HG3	1:L:153:PHE:O	2.14	0.48
3:S:109:ARG:H	3:S:111:TRP:HE1	1.61	0.48
1:V:299:LEU:HB3	1:V:300:PRO:HD2	1.95	0.48
2:W:4:MET:HE3	2:W:23:CYS:SG	2.54	0.48
2:W:194:CYS:O	2:W:206:THR:HA	2.13	0.48
3:X:12:VAL:HG21	3:X:18:LEU:HD13	1.96	0.48
2:c:136:LEU:HD21	2:c:196:VAL:HG13	1.95	0.48
1:I:92:TRP:CD1	1:Y:314:LYS:HZ1	2.31	0.48
3:K:204:CYS:O	3:K:216:ASP:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:69:MET:HG2	3:N:80:LEU:HD23	1.96	0.48
2:R:2:ILE:HD11	2:R:93:SER:HB2	1.95	0.48
3:X:142:GLY:O	3:X:193:PRO:HA	2.14	0.48
1:a:69:GLU:OE2	1:b:112:ARG:NH1	2.47	0.48
3:d:3:GLN:HB2	3:d:25:SER:OG	2.14	0.48
1:B:122:VAL:HG21	1:C:15:ILE:HD11	1.95	0.48
1:C:109:GLU:HB3	1:I:76:ARG:NH1	2.28	0.48
2:M:108:ARG:HE	2:M:171:SER:CB	2.26	0.48
1:V:135:VAL:C	1:V:163:GLN:HB2	2.38	0.48
1:B:74:GLU:HA	1:B:77:ILE:HD13	1.96	0.48
3:K:71:VAL:HG22	3:K:78:PHE:HB3	1.96	0.48
1:L:59:PRO:HG3	1:L:88:TYR:CE1	2.49	0.48
1:L:169:VAL:HG22	1:L:254:ASN:HB3	1.95	0.48
1:L:183:LEU:HD11	1:L:240:TRP:HB2	1.95	0.48
3:N:38:ARG:HH21	3:N:91:ALA:HB3	1.78	0.48
3:S:29:ILE:HG23	3:S:34:TRP:CD1	2.49	0.48
1:U:94:TYR:HE2	1:a:95:ASN:HB3	1.79	0.48
1:V:75:PRO:HG3	1:V:153:PHE:O	2.14	0.48
1:b:66:SER:OG	1:b:96:THR:HG22	2.14	0.48
1:Q:222:GLU:HA	1:V:218:ARG:HD3	1.96	0.48
3:S:47:TRP:O	3:S:47:TRP:CE3	2.67	0.48
1:V:111:LEU:HG	1:V:115:PHE:CE2	2.49	0.48
2:W:61:ARG:NH1	2:W:82:ASP:OD1	2.44	0.48
2:W:189:HIS:CD2	2:W:189:HIS:H	2.32	0.48
3:X:162:TRP:HB3	3:X:167:LEU:HB2	1.96	0.48
1:Y:105:LEU:O	1:Y:108:GLU:HB3	2.13	0.48
2:J:136:LEU:HD21	2:J:196:VAL:HG13	1.96	0.47
3:N:171:VAL:HG22	3:N:190:VAL:HG22	1.96	0.47
2:R:198:HIS:HB3	2:R:201:LEU:HG	1.96	0.47
2:W:23:CYS:HB2	2:W:35:TRP:CH2	2.49	0.47
3:X:167:LEU:HD11	3:X:202:TYR:HD1	1.78	0.47
1:Y:188:ILE:HD12	1:Y:239:TYR:CE1	2.48	0.47
1:C:213:GLU:C	1:Y:235:ARG:HH22	2.22	0.47
3:E:11:LEU:HD23	3:E:118:THR:HB	1.94	0.47
1:P:21:TRP:CD1	1:P:41:THR:HG23	2.44	0.47
3:S:152:ASP:HA	3:S:183:LEU:HD13	1.96	0.47
1:V:86:TRP:HE3	1:V:87:SER:C	2.22	0.47
1:B:80:LEU:HD13	1:H:81:ASN:HA	1.96	0.47
1:C:217:ARG:HH21	1:C:219:PHE:HE1	1.61	0.47
1:H:59:MET:HE3	1:L:301:PHE:HZ	1.79	0.47
2:J:87:TYR:HE2	3:K:44:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:25:ALA:CB	2:M:90:GLN:HE22	2.27	0.47
3:K:162:TRP:HB3	3:K:167:LEU:HD12	1.96	0.47
2:W:131:SER:HB2	2:W:181:LEU:O	2.13	0.47
1:b:289:CYS:HB2	1:b:296:ILE:O	2.14	0.47
1:H:22:TYR:H	1:H:41:THR:HG21	1.80	0.47
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.95	0.47
1:L:66:SER:HB3	1:L:95:PRO:HG3	1.95	0.47
1:L:91:GLU:O	1:L:276:ARG:HA	2.15	0.47
2:W:142:ARG:HB2	2:W:175:LEU:HD11	1.95	0.47
3:X:146:LEU:HB3	3:X:219:VAL:HG11	1.97	0.47
1:a:133:ILE:HD12	1:a:139:GLU:HB3	1.96	0.47
3:E:205:ASN:HA	3:E:216:ASP:OD1	2.15	0.47
1:L:59:PRO:HD3	1:L:87:SER:CB	2.37	0.47
1:Q:224:SER:HB3	1:Q:226:ARG:NH1	2.28	0.47
2:W:163:VAL:HG22	2:W:175:LEU:HD22	1.97	0.47
2:c:30:SER:HB3	2:c:32:TRP:CD1	2.50	0.47
2:c:135:LEU:HD22	3:d:189:VAL:HG11	1.95	0.47
1:C:156:ASN:HA	1:C:262:TYR:HD2	1.79	0.47
1:C:159:TRP:HZ2	1:C:200:LEU:HD13	1.78	0.47
1:C:180:ARG:HH12	1:C:267:VAL:HG13	1.80	0.47
3:K:97:ARG:NH2	3:K:99:GLU:OE1	2.48	0.47
1:Q:88:TYR:C	1:Q:89:ILE:HG13	2.40	0.47
3:S:38:ARG:HD3	3:S:93:TYR:CZ	2.48	0.47
3:S:142:GLY:O	3:S:194:SER:N	2.48	0.47
3:S:157:PRO:HG2	3:S:210:PRO:HD3	1.96	0.47
1:U:9:PHE:HE2	1:U:12:GLY:HA3	1.80	0.47
1:U:10:ILE:HG22	1:U:11:GLU:HG2	1.97	0.47
1:V:108:GLU:O	1:V:112:ARG:HG3	2.15	0.47
1:Y:275:PHE:HE2	1:Y:289:GLN:HG3	1.79	0.47
1:a:131:LYS:HE3	1:a:141:TYR:CE1	2.50	0.47
1:b:51:LEU:HD12	1:b:290:GLN:OE1	2.14	0.47
1:B:77:ILE:HG21	1:I:77:ILE:CG1	2.38	0.47
1:Q:26:VAL:HG12	1:Q:322:ARG:HB3	1.96	0.47
1:U:13:GLY:HA3	1:V:330:VAL:O	2.15	0.47
2:W:23:CYS:HB3	2:W:35:TRP:CZ2	2.50	0.47
2:W:32:TRP:HB3	2:W:91:TYR:HB2	1.95	0.47
2:W:123:GLU:HA	2:W:126:LYS:HD2	1.97	0.47
2:W:147:GLN:HB3	2:W:154:LEU:HD21	1.96	0.47
1:Y:56:GLY:H	1:Y:285:ASN:HB3	1.80	0.47
1:b:273:GLY:C	1:b:274(A):LYS:HG3	2.36	0.47
2:D:142:ARG:HG3	2:D:173:TYR:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:156:GLU:N	3:K:157:PRO:HD2	2.29	0.47
1:L:188:ILE:HG12	1:L:208:VAL:HG21	1.97	0.47
2:M:148:TRP:O	2:M:154:LEU:HA	2.14	0.47
1:U:77:ILE:HG23	1:a:70:PHE:CE1	2.50	0.47
2:W:117:ILE:H	3:X:135:SER:HB3	1.79	0.47
1:a:100:VAL:HG21	1:b:322:LEU:HD22	1.96	0.47
1:b:66:SER:O	1:b:91:GLU:HG2	2.15	0.47
1:B:94:TYR:OH	1:H:59:MET:SD	2.63	0.47
3:E:36:TRP:CB	3:E:48:ILE:HD12	2.42	0.47
2:J:33:LEU:CD2	2:J:90:GLN:HG2	2.45	0.47
3:N:127:PRO:HB2	3:N:150:VAL:HG13	1.97	0.47
1:Q:26:VAL:HG21	1:Q:324:ALA:HB2	1.97	0.47
1:Q:110:GLU:OE2	1:a:73:LEU:HA	2.15	0.47
1:Q:140:GLY:HA2	1:Q:159:TRP:HB3	1.97	0.47
2:R:29:ILE:HG21	2:R:33:LEU:HD23	1.97	0.47
2:W:21:ILE:HG13	2:W:21:ILE:O	2.15	0.47
2:W:33:LEU:HD22	2:W:91:TYR:CE2	2.45	0.47
2:W:83:PHE:CD1	2:W:105:GLU:HA	2.50	0.47
1:Y:187:GLY:HA3	1:Y:258:LEU:HD12	1.96	0.47
1:C:57:LYS:HE3	1:C:57:LYS:HB2	1.75	0.46
1:C:108:GLU:O	1:C:112:ARG:HG3	2.15	0.46
2:D:1:ASP:HB3	2:D:2:ILE:HD12	1.96	0.46
2:D:36:TYR:CZ	2:D:46:LEU:HD13	2.50	0.46
1:U:111:HIS:HB3	1:V:327:LEU:HD21	1.96	0.46
2:W:114:SER:OG	2:W:137:ASN:HB2	2.14	0.46
1:a:163:SER:O	1:a:167:LYS:CD	2.63	0.46
1:b:181:ARG:HH12	1:b:268:VAL:HG13	1.78	0.46
1:B:131:LYS:HB2	1:B:141:TYR:CZ	2.50	0.46
1:I:125:GLN:OE1	1:I:155:GLY:HA2	2.15	0.46
1:L:101:TYR:CD1	1:L:232:GLN:HG3	2.50	0.46
3:N:159:THR:HG23	3:N:209:LYS:HE3	1.98	0.46
1:U:133:ILE:CG2	1:U:137:CYS:HB2	2.45	0.46
2:W:139:PHE:HZ	2:W:175:LEU:HB2	1.81	0.46
1:Y:53:SER:O	1:Y:286:THR:HG22	2.15	0.46
1:b:41:ASN:HB2	1:b:323:ARG:CZ	2.45	0.46
1:b:63:GLY:O	1:b:66:SER:HB3	2.14	0.46
2:D:132:VAL:HG12	2:D:148:TRP:HH2	1.79	0.46
3:K:142:GLY:O	3:K:194:SER:N	2.37	0.46
1:L:74:ASN:ND2	1:L:100:CYS:SG	2.88	0.46
1:L:85(A):SER:HA	1:L:120:GLU:HG3	1.98	0.46
2:R:94:TYR:OH	3:S:50:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:183:LEU:HD11	1:V:240:TRP:HB2	1.96	0.46
2:W:113:PRO:HB2	2:W:136:LEU:HD22	1.97	0.46
1:b:88:TYR:HB2	1:b:274(A):LYS:O	2.15	0.46
1:b:172:LYS:HA	1:b:252:PHE:O	2.16	0.46
1:b:245:LYS:HB3	1:b:246:PRO:HD2	1.97	0.46
1:C:288:CYS:HB3	1:C:295:ILE:HG13	1.96	0.46
3:E:204:CYS:O	3:E:216:ASP:HA	2.14	0.46
1:I:42:GLN:OE1	2:J:32:TRP:NE1	2.48	0.46
1:L:121:PHE:CD1	1:L:266:ILE:HA	2.51	0.46
3:S:99:GLU:OE2	3:S:111:TRP:CZ2	2.68	0.46
1:Y:186:TRP:HH2	1:Y:241:THR:HG23	1.81	0.46
1:b:53:SER:HB3	1:b:290:GLN:HE22	1.79	0.46
2:c:197:THR:HG22	2:c:204:PRO:HB3	1.97	0.46
1:C:188:ILE:HD13	1:C:219:PHE:HB2	1.98	0.46
1:Q:86:TRP:CD2	1:Q:89:ILE:HD11	2.51	0.46
1:Q:188:ILE:HD12	1:Q:239:TYR:CE1	2.50	0.46
1:Y:302:GLN:O	1:Y:315:TYR:HA	2.14	0.46
1:b:112:ARG:C	1:b:114:LYS:H	2.23	0.46
1:C:84:THR:HG21	1:C:123:LYS:HG3	1.98	0.46
1:C:188:ILE:HG12	1:C:208:VAL:HG21	1.98	0.46
3:E:153:TYR:CE1	3:E:184:TYR:HB2	2.51	0.46
1:L:123:LYS:HG2	1:L:264:PHE:CD1	2.51	0.46
3:N:159:THR:OG1	3:N:207:ASN:HB2	2.15	0.46
1:Q:20:ASN:O	1:Q:329:ASN:ND2	2.49	0.46
1:U:59:MET:HE3	1:V:301:PHE:HZ	1.79	0.46
1:V:135:VAL:HG11	1:V:160:LEU:HB3	1.98	0.46
3:X:69:MET:HG2	3:X:80:LEU:HD23	1.97	0.46
2:D:120:PRO:HB2	2:D:125:LEU:HD21	1.97	0.46
2:D:142:ARG:HH21	2:D:165:GLU:HA	1.81	0.46
1:H:91:ILE:HD13	1:I:91:ILE:HD13	1.96	0.46
3:K:134:PRO:HG3	3:K:221:PRO:HA	1.96	0.46
1:L:101:TYR:HD1	1:L:232:GLN:HG3	1.81	0.46
1:U:94:TYR:CZ	1:U:98:LEU:HD11	2.51	0.46
1:V:54:ILE:HA	1:V:286:THR:O	2.15	0.46
3:d:155:PRO:HG3	3:d:210:PRO:HB2	1.98	0.46
2:J:21:ILE:HG23	2:J:102:THR:HG21	1.98	0.46
3:K:69:MET:HG2	3:K:80:LEU:HD23	1.98	0.46
2:M:122:ASP:HA	2:M:125:LEU:HG	1.97	0.46
1:P:70:PHE:CE1	1:a:77:ILE:HG23	2.51	0.46
1:b:100:CYS:HB3	1:b:146:CYS:SG	2.56	0.46
3:d:150:VAL:HG12	3:d:153:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:CE3	2:D:73:LEU:HD22	2.50	0.46
1:P:77:ILE:HD12	1:a:77:ILE:CG2	2.46	0.46
1:P:125:GLN:OE1	1:P:155:GLY:HA2	2.15	0.46
2:W:108:ARG:HB3	2:W:140:TYR:CD2	2.50	0.46
2:D:132:VAL:HG12	2:D:148:TRP:CH2	2.51	0.46
3:S:14:PRO:HA	3:S:119:VAL:CG1	2.45	0.46
3:S:90:THR:HG23	3:S:118:THR:HA	1.97	0.46
3:X:93:TYR:CE1	3:X:117:VAL:HB	2.51	0.46
1:b:61:SER:C	1:b:62:LEU:O	2.36	0.46
1:B:119:TYR:HD1	1:C:15:ILE:HG13	1.80	0.45
1:C:226:ARG:HE	1:C:235:ARG:HG2	1.82	0.45
1:H:13:GLY:N	1:L:332:SER:HA	2.31	0.45
3:K:11:LEU:HD23	3:K:11:LEU:O	2.16	0.45
3:K:18:LEU:O	3:K:81:LYS:HA	2.17	0.45
2:M:150:VAL:HG22	2:M:192:TYR:HD1	1.80	0.45
1:P:89:LEU:HG	1:Q:317:LYS:HE3	1.99	0.45
1:Q:48:ASN:O	1:Q:293:GLY:HA3	2.15	0.45
2:R:130:ALA:HB1	2:R:186:TYR:CE2	2.51	0.45
1:V:43:LEU:HG	1:V:321:LEU:HB2	1.97	0.45
1:V:53:SER:CB	1:V:58:GLN:HG2	2.46	0.45
1:Y:52:CYS:HB3	1:Y:284:CYS:C	2.41	0.45
1:Y:209:ALA:CB	1:Y:218:ARG:HG2	2.46	0.45
5:O:1:NAG:H4	5:O:2:NAG:H2	1.61	0.45
3:E:11:LEU:HA	3:E:118:THR:O	2.17	0.45
1:L:273:LYS:HB2	1:L:309:ILE:HD11	1.98	0.45
3:N:51:PHE:CD1	3:N:57:PRO:HB3	2.49	0.45
3:S:38:ARG:HG2	3:S:39:GLN:N	2.31	0.45
1:V:129:SER:HB3	1:V:261:ARG:HD2	1.98	0.45
1:V:175:ASN:HA	1:V:248:SER:HB3	1.98	0.45
3:X:38:ARG:NH2	3:X:46:GLU:OE1	2.49	0.45
1:a:141:TYR:CZ	1:a:170:ARG:HG3	2.52	0.45
1:b:62:LEU:H	1:b:80:LEU:HD11	1.80	0.45
3:E:6:GLU:OE2	3:E:95:CYS:N	2.43	0.45
3:E:134:PRO:HD2	3:E:221:PRO:HA	1.97	0.45
2:M:184:ALA:O	2:M:187:GLU:HB2	2.15	0.45
1:Q:60:ILE:HD12	1:Q:86:TRP:CE3	2.51	0.45
1:Q:253:SER:HB3	1:Q:257:PHE:CD2	2.51	0.45
3:S:18:LEU:HD12	3:S:18:LEU:O	2.16	0.45
2:W:25:ALA:HB3	2:W:69:SER:HB2	1.99	0.45
2:W:57:GLY:O	2:W:58:VAL:C	2.59	0.45
3:X:93:TYR:O	3:X:114:GLY:HA2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:51:LEU:HD21	1:Y:279:LEU:HD22	1.97	0.45
1:a:68:LYS:H	1:a:81:ASN:ND2	2.14	0.45
1:a:100:VAL:HG22	1:b:324:LEU:HD21	1.97	0.45
1:b:91:GLU:CD	1:b:92:LYS:N	2.74	0.45
1:B:23:GLY:HA3	1:B:36:ALA:HA	1.99	0.45
3:E:33:TYR:HB2	3:E:98:GLU:HB3	1.99	0.45
3:E:66:ARG:HB3	3:E:82:LEU:HD12	1.97	0.45
1:I:61:THR:HG21	1:Y:314:LYS:HZ3	1.80	0.45
2:J:113:PRO:HB3	2:J:139:PHE:HB3	1.98	0.45
2:J:117:ILE:HG12	2:J:194:CYS:SG	2.55	0.45
2:R:129:THR:HA	2:R:182:SER:CB	2.47	0.45
3:S:47:TRP:HZ2	3:S:50:ARG:CD	2.29	0.45
2:W:66:GLY:HA3	2:W:71:PHE:HA	1.98	0.45
3:X:6:GLU:OE2	3:X:94:TYR:HA	2.16	0.45
1:a:18:VAL:HB	3:d:100:HIS:ND1	2.32	0.45
3:d:158:VAL:HG11	3:d:186:LEU:HD22	1.98	0.45
3:E:51:PHE:CD1	3:E:57:PRO:HB3	2.51	0.45
1:V:174:PHE:O	1:V:248:SER:HA	2.16	0.45
1:Y:207:TYR:OH	1:Y:252:GLU:OE2	2.24	0.45
1:Y:287:THR:CG2	1:Y:296:ASN:HA	2.47	0.45
1:b:42:LEU:HB3	1:b:301:PRO:HG2	1.98	0.45
1:b:148:PHE:N	1:b:151:SER:O	2.46	0.45
1:C:121:PHE:HB2	1:C:267:VAL:HG21	1.99	0.45
2:J:121:SER:HB3	3:K:130:PHE:HB3	1.98	0.45
2:M:136:LEU:HD21	2:M:196:VAL:HG13	1.97	0.45
2:R:2:ILE:HG23	2:R:27:GLN:HG2	1.97	0.45
3:X:149:LEU:HD13	3:X:151:LYS:CE	2.46	0.45
1:Y:165:GLY:C	1:Y:166:THR:HG1	2.25	0.45
1:b:54:ILE:HG12	1:b:287:THR:O	2.15	0.45
1:b:60:ILE:HD11	1:b:282:ILE:HB	1.97	0.45
1:b:115:PHE:HB2	1:b:275:LEU:N	2.31	0.45
2:c:38:GLN:O	2:c:84:ALA:HB1	2.17	0.45
1:L:47:HIS:HA	1:L:295:ILE:HG23	1.99	0.45
1:L:56:GLY:O	1:L:58:GLN:N	2.42	0.45
1:L:180:ARG:HD2	1:L:266:ILE:O	2.17	0.45
3:N:22:CYS:HB2	3:N:36:TRP:CZ2	2.52	0.45
3:N:150:VAL:HG12	3:N:153:TYR:CD2	2.52	0.45
1:b:124:PHE:N	1:b:264:ALA:O	2.50	0.45
1:C:113:LEU:HD22	1:I:76:ARG:HG2	1.99	0.45
1:C:236:MET:SD	1:C:258:LEU:HD11	2.57	0.45
3:E:162:TRP:HB3	3:E:167:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:32:TRP:HB3	2:M:91:TYR:CE1	2.51	0.45
3:N:122:ALA:HB3	3:N:154:PHE:CE2	2.51	0.45
1:P:70:PHE:CD2	1:P:78:GLU:HA	2.52	0.45
2:W:145:LYS:HB2	2:W:197:THR:OG1	2.17	0.45
1:Y:135:VAL:C	1:Y:163:GLN:HB2	2.42	0.45
3:d:29:ILE:HD12	3:d:76:ASN:HA	1.99	0.45
1:C:132:TRP:H	1:C:132:TRP:CD1	2.34	0.45
2:D:32:TRP:HZ3	2:D:50:LYS:HG3	1.82	0.45
2:J:98:PHE:CG	3:K:45:LEU:HB2	2.51	0.45
3:S:48:ILE:HD11	3:S:80:LEU:HD11	1.98	0.45
3:S:125:LYS:HB2	3:S:154:PHE:HD1	1.82	0.45
2:W:49:TYR:C	2:W:51:ALA:H	2.23	0.45
1:a:67:GLY:HA2	1:a:81:ASN:HD21	1.82	0.45
3:d:136:SER:HA	3:d:139:THR:HG23	1.99	0.45
3:d:157:PRO:HB2	3:d:210:PRO:HD3	1.98	0.45
3:E:140:SER:OG	3:E:143:THR:OG1	2.24	0.45
3:K:134:PRO:HA	3:K:146:LEU:HD23	1.98	0.45
1:Q:143:ALA:HA	1:Q:151:ASN:CG	2.42	0.45
1:Q:226:ARG:NH2	1:Q:234:GLY:HA2	2.32	0.45
2:W:8:PRO:HG2	2:W:11:LEU:HG	1.98	0.45
2:W:18:ARG:HG2	2:W:76:SER:HA	1.99	0.45
2:W:33:LEU:HG	2:W:49:TYR:CB	2.46	0.45
1:b:37:THR:N	1:b:328:LEU:O	2.41	0.45
2:c:3:GLN:HG3	2:c:4:MET:N	2.31	0.45
2:c:192:TYR:O	2:c:208:SER:HA	2.17	0.45
3:K:20:LEU:O	3:K:79:SER:HA	2.16	0.44
1:Q:43:LEU:HD21	1:Q:303:ASN:ND2	2.28	0.44
3:S:93:TYR:HE2	3:S:117:VAL:HB	1.82	0.44
3:X:132:LEU:HD21	3:X:149:LEU:CD1	2.47	0.44
1:Y:72:LEU:HD23	1:Y:185:VAL:HG11	1.98	0.44
3:d:69:MET:HG2	3:d:80:LEU:HD23	1.99	0.44
5:G:2:NAG:H4	5:G:3:BMA:H2	1.55	0.44
1:C:216:ASN:C	1:C:217:ARG:HG2	2.43	0.44
3:E:142:GLY:O	3:E:193:PRO:HA	2.18	0.44
1:I:13:GLY:H	1:Y:330:VAL:HG23	1.81	0.44
1:I:51:LYS:NZ	1:I:103:GLU:O	2.51	0.44
2:J:6:GLN:NE2	2:J:86:TYR:O	2.50	0.44
2:J:32:TRP:CZ3	2:J:50:LYS:HG3	2.47	0.44
2:J:191:VAL:C	2:J:192:TYR:CD1	2.95	0.44
3:K:208:HIS:CE1	3:K:211:SER:H	2.36	0.44
1:Q:191:PRO:O	1:Q:223:ILE:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:6:GLN:OE1	2:W:99:GLY:CA	2.64	0.44
2:W:124:GLN:HE22	3:X:151:LYS:NZ	2.14	0.44
1:Y:153:PHE:HZ	1:Y:258:LEU:HD13	1.82	0.44
1:b:147:LYS:HG2	1:b:152:ASN:HA	1.98	0.44
1:b:184:LEU:HD11	1:b:241:TRP:HB2	1.99	0.44
2:c:19:VAL:O	2:c:74:THR:HA	2.17	0.44
1:H:76:ARG:NH1	1:Y:109:GLU:CB	2.80	0.44
1:H:100:VAL:HG13	1:L:323:LEU:HD23	1.99	0.44
2:R:87:TYR:HE2	3:S:44:GLY:HA2	1.81	0.44
1:U:41:THR:O	1:U:45:ILE:HG13	2.17	0.44
3:d:146:LEU:HD22	3:d:219:VAL:HG12	2.00	0.44
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.80	0.44
3:E:122:ALA:HB3	3:E:154:PHE:CE2	2.52	0.44
3:K:167:LEU:HD11	3:K:202:TYR:CD1	2.51	0.44
1:P:80:LEU:HD22	1:U:81:ASN:HB2	1.99	0.44
1:U:21:TRP:CZ3	1:V:326:GLY:HA3	2.51	0.44
2:W:121:SER:OG	3:X:130:PHE:HB3	2.17	0.44
2:W:133:VAL:HG21	3:X:187:SER:HB3	1.99	0.44
1:b:175:PHE:O	1:b:249:SER:HA	2.18	0.44
3:d:33:TYR:CE2	3:d:52:TYR:HB2	2.52	0.44
2:D:49:TYR:C	2:D:51:ALA:H	2.24	0.44
2:M:37:GLN:HB2	2:M:47:LEU:HD11	2.00	0.44
3:N:132:LEU:HD21	3:N:149:LEU:CD1	2.48	0.44
3:N:156:GLU:N	3:N:157:PRO:HD2	2.31	0.44
1:Y:120:GLU:HB3	1:Y:268:SER:HB2	1.98	0.44
1:Y:192:ALA:HB2	1:Y:233:ALA:HB3	2.00	0.44
1:a:41:THR:O	1:a:45:ILE:HG13	2.18	0.44
1:b:107:ASP:HB2	1:b:241:TRP:HE1	1.82	0.44
1:b:144:ALA:O	1:b:147:LYS:HG3	2.17	0.44
2:c:131:SER:HA	2:c:179:LEU:O	2.17	0.44
3:d:11:LEU:HD12	3:d:124:THR:HG22	1.99	0.44
1:P:26:HIS:O	1:P:32:SER:HA	2.18	0.44
2:R:21:ILE:HG23	2:R:102:THR:HG21	1.99	0.44
3:S:66:ARG:HD2	3:S:83:THR:O	2.17	0.44
2:W:47:LEU:HD23	2:W:47:LEU:HA	1.81	0.44
1:Y:194:LEU:HD12	1:Y:223:ILE:HD12	2.00	0.44
1:b:50:LYS:HE2	1:b:283:GLU:OE1	2.17	0.44
1:L:48:ASN:OD1	1:L:294:ALA:O	2.35	0.44
2:M:178:THR:HG22	2:M:180:THR:HG23	2.00	0.44
3:N:12:VAL:HG21	3:N:18:LEU:HD13	2.00	0.44
1:Q:165:GLY:C	1:Q:202:LYS:HG3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:135:LEU:HD22	3:S:189:VAL:HG11	1.99	0.44
1:U:10:ILE:O	1:U:11:GLU:C	2.61	0.44
2:W:124:GLN:CD	3:X:151:LYS:HZ2	2.25	0.44
1:Y:191:PRO:HB3	1:Y:196:GLU:HG2	1.98	0.44
1:a:14:TRP:O	1:b:19:ALA:N	2.51	0.44
2:c:32:TRP:CZ3	2:c:50:LYS:HE2	2.53	0.44
3:d:51:PHE:CD1	3:d:57:PRO:HB3	2.48	0.44
1:C:215:TYR:CZ	1:C:241:THR:HB	2.52	0.44
2:D:115:VAL:HG21	2:D:196:VAL:HG21	1.99	0.44
2:D:129:THR:HA	2:D:185:ASP:OD2	2.17	0.44
1:H:111:HIS:CB	1:L:327:LEU:HD21	2.47	0.44
1:H:131:LYS:HB2	1:H:141:TYR:CZ	2.52	0.44
2:J:150:VAL:HA	2:J:191:VAL:O	2.17	0.44
2:J:186:TYR:O	2:J:186:TYR:HD1	1.98	0.44
1:U:77:ILE:CG2	1:a:77:ILE:HD12	2.47	0.44
1:U:97:GLU:OE2	1:V:321:LEU:HD21	2.17	0.44
1:V:111:LEU:HD13	1:V:240:TRP:CD2	2.52	0.44
3:X:155:PRO:HB2	3:X:208:HIS:CE1	2.53	0.44
1:Y:108:GLU:O	1:Y:112:ARG:HG3	2.17	0.44
1:b:158:MET:HE3	1:b:158:MET:HB2	1.86	0.44
2:c:142:ARG:HG3	2:c:173:TYR:CE2	2.53	0.44
3:d:209:LYS:HB2	3:d:210:PRO:HD3	2.00	0.44
1:C:50:LYS:HA	1:C:282:GLU:HG3	2.00	0.44
1:C:302:GLN:O	1:C:315:TYR:HA	2.17	0.44
2:D:105:GLU:OE2	2:D:142:ARG:NH1	2.51	0.44
2:J:190:LYS:O	2:J:210:ASN:HA	2.17	0.44
3:N:20:LEU:HD21	3:N:117:VAL:HG21	2.00	0.44
1:b:44:GLU:OE2	1:b:46:LYS:HG2	2.17	0.44
1:b:119:LEU:HB2	1:b:271:GLY:H	1.80	0.44
3:d:98:GLU:CD	3:d:99:GLU:O	2.61	0.44
2:D:197:THR:HG22	2:D:204:PRO:HB3	2.00	0.43
3:E:209:LYS:HB2	3:E:210:PRO:HD3	2.00	0.43
3:K:11:LEU:HD21	3:K:122:ALA:O	2.18	0.43
1:L:222:GLU:HA	1:Y:218:ARG:HH11	1.83	0.43
1:P:87:GLY:HA2	1:U:63:PHE:HZ	1.83	0.43
1:Q:86:TRP:O	1:Q:119:LEU:HG	2.17	0.43
1:U:23:GLY:HA3	1:U:36:ALA:HA	1.99	0.43
1:U:169:ASN:O	1:U:173:ILE:HG13	2.18	0.43
1:b:121:PHE:O	1:b:268:VAL:HG23	2.18	0.43
2:c:186:TYR:C	2:c:188:LYS:N	2.74	0.43
1:B:80:LEU:HD21	1:H:80:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:162:TRP:CE2	3:E:190:VAL:HG23	2.53	0.43
1:H:133:ILE:HD12	1:H:137:CYS:CB	2.43	0.43
2:M:182:SER:O	2:M:186:TYR:N	2.38	0.43
1:P:119:TYR:CE1	1:P:136:GLY:HA2	2.54	0.43
1:P:122:VAL:HG21	1:Q:15:ILE:HD11	2.00	0.43
1:P:133:ILE:O	1:P:133:ILE:HG22	2.18	0.43
1:V:140:GLY:O	1:V:142:THR:HG23	2.18	0.43
1:Y:169:VAL:HG22	1:Y:254:ASN:HB3	1.99	0.43
1:Y:182:VAL:O	1:Y:243:VAL:HG12	2.18	0.43
1:Y:290:THR:OG1	1:Y:293:GLY:O	2.27	0.43
3:d:208:HIS:CE1	3:d:211:SER:H	2.36	0.43
1:B:54:SER:O	1:B:58:LYS:HG2	2.17	0.43
1:C:50:LYS:HZ2	1:C:282:GLU:HB3	1.84	0.43
2:D:21:ILE:HG23	2:D:102:THR:HG21	2.00	0.43
2:D:32:TRP:CZ3	2:D:50:LYS:HG3	2.53	0.43
1:P:9:PHE:O	1:P:9:PHE:CG	2.71	0.43
1:Q:182:VAL:HG22	1:Q:265:GLU:HG2	2.00	0.43
1:Y:51:LEU:CD2	1:Y:279:LEU:HD22	2.48	0.43
1:Y:273:LYS:HD3	1:Y:307:ILE:HG22	1.99	0.43
1:Y:289:GLN:OE1	1:Y:294:ALA:HB2	2.17	0.43
1:b:203:LYS:HA	1:b:203:LYS:HD3	1.78	0.43
1:C:30:LEU:HD23	1:H:51:LYS:HB2	1.99	0.43
1:C:169:VAL:HG22	1:C:254:ASN:HB3	2.00	0.43
1:H:23:GLY:HA3	1:H:36:ALA:HA	2.00	0.43
1:H:83:LYS:HE3	1:I:84:VAL:HG11	2.01	0.43
2:J:49:TYR:C	2:J:51:ALA:H	2.25	0.43
1:Q:304:ILE:O	1:Q:315:TYR:CD1	2.71	0.43
3:S:6:GLU:OE2	3:S:94:TYR:HA	2.18	0.43
2:W:55:GLU:O	2:W:55:GLU:CG	2.67	0.43
2:W:124:GLN:HG2	2:W:129:THR:OG1	2.19	0.43
1:Y:47:HIS:CD2	1:Y:47:HIS:H	2.36	0.43
3:d:6:GLU:OE2	3:d:94:TYR:HA	2.18	0.43
3:E:36:TRP:CD1	3:E:69:MET:HE2	2.52	0.43
1:H:42:GLN:OE1	2:M:32:TRP:NE1	2.51	0.43
3:N:38:ARG:HD3	3:N:46:GLU:OE1	2.18	0.43
1:P:136:GLY:O	1:Q:15:ILE:N	2.51	0.43
1:V:110:GLU:O	1:V:114:LYS:HG3	2.19	0.43
2:W:37:GLN:O	2:W:44:PRO:HA	2.19	0.43
3:X:150:VAL:HG12	3:X:153:TYR:CD1	2.54	0.43
1:Y:141:VAL:HG21	1:Y:151:ASN:O	2.17	0.43
1:b:111:LEU:HD22	1:b:241:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:20:LEU:O	3:d:79:SER:HA	2.19	0.43
2:J:145:LYS:HB2	2:J:197:THR:OG1	2.19	0.43
1:L:305:HIS:CD2	1:L:307:ILE:HB	2.53	0.43
1:Q:110:GLU:HG2	1:a:76:ARG:HE	1.83	0.43
1:Q:248:SER:O	1:b:228:PRO:HG2	2.18	0.43
1:V:36:VAL:HA	1:V:328:ARG:HA	2.01	0.43
1:V:310:GLY:O	1:V:311:LYS:C	2.62	0.43
2:W:6:GLN:CG	2:W:88:CYS:SG	3.07	0.43
1:B:80:LEU:HG	1:I:80:LEU:HD21	2.00	0.43
2:J:2:ILE:HG21	2:J:29:ILE:HD11	1.99	0.43
3:K:155:PRO:CB	3:K:210:PRO:HG2	2.42	0.43
1:P:69:GLU:OE1	1:Q:112:ARG:HD3	2.19	0.43
1:Q:273:LYS:HD3	1:Q:307:ILE:HG23	2.00	0.43
1:Q:290:THR:HB	1:Q:305:HIS:HB3	1.99	0.43
2:W:135:LEU:HD21	2:W:137:ASN:ND2	2.34	0.43
2:c:6:GLN:NE2	2:c:102:THR:HG23	2.32	0.43
2:D:94:TYR:OH	3:E:50:ARG:NH1	2.51	0.43
3:K:29:ILE:HG23	3:K:34:TRP:HE1	1.80	0.43
1:L:171:LYS:HA	1:L:251:PHE:O	2.18	0.43
1:Q:224:SER:HB3	1:Q:226:ARG:HH11	1.84	0.43
2:R:29:ILE:HG23	2:R:92:ASN:HB2	2.00	0.43
3:X:51:PHE:CD1	3:X:57:PRO:HB3	2.53	0.43
3:X:59:TYR:O	3:X:64:ARG:NH2	2.50	0.43
1:Y:74:ASN:OD1	1:Y:75:PRO:CD	2.66	0.43
1:Y:135:VAL:HG12	1:Y:168:PRO:HD2	1.99	0.43
1:Y:243:VAL:HB	1:Y:249:ILE:HD12	2.00	0.43
2:c:148:TRP:O	2:c:149:LYS:HD2	2.18	0.43
3:d:36:TRP:CZ3	3:d:95:CYS:HB3	2.54	0.43
2:M:142:ARG:HH21	2:M:165:GLU:HA	1.84	0.43
3:N:129:VAL:HG12	3:N:217:LYS:HD2	2.00	0.43
2:R:59:PRO:HB2	2:R:61:ARG:HG2	2.01	0.43
1:U:26:HIS:O	1:U:32:SER:HA	2.18	0.43
1:V:115:PHE:HA	1:V:118:VAL:HG23	2.00	0.43
1:Y:101:TYR:CZ	1:Y:232:GLN:HB3	2.53	0.43
2:c:21:ILE:HG23	2:c:102:THR:HG21	2.00	0.43
2:c:144:ALA:HB2	2:c:198:HIS:CD2	2.47	0.43
3:d:35:ILE:CD1	3:d:50:ARG:CG	2.82	0.43
2:D:87:TYR:HE2	3:E:44:GLY:HA2	1.84	0.43
2:D:117:ILE:HG12	2:D:194:CYS:SG	2.59	0.43
2:J:12:SER:O	2:J:107:LYS:HE3	2.19	0.43
2:J:120:PRO:HB2	2:J:125:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:155:PRO:CG	3:N:210:PRO:HG2	2.48	0.43
2:W:91:TYR:CD1	2:W:96:TRP:CD2	3.07	0.43
1:C:302:GLN:HG2	1:C:314:LYS:O	2.19	0.42
2:J:49:TYR:C	2:J:51:ALA:N	2.75	0.42
1:L:65:CYS:HA	1:L:97:ASN:HB2	2.01	0.42
1:Q:50:LYS:HD3	1:Q:282:GLU:OE1	2.19	0.42
2:W:95:PRO:O	2:W:97:THR:HG23	2.19	0.42
1:Y:212:SER:HB3	1:Y:249:ILE:HG12	2.01	0.42
2:J:150:VAL:O	2:J:151:ASP:C	2.62	0.42
3:K:146:LEU:HD22	3:K:219:VAL:HG12	2.00	0.42
1:a:152:VAL:HG22	1:a:157:TYR:HB2	2.01	0.42
1:b:59:PRO:HD3	1:b:86:TRP:CB	2.48	0.42
1:B:74:GLU:OE1	1:I:76:ARG:NH2	2.52	0.42
1:C:161:ILE:HG22	1:C:162:HIS:HD2	1.84	0.42
1:I:68:LYS:HB2	1:I:81:ASN:ND2	2.34	0.42
2:J:142:ARG:HG3	2:J:173:TYR:CG	2.54	0.42
2:J:193:ALA:HB1	2:J:206:THR:CG2	2.49	0.42
1:L:305:HIS:NE2	1:L:307:ILE:HB	2.34	0.42
3:N:132:LEU:HD21	3:N:149:LEU:HD11	2.00	0.42
1:P:111:HIS:O	1:P:115:VAL:HG23	2.19	0.42
2:W:30:SER:HB3	2:W:71:PHE:CZ	2.55	0.42
3:X:36:TRP:HB3	3:X:48:ILE:HD12	2.00	0.42
1:b:94:ASN:HB3	1:b:95:PRO:HD3	2.01	0.42
2:c:187:GLU:H	2:c:187:GLU:CD	2.27	0.42
3:d:31:SER:O	3:d:100:HIS:HE1	2.03	0.42
1:C:99:ILE:HG22	1:C:101:TYR:O	2.19	0.42
3:S:18:LEU:HD22	3:S:117:VAL:HG11	2.02	0.42
2:W:210:ASN:HB2	3:X:137:LYS:HZ2	1.84	0.42
3:X:205:ASN:HA	3:X:216:ASP:OD1	2.18	0.42
1:Y:175:ASN:OD1	1:Y:175:ASN:C	2.62	0.42
2:c:115:VAL:HG12	2:c:207:LYS:HD2	2.01	0.42
3:d:205:ASN:HA	3:d:216:ASP:OD1	2.20	0.42
1:B:94:TYR:CZ	1:B:98:LEU:HD11	2.54	0.42
2:D:59:PRO:HB2	2:D:61:ARG:HG2	2.00	0.42
2:D:91:TYR:HA	2:D:96:TRP:NE1	2.35	0.42
3:E:33:TYR:CD2	3:E:52:TYR:HB2	2.54	0.42
3:E:132:LEU:HD21	3:E:149:LEU:HG	2.01	0.42
1:H:10:ILE:CG2	1:L:17:TYR:CE2	2.93	0.42
2:J:35:TRP:CE3	2:J:73:LEU:HD22	2.54	0.42
2:J:191:VAL:C	2:J:192:TYR:HD1	2.27	0.42
1:L:35:THR:HG22	1:L:329:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:41:THR:O	1:P:45:ILE:HG13	2.19	0.42
1:Q:120:GLU:HG3	1:Q:268:SER:HB3	2.02	0.42
2:R:107:LYS:HB3	2:R:107:LYS:HE2	1.94	0.42
1:U:12:GLY:O	1:V:17:TYR:CZ	2.72	0.42
1:V:289:GLN:H	1:V:309:ILE:HG21	1.85	0.42
2:W:135:LEU:HD22	3:X:189:VAL:HG11	2.01	0.42
2:W:143:GLU:OE1	2:W:199:GLN:NE2	2.52	0.42
3:X:11:LEU:HD23	3:X:11:LEU:HA	1.80	0.42
1:B:25:HIS:HB3	1:C:14:CYS:HB2	2.01	0.42
1:B:41:THR:O	1:B:45:ILE:HG13	2.19	0.42
1:C:84:THR:OG1	1:C:123:LYS:HE3	2.18	0.42
3:K:122:ALA:HB3	3:K:154:PHE:CE2	2.54	0.42
3:K:205:ASN:HA	3:K:216:ASP:OD1	2.19	0.42
2:W:50:LYS:HD2	3:X:104:GLY:CA	2.48	0.42
3:X:98:GLU:HA	3:X:108:VAL:HG12	2.00	0.42
1:b:157:ASN:HA	1:b:263:TYR:CD2	2.48	0.42
1:C:78:ASP:CG	1:C:155:ARG:HE	2.27	0.42
1:I:62:GLN:OE1	1:I:62:GLN:N	2.52	0.42
2:J:189:HIS:CG	2:J:190:LYS:N	2.87	0.42
3:S:35:ILE:CD1	3:S:98:GLU:CB	2.75	0.42
1:V:291:PRO:HD2	1:V:305:HIS:CG	2.54	0.42
1:Y:50:LYS:O	1:Y:294:ALA:N	2.47	0.42
1:Y:188:ILE:HD13	1:Y:219:PHE:HB2	2.01	0.42
2:c:2:ILE:HG22	2:c:90:GLN:HE22	1.83	0.42
2:c:155:GLN:N	2:c:155:GLN:CD	2.78	0.42
1:H:38:LEU:O	1:H:42:GLN:HB2	2.20	0.42
1:L:56:GLY:O	1:L:59:PRO:HD2	2.20	0.42
1:Q:58:GLN:NE2	1:Q:85(A):SER:O	2.53	0.42
2:R:62:PHE:CD1	2:R:75:ILE:HG12	2.54	0.42
2:R:166:GLN:HB2	2:R:173:TYR:CE1	2.55	0.42
1:U:104:ASN:OD1	1:V:323:LEU:HD12	2.20	0.42
1:a:132:GLU:HG2	1:a:138:PHE:HE1	1.85	0.42
2:c:150:VAL:HB	2:c:155:GLN:NE2	2.35	0.42
1:C:48:ASN:ND2	1:C:294:ALA:HB3	2.33	0.42
1:C:212:SER:O	1:Y:235:ARG:NH2	2.53	0.42
2:D:1:ASP:CB	2:D:2:ILE:HD12	2.50	0.42
3:E:50:ARG:NH2	3:E:98:GLU:OE2	2.52	0.42
1:H:73:LEU:HD22	1:Y:107:ASP:OD2	2.20	0.42
3:N:87:ALA:HA	3:N:119:VAL:HB	2.02	0.42
3:N:155:PRO:HG3	3:N:210:PRO:CG	2.49	0.42
2:R:128:GLY:O	2:R:182:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:205:ASN:HA	3:S:216:ASP:OD1	2.20	0.42
1:V:297:THR:HG23	1:V:313:PRO:HG2	2.01	0.42
3:d:150:VAL:HG12	3:d:153:TYR:CE1	2.55	0.42
1:C:56:GLY:HA2	1:C:284:CYS:HA	2.01	0.42
1:C:100:CYS:HB3	1:C:144:ALA:O	2.20	0.42
1:C:120:GLU:HA	1:C:268:SER:H	1.85	0.42
2:J:116:PHE:HE1	3:K:140:SER:HB3	1.85	0.42
1:L:158:VAL:HG23	1:L:261:ARG:HB2	2.00	0.42
2:M:155:GLN:NE2	2:M:179:LEU:HD13	2.34	0.42
3:S:4:LEU:HD22	3:S:24:VAL:HG22	2.01	0.42
2:W:186:TYR:HB3	2:W:188:LYS:HG2	2.02	0.42
1:Y:291:PRO:HD2	1:Y:305:HIS:CG	2.54	0.42
1:b:112:ARG:C	1:b:114:LYS:N	2.78	0.42
2:c:50:LYS:C	2:c:52:SER:N	2.78	0.42
2:c:184:ALA:C	2:c:186:TYR:N	2.74	0.42
3:d:32:TYR:HD2	3:d:98:GLU:O	2.02	0.42
2:D:35:TRP:NE1	2:D:71:PHE:CE2	2.88	0.41
2:M:157:GLY:O	2:M:158:ASN:C	2.63	0.41
1:P:59:MET:HE2	1:a:94:TYR:CZ	2.55	0.41
2:R:158:ASN:O	2:R:179:LEU:HD12	2.20	0.41
2:W:161:GLU:HG2	2:W:177:SER:HA	2.02	0.41
3:X:157:PRO:HD2	3:X:210:PRO:HG2	2.02	0.41
3:d:36:TRP:CH2	3:d:95:CYS:HB3	2.54	0.41
1:C:52:CYS:SG	1:C:282:GLU:HB2	2.60	0.41
3:E:29:ILE:HG23	3:E:34:TRP:CD1	2.55	0.41
1:I:70:PHE:CD1	1:I:77:ILE:HG22	2.55	0.41
2:J:162:SER:HB2	3:K:175:PRO:HD2	2.02	0.41
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.55	0.41
1:L:58:GLN:N	1:L:59:PRO:CD	2.82	0.41
2:R:105:GLU:OE2	2:R:142:ARG:NH1	2.51	0.41
2:R:181:LEU:HD23	2:R:181:LEU:HA	1.79	0.41
3:S:196:SER:O	3:S:200:GLN:N	2.53	0.41
1:V:122:SER:OG	1:V:265:GLU:HB3	2.20	0.41
2:W:38:GLN:HB2	2:W:85:ILE:HB	2.02	0.41
1:Y:121:PHE:HE2	1:Y:264:PHE:HD1	1.68	0.41
1:b:58:GLN:HA	1:b:88:TYR:O	2.20	0.41
2:D:39:LYS:HB2	2:D:42:LYS:HD3	2.01	0.41
2:D:144:ALA:HB2	2:D:198:HIS:CD2	2.47	0.41
3:E:149:LEU:HB3	3:E:151:LYS:HE3	2.02	0.41
1:I:19:ASP:HB3	3:K:33:TYR:CE1	2.55	0.41
1:I:58:LYS:HD3	1:I:58:LYS:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:GLU:HG2	1:I:77:ILE:HD12	2.02	0.41
2:J:115:VAL:HG12	2:J:207:LYS:HD2	2.02	0.41
1:P:91:ILE:HG12	1:U:91:ILE:HG21	2.00	0.41
1:P:121:LYS:HE2	1:P:121:LYS:HB2	1.83	0.41
1:P:141:TYR:HE1	1:P:173:ILE:HD12	1.85	0.41
1:Q:115:PHE:HD2	1:Q:274:LEU:HD11	1.85	0.41
2:R:35:TRP:O	2:R:47:LEU:N	2.47	0.41
3:S:154:PHE:CE1	3:S:183:LEU:HD21	2.55	0.41
1:V:135:VAL:HG21	1:V:170:ILE:HG21	2.02	0.41
2:W:138:ASN:H	2:W:174:SER:HB3	1.85	0.41
2:W:152:ASN:OD1	2:W:153:ALA:N	2.54	0.41
3:X:13:LYS:HZ3	3:X:121:SER:C	2.26	0.41
3:X:33:TYR:CD2	3:X:52:TYR:HB2	2.56	0.41
3:X:146:LEU:HD22	3:X:219:VAL:HG12	2.02	0.41
1:a:13:GLY:HA3	1:b:331:VAL:O	2.20	0.41
1:a:140:PHE:CD2	1:b:11:ASP:HB2	2.55	0.41
3:d:33:TYR:HB2	3:d:98:GLU:CB	2.49	0.41
1:B:20:GLY:H	3:E:101:ILE:HD11	1.85	0.41
3:E:37:ILE:HB	3:E:94:TYR:HB2	2.02	0.41
1:L:273:LYS:HD3	1:L:307:ILE:HG23	2.03	0.41
2:M:166:GLN:NE2	2:M:171:SER:HB3	2.31	0.41
3:S:69:MET:HE2	3:S:80:LEU:HD21	2.02	0.41
1:U:76:ARG:NH1	1:b:109:GLU:HB2	2.33	0.41
1:V:141:VAL:HG12	1:V:152:SER:HA	2.02	0.41
3:X:33:TYR:HB2	3:X:98:GLU:HB3	2.01	0.41
3:X:153:TYR:OH	3:X:186:LEU:HB2	2.20	0.41
1:a:21:TRP:CH2	1:b:327:GLY:HA2	2.55	0.41
1:b:159:VAL:HG23	1:b:262:ARG:HB2	2.01	0.41
2:c:94:TYR:CE1	3:d:50:ARG:NH1	2.88	0.41
1:H:21:TRP:HH2	1:L:326:GLY:HA3	1.85	0.41
1:I:138:PHE:O	1:Y:12:THR:HA	2.20	0.41
2:J:59:PRO:HB2	2:J:61:ARG:HG2	2.02	0.41
3:K:43:LYS:HE3	3:K:43:LYS:HB2	1.88	0.41
3:N:20:LEU:O	3:N:79:SER:HA	2.20	0.41
3:N:36:TRP:CH2	3:N:95:CYS:HB3	2.55	0.41
1:Q:48:ASN:N	1:Q:294:ALA:O	2.53	0.41
1:V:62:LEU:HD12	1:V:91:GLU:HG2	2.02	0.41
3:X:154:PHE:HB3	3:X:155:PRO:HD3	2.02	0.41
1:Y:54:ILE:O	1:Y:285:ASN:HB2	2.20	0.41
2:c:4:MET:SD	2:c:90:GLN:NE2	2.94	0.41
2:J:139:PHE:HE1	2:J:142:ARG:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:PRO:HG2	1:L:235:ARG:HD3	2.03	0.41
1:Q:91:GLU:HG3	1:Q:112:ARG:NH2	2.35	0.41
1:V:99:ILE:HD13	1:V:99:ILE:HA	1.95	0.41
1:V:216:ASN:O	1:V:217:ARG:C	2.62	0.41
1:b:45:ASP:HA	1:b:304:ASN:OD1	2.21	0.41
1:b:65:CYS:O	1:b:65:CYS:SG	2.78	0.41
3:d:18:LEU:O	3:d:81:LYS:HA	2.21	0.41
1:B:74:GLU:HA	1:B:77:ILE:CD1	2.50	0.41
1:C:29:LEU:HD13	1:H:51:LYS:CG	2.50	0.41
1:C:57:LYS:NZ	1:C:119:LEU:HD21	2.36	0.41
2:D:181:LEU:HB2	2:D:185:ASP:OD1	2.20	0.41
1:H:90:ASP:OD2	1:I:61:THR:HA	2.20	0.41
3:N:6:GLU:OE2	3:N:94:TYR:HA	2.21	0.41
2:R:91:TYR:HA	2:R:96:TRP:CD1	2.56	0.41
3:S:11:LEU:HD12	3:S:124:THR:CG2	2.51	0.41
1:V:120(A):GLU:HB2	1:V:268:SER:HB2	2.02	0.41
1:V:242:MET:HE1	1:V:266:ILE:HD12	2.03	0.41
3:X:127:PRO:HG3	3:X:208:HIS:HB2	2.01	0.41
3:X:167:LEU:HD11	3:X:202:TYR:CD1	2.55	0.41
1:Y:191:PRO:HD2	1:Y:223:ILE:HG12	2.02	0.41
1:a:125:GLN:OE1	1:a:155:GLY:HA2	2.19	0.41
1:a:133:ILE:O	1:a:137:CYS:HB2	2.19	0.41
1:b:52:CYS:HB2	1:b:285:CYS:H	1.86	0.41
1:b:52:CYS:CB	1:b:285:CYS:H	2.34	0.41
2:c:32:TRP:HB3	2:c:91:TYR:CE1	2.55	0.41
2:c:135:LEU:CD2	3:d:189:VAL:HG11	2.50	0.41
1:C:113:LEU:CD2	1:I:75:LYS:CG	2.98	0.41
3:K:162:TRP:CB	3:K:167:LEU:HB2	2.49	0.41
1:L:58:GLN:C	1:L:86:TRP:HA	2.44	0.41
1:L:121:PHE:CE1	1:L:266:ILE:HG12	2.56	0.41
3:N:129:VAL:HG13	3:N:148:CYS:SG	2.61	0.41
2:R:166:GLN:HB2	2:R:173:TYR:HE1	1.84	0.41
3:S:132:LEU:HD21	3:S:149:LEU:HG	2.02	0.41
1:V:236:MET:SD	1:V:258:LEU:HD11	2.61	0.41
3:X:39:GLN:O	3:X:91:ALA:HA	2.21	0.41
3:X:93:TYR:HE1	3:X:117:VAL:HB	1.85	0.41
1:H:76:ARG:NH2	1:I:69:GLU:O	2.52	0.41
2:J:19:VAL:O	2:J:74:THR:HA	2.20	0.41
2:J:35:TRP:CG	2:J:73:LEU:HD13	2.56	0.41
2:J:162:SER:OG	2:J:176:SER:OG	2.38	0.41
2:J:181:LEU:HA	2:J:181:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:87:ALA:O	3:K:90:THR:HG22	2.21	0.41
1:L:60:ILE:HG23	1:L:83:LYS:NZ	2.35	0.41
3:N:36:TRP:CD1	3:N:80:LEU:HG	2.55	0.41
1:P:77:ILE:HG23	1:U:70:PHE:HE1	1.84	0.41
1:Q:74:ASN:HB3	1:Q:77:CYS:SG	2.61	0.41
1:Q:279:LEU:HD23	1:Q:279:LEU:HA	1.93	0.41
3:S:36:TRP:HB3	3:S:48:ILE:HD11	2.02	0.41
1:U:77:ILE:HG21	1:a:77:ILE:HD12	2.03	0.41
2:W:137:ASN:HA	2:W:174:SER:CB	2.50	0.41
3:X:66:ARG:HD2	3:X:83:THR:O	2.21	0.41
3:X:122:ALA:HB3	3:X:154:PHE:CE2	2.54	0.41
3:X:204:CYS:O	3:X:216:ASP:HA	2.20	0.41
1:Y:75:PRO:HG3	1:Y:153:PHE:O	2.20	0.41
1:Y:143:ALA:HA	1:Y:151:ASN:HB2	2.03	0.41
1:a:159:TYR:HB3	1:a:160:PRO:HD3	2.03	0.41
1:b:102:PRO:HB2	1:b:236:ARG:CD	2.51	0.41
1:b:142:VAL:HG12	1:b:153:SER:HA	2.03	0.41
2:c:182:SER:O	2:c:182:SER:OG	2.13	0.41
3:d:29:ILE:HG23	3:d:34:TRP:HE1	1.86	0.41
1:B:51:LYS:CG	1:Y:29:LEU:HD13	2.50	0.41
1:B:88:PHE:HE2	1:I:83:LYS:HG2	1.86	0.41
2:D:38:GLN:O	2:D:84:ALA:HB1	2.21	0.41
2:D:95:PRO:HA	3:E:47:TRP:CZ3	2.56	0.41
3:S:146:LEU:HD22	3:S:219:VAL:CG1	2.50	0.41
1:V:111:LEU:HD22	1:V:240:TRP:CD1	2.56	0.41
2:W:132:VAL:HG22	2:W:133:VAL:H	1.86	0.41
1:Y:183:LEU:HB3	1:Y:264:PHE:HB2	2.02	0.41
2:c:186:TYR:C	2:c:188:LYS:H	2.27	0.41
1:C:116:SER:HA	1:C:273:LYS:HA	2.03	0.40
1:H:91:ILE:HG12	1:I:91:ILE:HG21	2.02	0.40
1:I:122:VAL:HG21	1:Y:15:ILE:HD11	2.03	0.40
2:J:105:GLU:OE2	2:J:142:ARG:NH1	2.52	0.40
2:J:166:GLN:HG2	2:J:171:SER:HA	2.03	0.40
2:M:49:TYR:C	2:M:51:ALA:H	2.29	0.40
1:Q:43:LEU:HD13	1:Q:321:LEU:HD13	2.03	0.40
2:R:33:LEU:CD2	2:R:90:GLN:HG2	2.51	0.40
1:V:54:ILE:HG13	1:V:289:GLN:HG3	2.02	0.40
2:W:61:ARG:CD	2:W:79:GLN:HG2	2.51	0.40
2:W:134:CYS:HB2	2:W:148:TRP:CH2	2.55	0.40
2:W:151:ASP:CG	2:W:152:ASN:H	2.29	0.40
3:X:17:THR:HA	3:X:82:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:182:VAL:HG22	1:Y:265:GLU:HA	2.02	0.40
1:a:122:VAL:HG21	1:b:15:ILE:HD11	2.03	0.40
1:b:20:ASN:C	1:b:330:ASN:HD21	2.29	0.40
3:d:90:THR:HB	3:d:119:VAL:H	1.86	0.40
5:F:1:NAG:O4	5:F:2:NAG:O7	2.38	0.40
1:C:56:GLY:O	1:C:57:LYS:C	2.64	0.40
1:C:153:PHE:CG	1:C:154:PHE:N	2.89	0.40
3:N:35:ILE:HA	3:N:49:GLY:O	2.21	0.40
1:P:159:TYR:HB3	1:P:160:PRO:HD3	2.04	0.40
2:R:18:ARG:HG2	2:R:76:SER:O	2.21	0.40
2:R:162:SER:OG	2:R:176:SER:OG	2.39	0.40
3:S:90:THR:HG23	3:S:118:THR:HG22	2.03	0.40
1:U:71:ASN:N	1:V:109:GLU:OE1	2.54	0.40
1:V:157:MET:HE1	1:V:186:TRP:HA	2.03	0.40
1:V:289:GLN:CG	1:V:294:ALA:HB2	2.51	0.40
1:b:67:PHE:O	1:b:67:PHE:CG	2.75	0.40
1:b:331:VAL:HG12	1:b:333:SER:H	1.87	0.40
2:c:185:ASP:O	2:c:186:TYR:C	2.63	0.40
3:d:33:TYR:CD2	3:d:52:TYR:HB2	2.56	0.40
1:C:209:ALA:HB1	1:Y:224:SER:CB	2.51	0.40
1:C:218:ARG:HD2	1:Y:223:ILE:O	2.21	0.40
1:H:76:ARG:HD2	1:Y:110:GLU:HA	2.04	0.40
2:J:149:LYS:HG2	2:J:152:ASN:HA	2.02	0.40
1:L:305:HIS:ND1	1:L:306:PRO:HD2	2.35	0.40
2:M:62:PHE:CD1	2:M:75:ILE:HG12	2.57	0.40
2:M:194:CYS:O	2:M:206:THR:HA	2.22	0.40
1:Q:137:SER:C	1:Q:139:ALA:H	2.28	0.40
2:R:2:ILE:HB	2:R:90:GLN:OE1	2.22	0.40
3:S:11:LEU:HD12	3:S:124:THR:HG22	2.04	0.40
2:W:19:VAL:O	2:W:74:THR:HA	2.21	0.40
2:W:55:GLU:C	2:W:57:GLY:N	2.78	0.40
1:Y:41:ASN:HB2	1:Y:322:ARG:NH2	2.37	0.40
3:E:125:LYS:HD2	3:E:183:LEU:HD21	2.03	0.40
1:H:56:ILE:HA	1:H:59:MET:HE2	2.03	0.40
1:I:23:GLY:HA3	1:I:36:ALA:HA	2.02	0.40
2:J:114:SER:OG	2:J:137:ASN:HB2	2.22	0.40
3:K:124:THR:O	3:K:124:THR:HG23	2.21	0.40
3:K:152:ASP:HA	3:K:183:LEU:HD13	2.02	0.40
2:M:142:ARG:HG3	2:M:173:TYR:CG	2.56	0.40
2:M:197:THR:HG22	2:M:204:PRO:HB3	2.02	0.40
3:N:38:ARG:HD2	3:N:48:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:94:TYR:CZ	1:P:98:LEU:HD11	2.56	0.40
1:Q:72:LEU:HD13	1:Q:238:PHE:HD2	1.85	0.40
1:Q:132:TRP:C	1:Q:134:ALA:N	2.80	0.40
2:R:160:GLN:HB2	3:S:177:VAL:HG11	2.03	0.40
1:U:8:GLY:H	1:U:112:ASP:CG	2.29	0.40
1:U:101:LEU:HD22	1:V:28:THR:C	2.47	0.40
1:V:62:LEU:HD22	1:V:80:LEU:HD13	2.03	0.40
1:a:96:ALA:O	1:a:100:VAL:HG23	2.22	0.40
1:a:140:PHE:HD2	1:b:11:ASP:HB2	1.86	0.40
2:c:39:LYS:HB2	2:c:42:LYS:HD3	2.04	0.40
3:d:149:LEU:HD13	3:d:151:LYS:HE3	2.02	0.40
2:D:121:SER:HB3	3:E:130:PHE:HB3	2.03	0.40
3:E:6:GLU:OE2	3:E:94:TYR:HA	2.22	0.40
1:I:125:GLN:C	1:I:126:LEU:HD12	2.46	0.40
1:L:117:GLY:O	1:L:270:GLY:N	2.51	0.40
1:L:123:LYS:HE2	1:L:264:PHE:CE1	2.56	0.40
1:L:327:LEU:HD23	1:L:327:LEU:HA	1.87	0.40
1:Q:43:LEU:HD22	1:Q:321:LEU:HD13	2.04	0.40
2:R:142:ARG:HG3	2:R:173:TYR:CG	2.57	0.40
1:U:22:TYR:H	1:U:41:THR:HG21	1.86	0.40
1:V:29:LEU:HD12	1:V:30:LEU:N	2.36	0.40
1:V:157:MET:CE	1:V:186:TRP:HA	2.50	0.40
2:W:19:VAL:HG21	2:W:78:LEU:HD21	2.02	0.40
2:W:80:PRO:HB3	2:W:169:LYS:H	1.87	0.40
2:W:176:SER:HB3	3:X:174:PHE:CZ	2.56	0.40
1:b:41:ASN:ND2	1:b:43:LEU:O	2.51	0.40
1:b:293:LYS:NZ	1:b:305:ILE:O	2.49	0.40

All (3) 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)
3:S:199:THR:CA	2:c:182:SER:OG[3_654]	1.70	0.50
3:S:199:THR:C	2:c:182:SER:OG[3_654]	1.70	0.50
2:M:3:GLN:CD	3:d:84:SER:OG[3_554]	2.13	0.07

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	B	166/504 (33%)	162 (98%)	4 (2%)	0	100	100
1	C	321/504 (64%)	290 (90%)	31 (10%)	0	100	100
1	H	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	I	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	L	321/504 (64%)	295 (92%)	26 (8%)	0	100	100
1	P	166/504 (33%)	158 (95%)	8 (5%)	0	100	100
1	Q	321/504 (64%)	299 (93%)	22 (7%)	0	100	100
1	U	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	V	321/504 (64%)	287 (89%)	33 (10%)	1 (0%)	36	71
1	Y	321/504 (64%)	293 (91%)	28 (9%)	0	100	100
1	a	166/504 (33%)	157 (95%)	9 (5%)	0	100	100
1	b	321/504 (64%)	288 (90%)	33 (10%)	0	100	100
2	D	210/214 (98%)	200 (95%)	10 (5%)	0	100	100
2	J	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	M	210/214 (98%)	195 (93%)	15 (7%)	0	100	100
2	R	210/214 (98%)	197 (94%)	13 (6%)	0	100	100
2	W	207/214 (97%)	176 (85%)	31 (15%)	0	100	100
2	c	210/214 (98%)	194 (92%)	16 (8%)	0	100	100
3	E	219/224 (98%)	195 (89%)	24 (11%)	0	100	100
3	K	219/224 (98%)	207 (94%)	12 (6%)	0	100	100
3	N	219/224 (98%)	203 (93%)	16 (7%)	0	100	100
3	S	219/224 (98%)	198 (90%)	21 (10%)	0	100	100
3	X	219/224 (98%)	204 (93%)	15 (7%)	0	100	100
3	d	219/224 (98%)	205 (94%)	14 (6%)	0	100	100
All	All	5493/8676 (63%)	5071 (92%)	421 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	300	PRO

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	B	146/434 (34%)	146 (100%)	0	100	100
1	C	279/434 (64%)	279 (100%)	0	100	100
1	H	146/434 (34%)	146 (100%)	0	100	100
1	I	146/434 (34%)	146 (100%)	0	100	100
1	L	279/434 (64%)	278 (100%)	1 (0%)	84	82
1	P	146/434 (34%)	146 (100%)	0	100	100
1	Q	279/434 (64%)	275 (99%)	4 (1%)	59	71
1	U	146/434 (34%)	146 (100%)	0	100	100
1	V	279/434 (64%)	276 (99%)	3 (1%)	65	74
1	Y	279/434 (64%)	278 (100%)	1 (0%)	84	82
1	a	146/434 (34%)	145 (99%)	1 (1%)	76	79
1	b	279/434 (64%)	276 (99%)	3 (1%)	65	74
2	D	186/188 (99%)	186 (100%)	0	100	100
2	J	186/188 (99%)	186 (100%)	0	100	100
2	M	186/188 (99%)	186 (100%)	0	100	100
2	R	186/188 (99%)	186 (100%)	0	100	100
2	W	185/188 (98%)	183 (99%)	2 (1%)	65	74
2	c	186/188 (99%)	186 (100%)	0	100	100
3	E	190/193 (98%)	190 (100%)	0	100	100
3	K	190/193 (98%)	190 (100%)	0	100	100
3	N	190/193 (98%)	189 (100%)	1 (0%)	81	81
3	S	190/193 (98%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	X	190/193 (98%)	189 (100%)	1 (0%)	81	81
3	d	190/193 (98%)	190 (100%)	0	100	100
All	All	4805/7494 (64%)	4788 (100%)	17 (0%)	84	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	218	ARG
3	N	90	THR
1	Q	52	CYS
1	Q	58	GLN
1	Q	303	ASN
1	Q	304	ILE
1	V	54	ILE
1	V	216	ASN
1	V	309	ILE
2	W	50	LYS
2	W	189	HIS
3	X	11	LEU
1	Y	284	CYS
1	a	127	LYS
1	b	142	VAL
1	b	143	THR
1	b	286	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	41	ASN
1	C	305	HIS
2	D	38	GLN
1	H	135	ASN
1	I	95	ASN
1	L	97	ASN
1	L	136	ASN
2	M	90	GLN
2	M	138	ASN
2	M	158	ASN
1	Q	41	ASN
1	Q	163	GLN

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Mol	Chain	Res	Type
1	Q	285	ASN
2	R	155	GLN
2	R	166	GLN
3	S	58	ASN
1	U	26	HIS
1	V	41	ASN
1	V	97	ASN
1	V	216	ASN
2	W	38	GLN
2	W	92	ASN
2	W	189	HIS
1	Y	47	HIS
1	Y	48	ASN
1	Y	136	ASN
1	Y	151	ASN
1	Y	156	ASN
1	Y	302	GLN
1	a	26	HIS
1	b	21	ASN
1	b	217	ASN
1	b	290	GLN
1	b	303	GLN
2	c	92	ASN
2	c	158	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](#)

19 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	$\# Z > 2$
4	NAG	A	1	4	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	A	2	4	14,14,15	0.35	0	17,19,21	0.67	1 (5%)
5	NAG	F	1	5	14,14,15	0.39	0	17,19,21	0.42	0
5	NAG	F	2	5	14,14,15	0.58	0	17,19,21	0.54	0
5	BMA	F	3	5	11,11,12	0.74	0	15,15,17	0.74	0
5	NAG	G	1	5	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	G	2	5	14,14,15	0.35	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	0.76	0	15,15,17	0.66	0
5	NAG	O	1	5	14,14,15	0.54	0	17,19,21	1.38	3 (17%)
5	NAG	O	2	5	14,14,15	2.19	2 (14%)	17,19,21	1.15	2 (11%)
5	BMA	O	3	5	11,11,12	1.99	5 (45%)	15,15,17	0.94	1 (6%)
5	NAG	T	1	5	14,14,15	0.37	0	17,19,21	0.50	0
5	NAG	T	2	5	14,14,15	0.33	0	17,19,21	0.80	0
5	BMA	T	3	5	11,11,12	1.25	1 (9%)	15,15,17	0.81	1 (6%)
4	NAG	Z	1	4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	Z	2	4	14,14,15	0.43	0	17,19,21	0.42	0
5	NAG	e	1	5	14,14,15	0.23	0	17,19,21	0.67	0
5	NAG	e	2	5	14,14,15	0.27	0	17,19,21	0.81	0
5	BMA	e	3	5	11,11,12	0.72	0	15,15,17	0.83	1 (6%)

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
4	NAG	A	1	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	NAG	G	1	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5	-	4/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	T	1	5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	1/2/19/22	0/1/1/1
4	NAG	Z	1	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	1/6/23/26	0/1/1/1
5	NAG	e	1	5	-	2/6/23/26	0/1/1/1
5	NAG	e	2	5	-	2/6/23/26	0/1/1/1
5	BMA	e	3	5	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2	NAG	C1-C2	6.68	1.61	1.52
5	O	2	NAG	O5-C1	-4.15	1.36	1.43
5	O	3	BMA	C2-C3	3.88	1.58	1.52
5	O	3	BMA	C1-C2	2.50	1.58	1.52
5	T	3	BMA	C4-C5	2.49	1.58	1.53
5	O	3	BMA	O5-C5	-2.37	1.38	1.43
5	O	3	BMA	O3-C3	2.24	1.48	1.43
5	O	3	BMA	O4-C4	2.10	1.48	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1	NAG	C4-C3-C2	2.99	115.40	111.02
5	O	1	NAG	O4-C4-C3	-2.72	103.96	110.38
5	O	2	NAG	C4-C3-C2	2.36	114.48	111.02
5	T	3	BMA	O2-C2-C3	-2.22	105.55	110.15
5	O	2	NAG	O5-C5-C4	-2.20	105.47	110.83
5	O	1	NAG	C2-N2-C7	2.11	125.73	122.90
4	A	2	NAG	C1-O5-C5	2.08	114.98	112.19
5	e	3	BMA	C1-O5-C5	2.08	114.97	112.19
5	O	3	BMA	O2-C2-C3	-2.01	105.99	110.15

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	e	2	NAG	C1-C2-N2-C7
5	O	3	BMA	C4-C5-C6-O6

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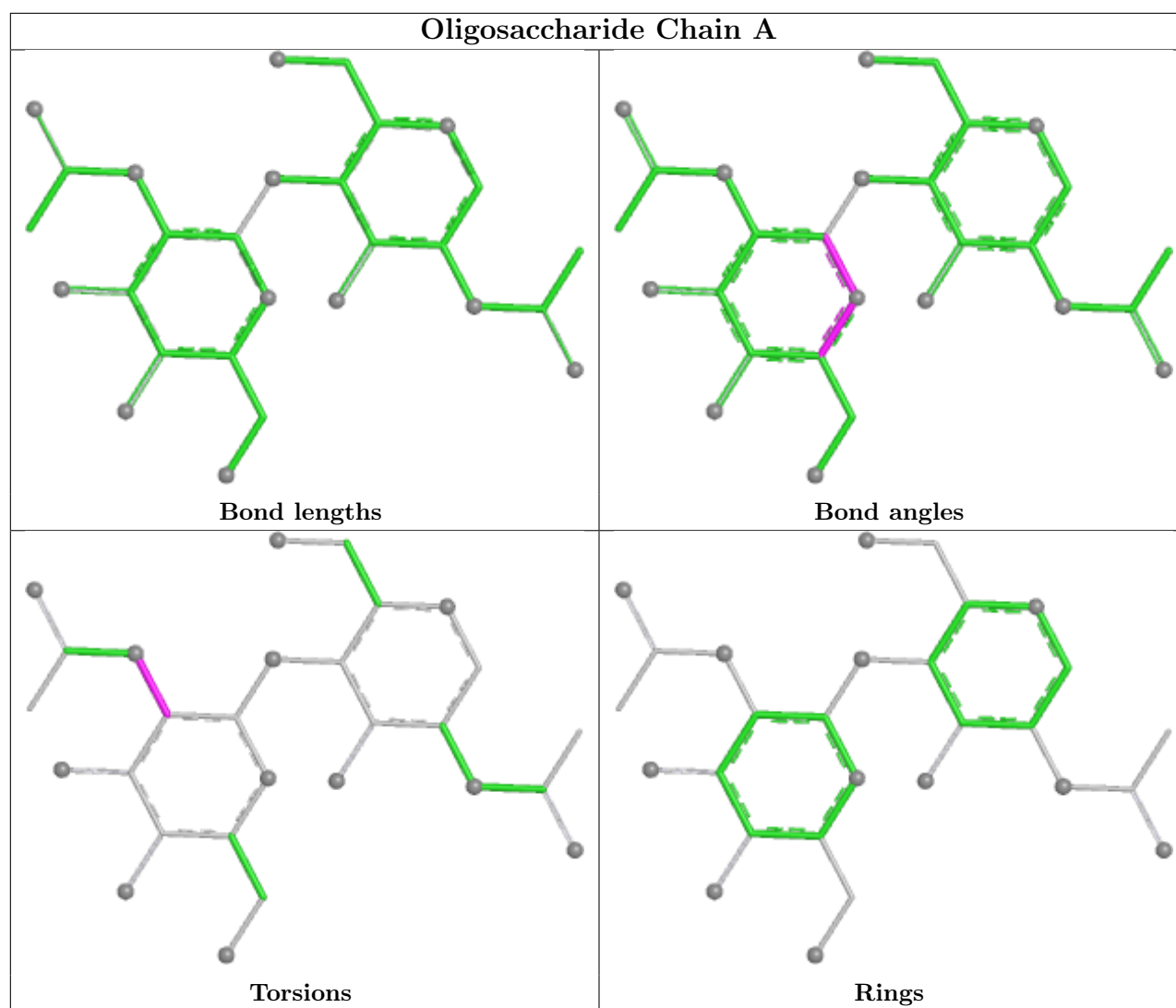
Mol	Chain	Res	Type	Atoms
5	O	3	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
5	e	2	NAG	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
4	A	2	NAG	C3-C2-N2-C7
5	T	2	NAG	C3-C2-N2-C7
5	e	1	NAG	C3-C2-N2-C7
4	A	2	NAG	C1-C2-N2-C7
5	F	2	NAG	C1-C2-N2-C7
5	O	1	NAG	C1-C2-N2-C7
5	T	2	NAG	C1-C2-N2-C7
5	e	1	NAG	C1-C2-N2-C7
5	O	1	NAG	C3-C2-N2-C7

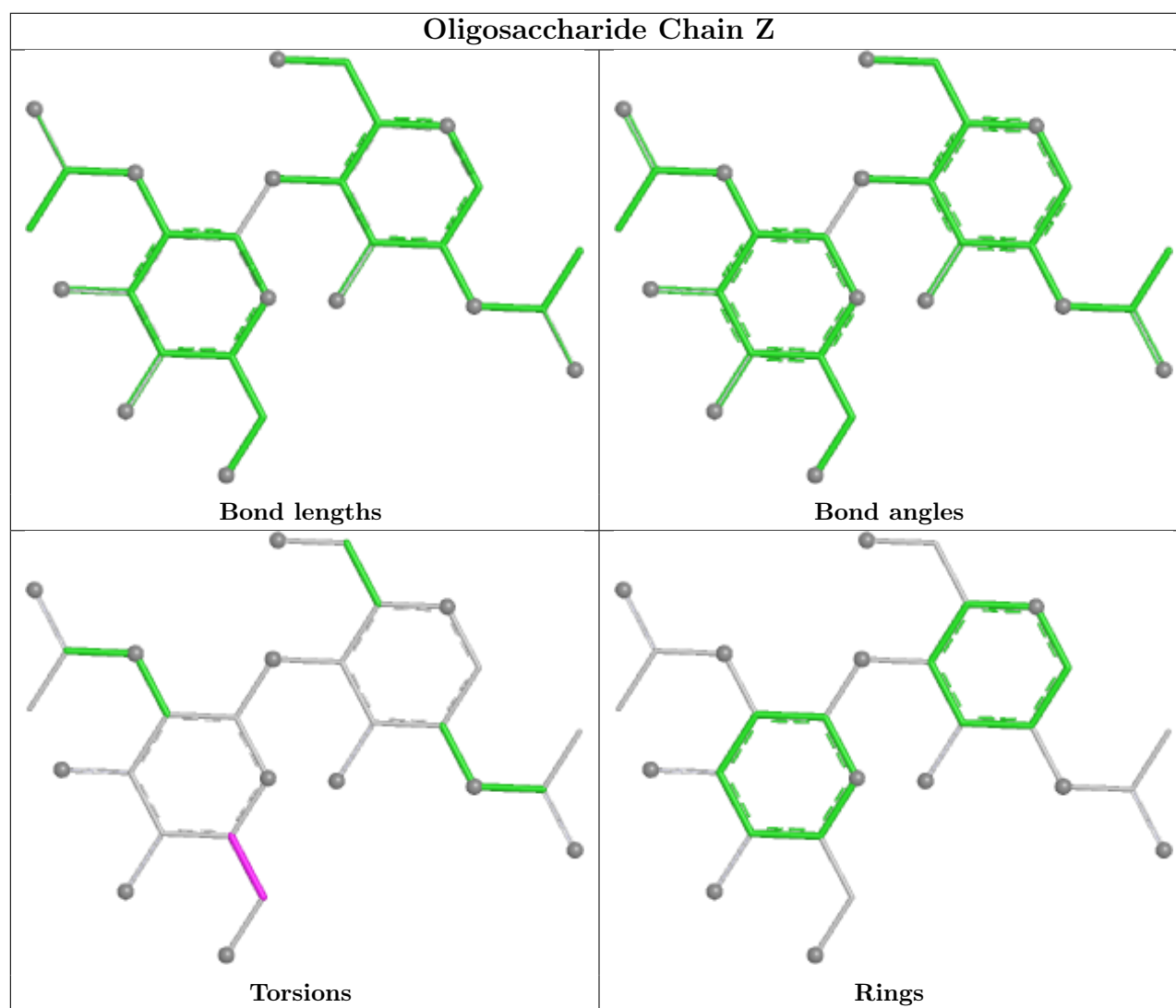
There are no ring outliers.

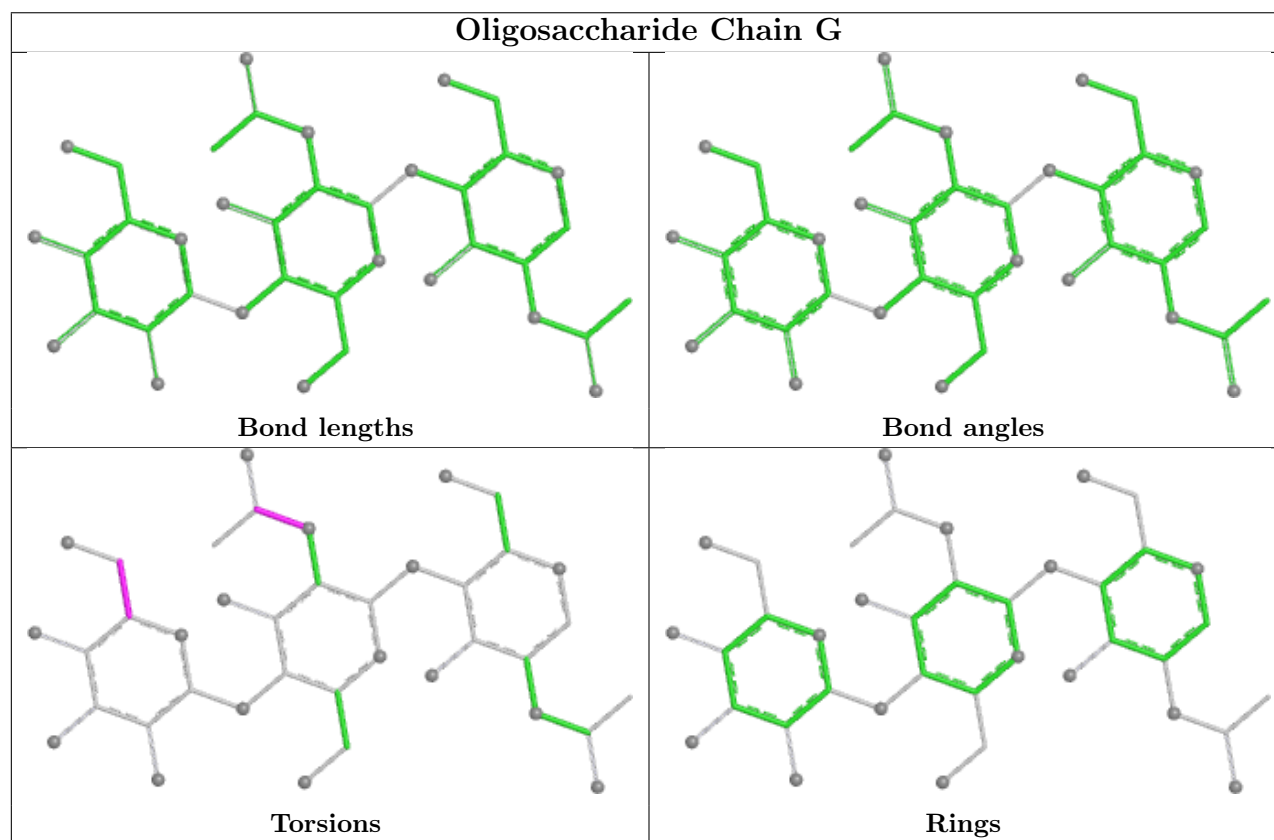
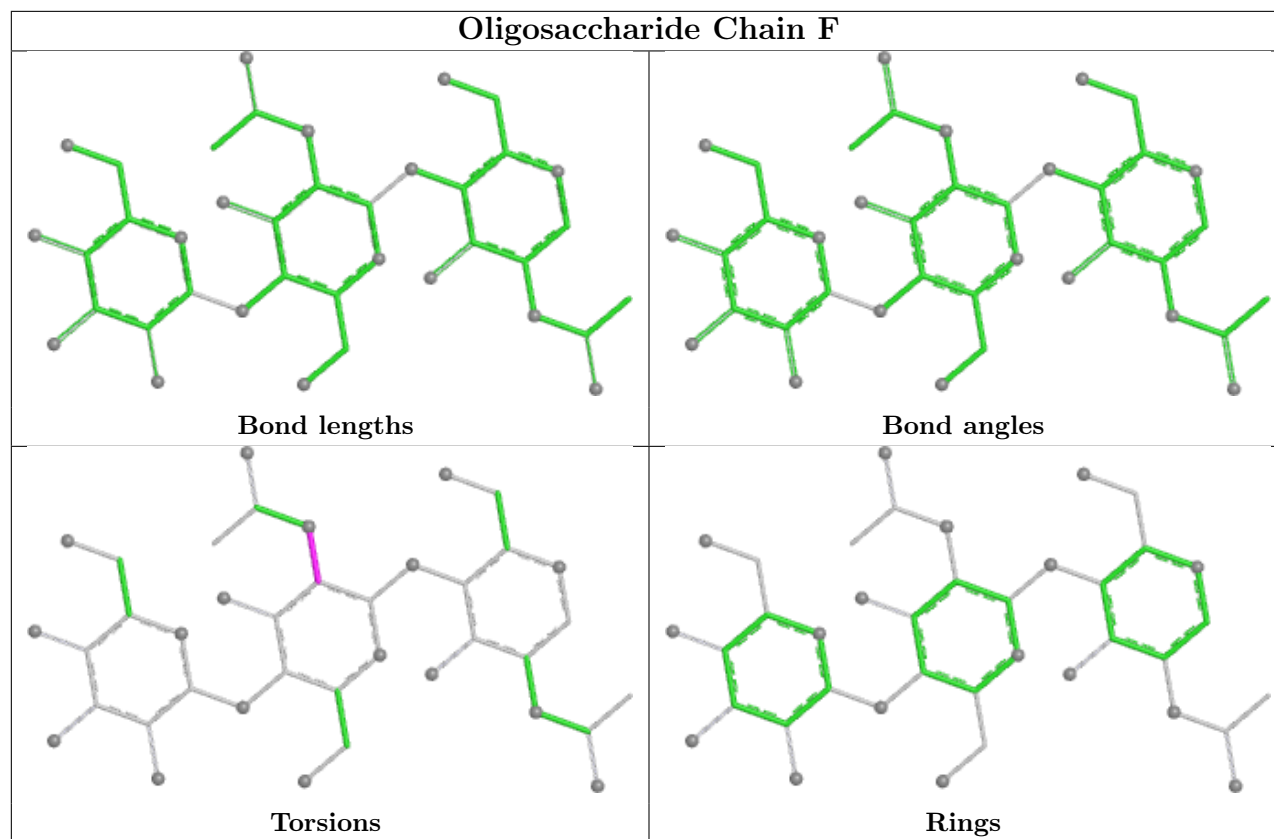
6 monomers are involved in 4 short contacts:

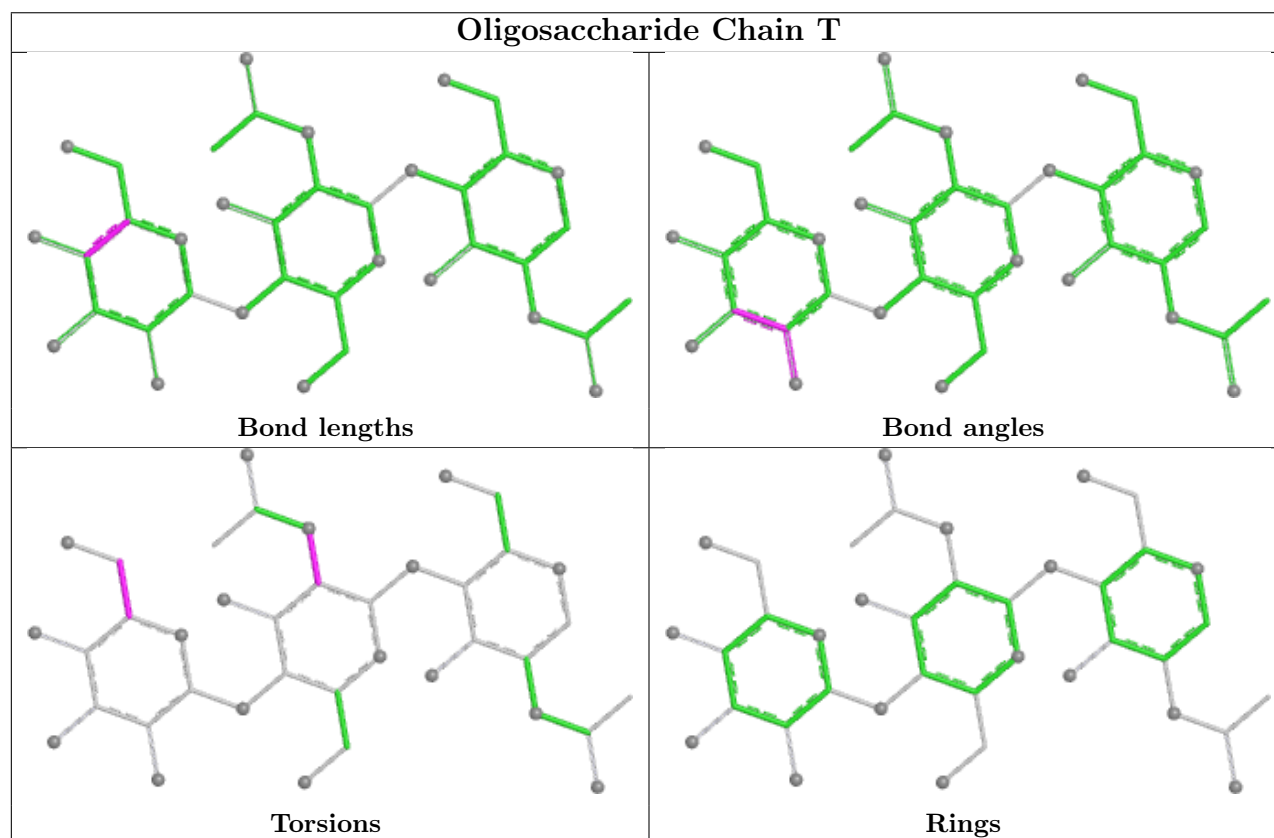
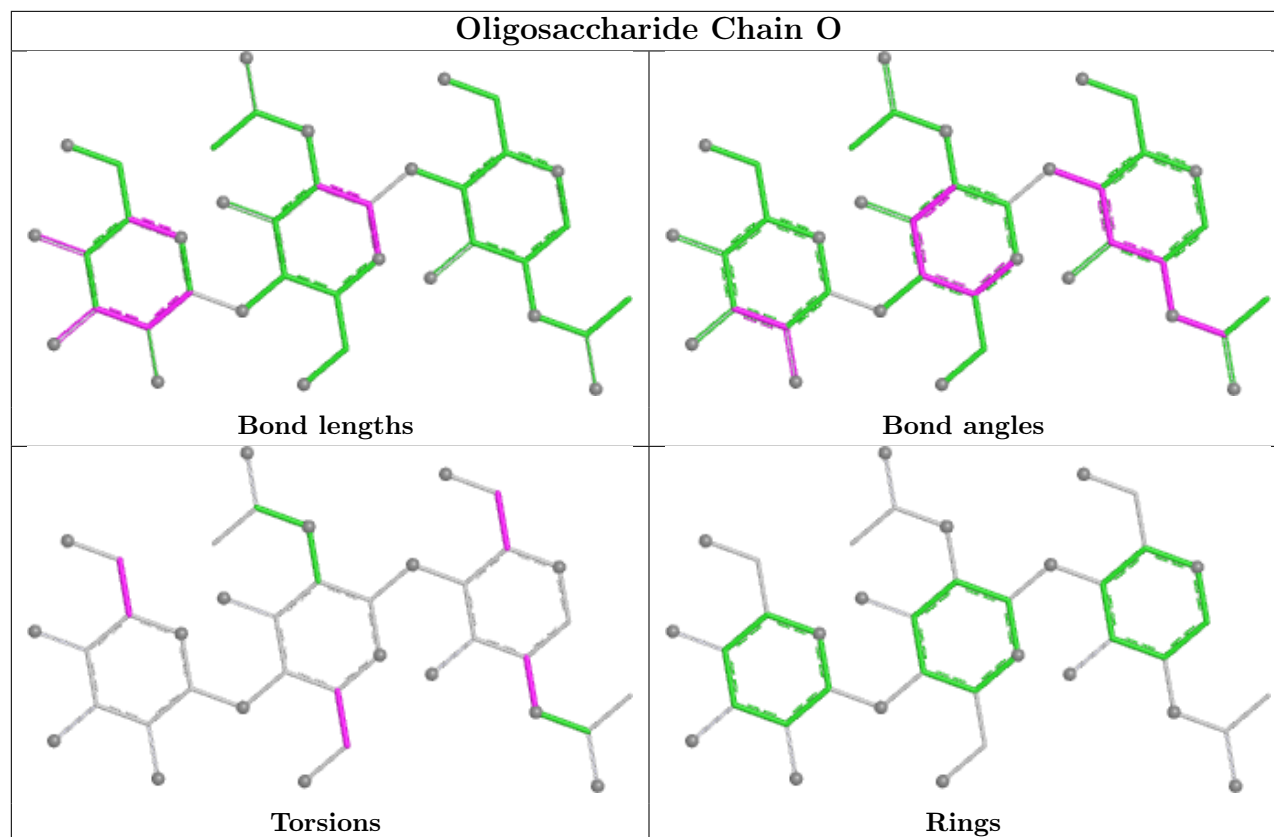
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	1	0
5	F	2	NAG	1	0
5	G	3	BMA	1	0
5	O	2	NAG	1	0
5	O	1	NAG	2	0
5	G	2	NAG	1	0

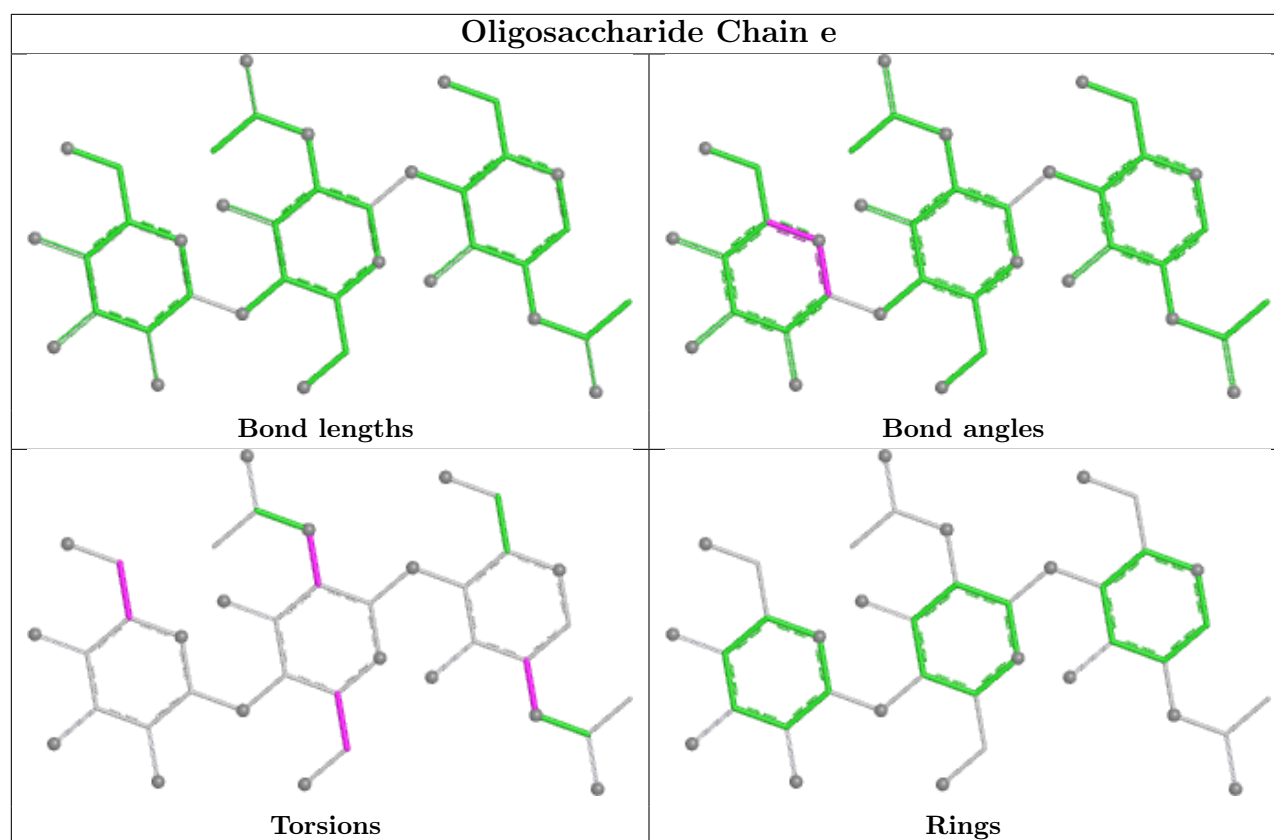
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	V	601	-	14,14,15	0.27	0	17,19,21	0.42	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
6	NAG	V	601	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

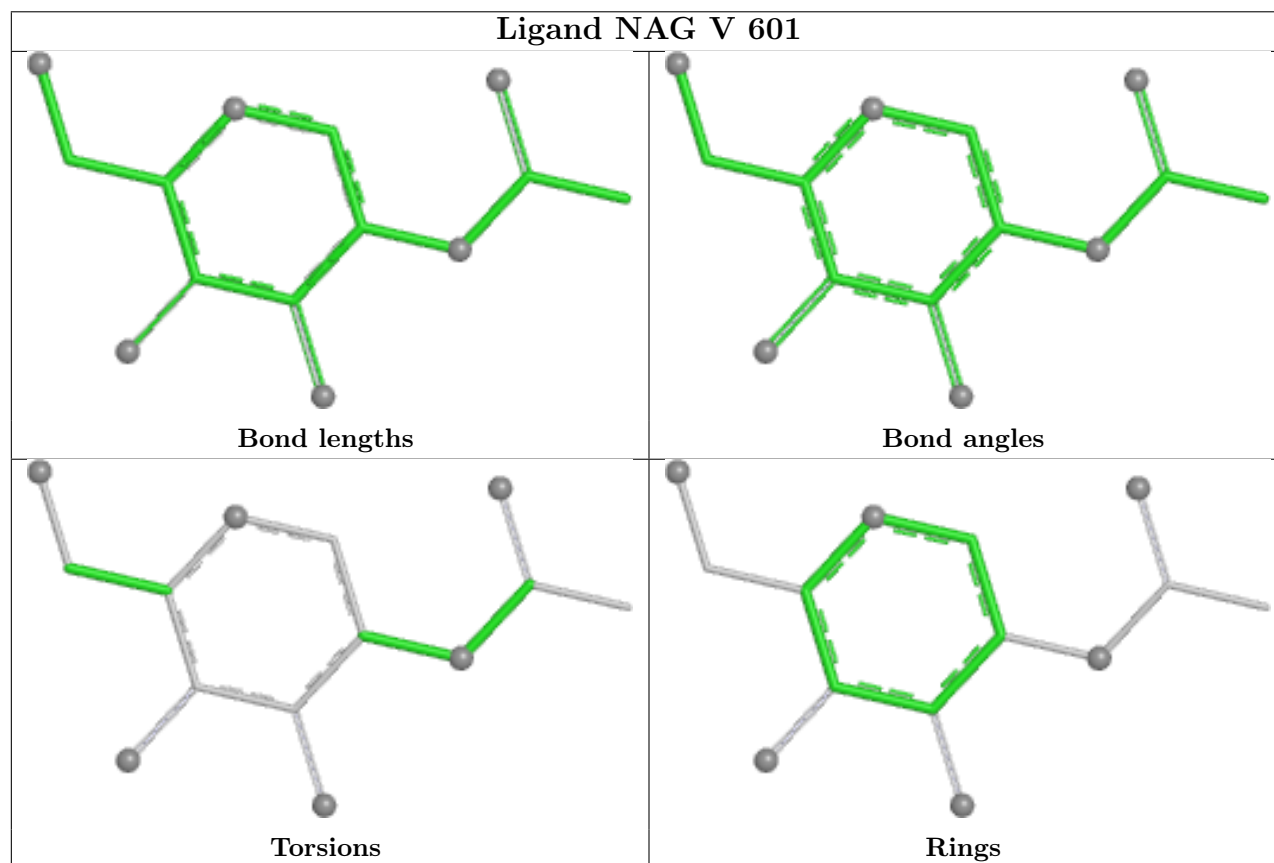
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	B	168/504 (33%)	0.18	2 (1%) 76 61	143, 193, 240, 248	0
1	C	323/504 (64%)	0.42	21 (6%) 25 26	159, 225, 243, 254	0
1	H	168/504 (33%)	0.31	8 (4%) 35 33	133, 170, 239, 251	0
1	I	168/504 (33%)	0.45	10 (5%) 27 29	147, 180, 248, 258	0
1	L	323/504 (64%)	0.30	10 (3%) 51 41	87, 193, 207, 218	0
1	P	168/504 (33%)	0.41	11 (6%) 25 26	161, 184, 266, 273	0
1	Q	323/504 (64%)	0.37	10 (3%) 51 41	171, 239, 258, 266	0
1	U	168/504 (33%)	0.32	10 (5%) 27 29	174, 224, 269, 277	0
1	V	323/504 (64%)	0.42	21 (6%) 25 26	175, 266, 280, 295	0
1	Y	323/504 (64%)	0.38	20 (6%) 26 28	146, 212, 228, 240	0
1	a	168/504 (33%)	0.38	12 (7%) 22 24	135, 180, 255, 267	0
1	b	323/504 (64%)	0.29	13 (4%) 42 37	30, 228, 247, 258	0
2	D	212/214 (99%)	0.37	11 (5%) 33 31	202, 249, 297, 303	0
2	J	212/214 (99%)	0.09	1 (0%) 87 75	142, 171, 208, 222	0
2	M	212/214 (99%)	0.38	14 (6%) 24 26	118, 152, 179, 190	0
2	R	212/214 (99%)	0.15	7 (3%) 49 40	153, 191, 222, 226	0
2	W	211/214 (98%)	0.61	18 (8%) 16 20	263, 324, 370, 376	0
2	c	212/214 (99%)	0.28	13 (6%) 27 28	124, 153, 184, 204	0
3	E	221/224 (98%)	0.42	8 (3%) 46 39	126, 257, 310, 317	0
3	K	221/224 (98%)	0.16	3 (1%) 73 58	77, 165, 177, 188	0
3	N	221/224 (98%)	0.27	10 (4%) 38 35	82, 149, 197, 224	0
3	S	221/224 (98%)	0.23	9 (4%) 41 37	87, 183, 212, 223	0
3	X	221/224 (98%)	0.56	10 (4%) 38 35	152, 325, 375, 379	0
3	d	221/224 (98%)	0.20	11 (4%) 34 32	83, 148, 186, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5543/8676 (63%)	0.33	263 (4%)	36	34	30, 199, 308, 379	0

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	185	VAL	7.1
1	V	71	ILE	6.8
1	Y	13	LEU	5.4
3	N	146	LEU	5.1
1	V	115	PHE	4.9
2	W	133	VAL	4.8
1	C	187	GLY	4.8
1	Q	71	ILE	4.6
1	C	189	HIS	4.6
1	Y	184	ILE	4.6
1	Q	67	PHE	4.6
1	C	275	PHE	4.6
2	W	134	CYS	4.6
1	a	7	ALA	4.4
1	V	159	TRP	4.4
1	b	306	HIS	4.4
2	D	73	LEU	4.3
1	C	159	TRP	4.2
3	X	35	ILE	4.2
1	C	67	PHE	4.2
2	J	70	GLU	4.1
1	Y	160	LEU	3.9
1	Y	260	PRO	3.8
1	b	276	PHE	3.8
1	C	258	LEU	3.8
1	U	91	ILE	3.8
1	P	66	VAL	3.7
1	Y	159	TRP	3.7
3	X	96	ALA	3.7
1	Y	71	ILE	3.6
2	c	98	PHE	3.6
1	C	68	ALA	3.6
1	P	20	GLY	3.6
1	H	141	TYR	3.6
2	c	47	LEU	3.6
3	N	145	ALA	3.6
2	W	21	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	U	103	GLU	3.5
1	V	156	ASN	3.5
1	C	188	ILE	3.5
2	D	135	LEU	3.4
2	W	135	LEU	3.4
2	M	86	TYR	3.4
1	C	158	VAL	3.4
1	L	200	LEU	3.4
1	L	191	PRO	3.4
1	Y	157	MET	3.4
1	C	323	LEU	3.4
1	Q	13	LEU	3.4
1	C	115	PHE	3.3
3	d	105	GLY	3.3
2	W	212	GLY	3.3
2	M	118	PHE	3.2
1	H	7	ALA	3.2
1	Y	132	TRP	3.2
1	U	139	GLU	3.2
1	V	301	PHE	3.2
1	a	21	TRP	3.2
1	L	185	VAL	3.2
1	Q	298	SER	3.1
2	M	35	TRP	3.1
1	B	103	GLU	3.1
1	I	66	VAL	3.1
1	Y	115	PHE	3.1
2	M	78	LEU	3.1
1	Q	159	TRP	3.1
2	R	135	LEU	3.1
1	P	24	TYR	3.1
2	M	19	VAL	3.0
1	Y	298	SER	3.0
3	E	127	PRO	3.0
2	c	73	LEU	3.0
1	I	112	ASP	3.0
3	N	189	VAL	3.0
3	S	189	VAL	3.0
2	c	177	SER	3.0
3	S	173	THR	3.0
1	V	258	LEU	3.0
1	Q	15	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	V	298	SER	2.9
1	Y	251	PHE	2.9
2	M	89	GLN	2.9
1	V	139	ALA	2.9
2	R	176	SER	2.9
1	H	79	ASN	2.9
1	H	140	PHE	2.9
2	M	34	ALA	2.8
1	V	184	ILE	2.8
1	H	60	ASN	2.8
1	b	117	GLY	2.8
3	X	131	PRO	2.8
1	Q	257	PHE	2.8
1	Q	186	TRP	2.8
3	d	150	VAL	2.8
2	c	89	GLN	2.8
2	c	145	LYS	2.8
1	U	65	ALA	2.8
3	S	174	PHE	2.7
1	C	71	ILE	2.7
3	d	129	VAL	2.7
3	d	37	ILE	2.7
1	a	72	HIS	2.7
1	P	7	ALA	2.7
3	d	127	PRO	2.7
2	M	73	LEU	2.7
1	Q	184	ILE	2.7
1	b	303	GLN	2.7
1	C	236	MET	2.7
3	d	151	LYS	2.7
1	b	250	ILE	2.7
3	d	215	VAL	2.7
2	W	116	PHE	2.7
1	C	321	LEU	2.7
2	M	212	GLY	2.7
1	P	140	PHE	2.7
2	R	136	LEU	2.6
2	R	175	LEU	2.6
1	b	65	CYS	2.6
3	E	187	SER	2.6
3	d	187	SER	2.6
1	a	57	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	W	178	THR	2.6
1	H	40	SER	2.6
1	V	81	ILE	2.6
1	Y	170	ILE	2.6
1	a	66	VAL	2.6
1	L	302	GLN	2.6
1	V	275	PHE	2.5
1	a	118	LEU	2.5
2	M	196	VAL	2.5
1	V	153	PHE	2.5
2	R	133	VAL	2.5
2	c	146	VAL	2.5
2	D	165	GLU	2.5
1	L	201	TYR	2.5
2	D	134	CYS	2.5
2	D	21	ILE	2.5
1	P	22	TYR	2.5
1	b	302	PHE	2.5
2	D	35	TRP	2.5
2	W	163	VAL	2.5
1	I	24	TYR	2.5
1	V	224	SER	2.5
1	a	40	SER	2.5
2	W	30	SER	2.5
2	W	142	ARG	2.5
1	I	56	ILE	2.4
3	X	34	TRP	2.4
2	D	206	THR	2.4
3	K	106	VAL	2.4
1	b	88	TYR	2.4
3	d	20	LEU	2.4
1	I	65	ALA	2.4
1	Y	263	ALA	2.4
2	D	118	PHE	2.4
1	V	82	GLY	2.3
1	Q	142	THR	2.3
1	V	289	GLN	2.3
1	C	139	ALA	2.3
3	X	50	ARG	2.3
2	W	73	LEU	2.3
1	L	91	GLU	2.3
3	K	98	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	X	27	ALA	2.3
1	L	275	PHE	2.3
1	U	84	VAL	2.3
1	b	90	VAL	2.3
1	V	328	ARG	2.3
3	N	180	SER	2.3
3	S	187	SER	2.3
1	a	67	GLY	2.3
1	B	66	VAL	2.3
1	V	104	THR	2.3
1	P	149	MET	2.3
2	M	90	GLN	2.3
1	b	291	THR	2.3
1	I	91	ILE	2.3
1	b	185	ILE	2.3
3	K	104	GLY	2.3
3	S	190	VAL	2.3
1	H	76	ARG	2.3
3	E	110	TYR	2.2
1	H	122	VAL	2.2
1	U	66	VAL	2.2
2	D	116	PHE	2.2
1	P	67	GLY	2.2
2	D	114	SER	2.2
2	c	131	SER	2.2
3	d	189	VAL	2.2
1	C	99	ILE	2.2
1	Y	215	TYR	2.2
1	b	322	LEU	2.2
3	X	176	ALA	2.2
2	M	156	SER	2.2
1	Y	70	TRP	2.2
1	V	187	GLY	2.2
1	Y	158	VAL	2.2
3	N	71	VAL	2.2
1	a	76	ARG	2.2
1	L	88	TYR	2.2
1	U	108	LEU	2.2
1	P	23	GLY	2.2
2	W	113	PRO	2.2
3	E	41	ALA	2.2
3	E	145	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	X	143	THR	2.2
1	C	298	SER	2.2
3	S	149	LEU	2.2
2	R	186	TYR	2.2
3	X	87	ALA	2.2
1	U	60	ASN	2.2
2	W	145	LYS	2.2
2	W	201	LEU	2.2
3	E	42	GLY	2.1
1	C	160	LEU	2.1
1	Y	164	SER	2.1
1	I	59	MET	2.1
3	N	22	CYS	2.1
1	P	73	LEU	2.1
1	V	183	LEU	2.1
2	c	48	ILE	2.1
1	Y	20	ASN	2.1
2	D	164	THR	2.1
2	c	133	VAL	2.1
1	V	236	MET	2.1
1	Y	122	SER	2.1
2	c	108	ARG	2.1
2	R	134	CYS	2.1
2	W	45	LYS	2.1
1	I	79	ASN	2.1
3	E	97	ARG	2.1
3	N	147	GLY	2.1
3	X	194	SER	2.1
1	V	266	ILE	2.1
2	c	178	THR	2.1
1	U	8	GLY	2.1
1	a	75	LYS	2.1
1	C	161	ILE	2.1
1	U	10	ILE	2.1
2	M	98	PHE	2.1
3	S	48	ILE	2.1
2	M	104	VAL	2.1
1	I	144	CYS	2.1
1	L	153	PHE	2.1
3	N	42	GLY	2.1
2	W	40	PRO	2.1
1	a	10	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	W	72	THR	2.1
3	E	173	THR	2.1
2	c	35	TRP	2.1
3	N	151	LYS	2.0
1	C	88	TYR	2.0
1	P	65	ALA	2.0
3	N	37	ILE	2.0
1	a	79	ASN	2.0
1	C	257	PHE	2.0
1	I	10	ILE	2.0
2	W	9	ALA	2.0
3	S	135	SER	2.0
3	d	42	GLY	2.0
1	b	128	THR	2.0
3	S	132	LEU	2.0
1	L	67	PHE	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.

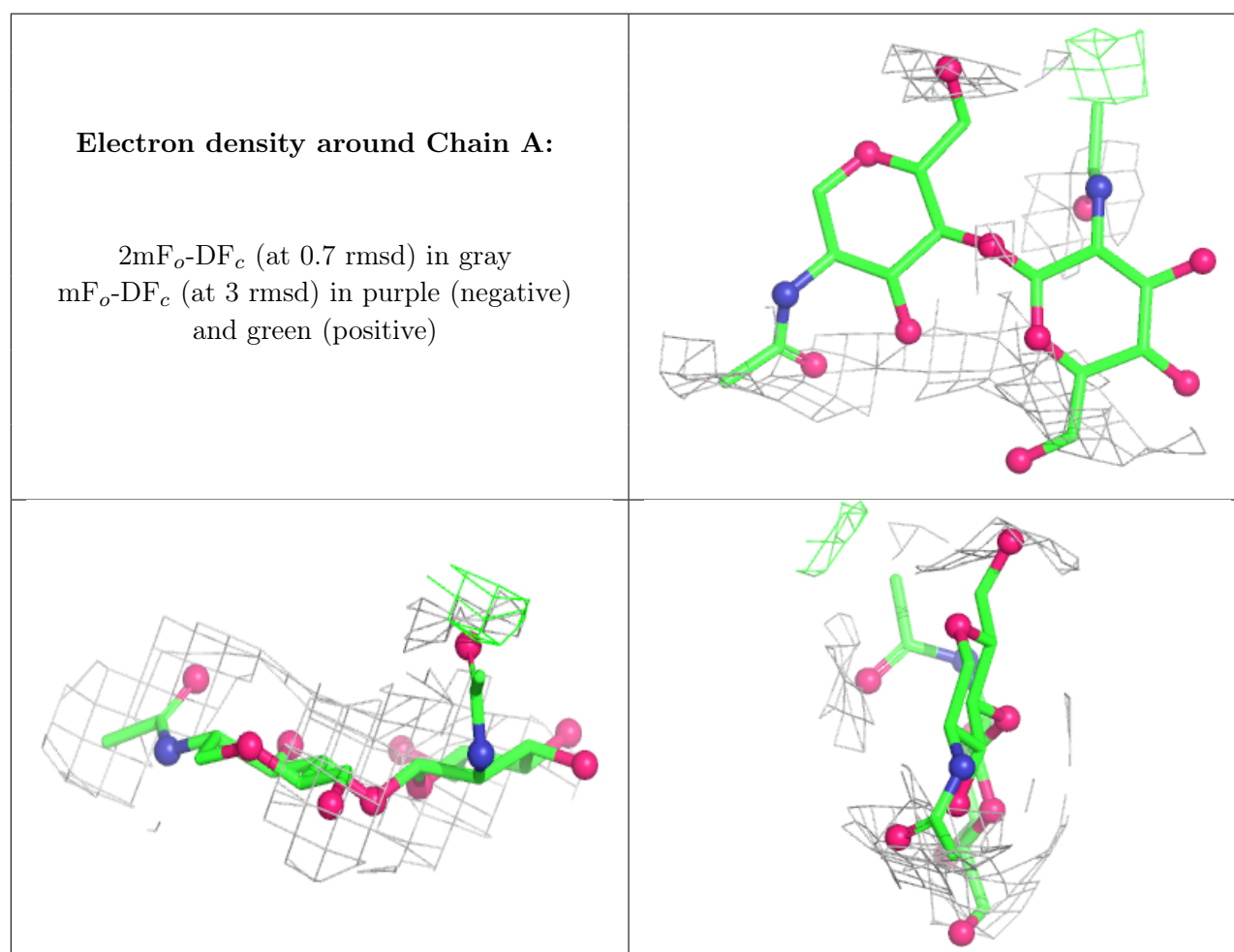
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	203,203,203,203	0
4	NAG	A	2	14/15	-	-	208,208,208,208	0
4	NAG	Z	2	14/15	0.83	0.09	192,192,192,192	0
4	NAG	Z	1	14/15	0.88	0.17	181,181,181,181	0
5	NAG	F	1	14/15	-	-	206,206,206,206	0
5	NAG	F	2	14/15	-	-	212,212,212,212	0
5	BMA	F	3	11/12	-	-	218,218,218,218	0
5	NAG	G	1	14/15	-	-	184,184,184,184	0
5	NAG	G	2	14/15	-	-	188,188,188,188	0
5	BMA	G	3	11/12	-	-	191,191,191,191	0
5	NAG	O	1	14/15	-	-	233,233,233,233	0
5	NAG	O	2	14/15	-	-	243,243,243,243	0

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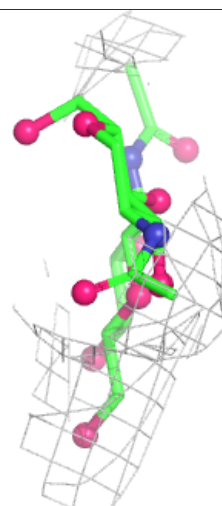
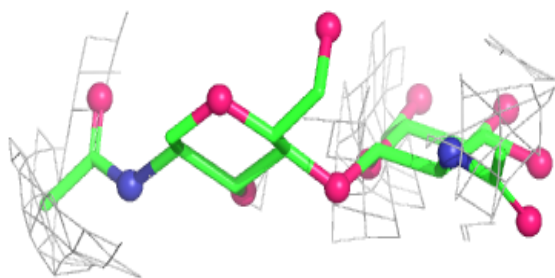
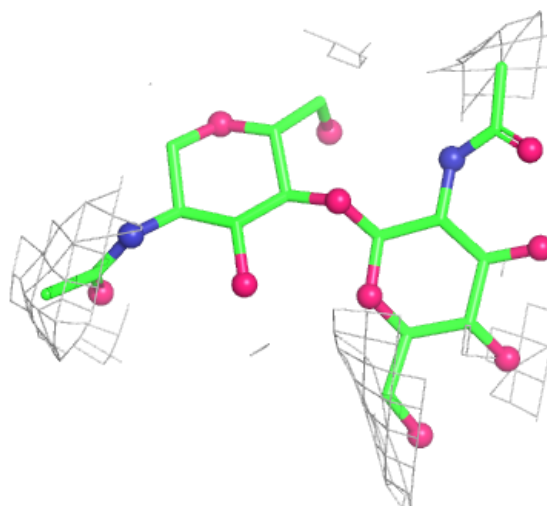
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	O	3	11/12	-	-	250,250,250,250	0
5	NAG	T	1	14/15	-	-	238,238,238,238	0
5	NAG	T	2	14/15	-	-	250,250,250,250	0
5	BMA	T	3	11/12	-	-	256,256,256,256	0
5	NAG	e	1	14/15	-	-	202,202,202,202	0
5	NAG	e	2	14/15	-	-	206,206,206,206	0
5	BMA	e	3	11/12	-	-	204,204,204,204	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.



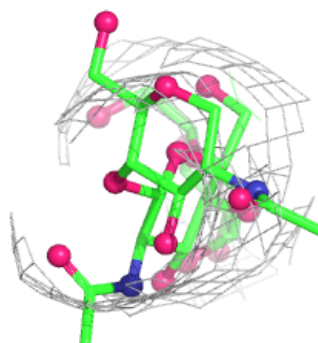
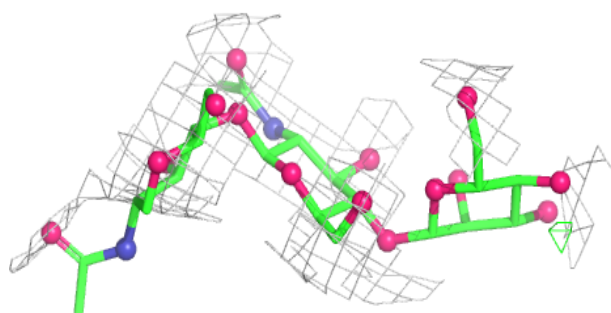
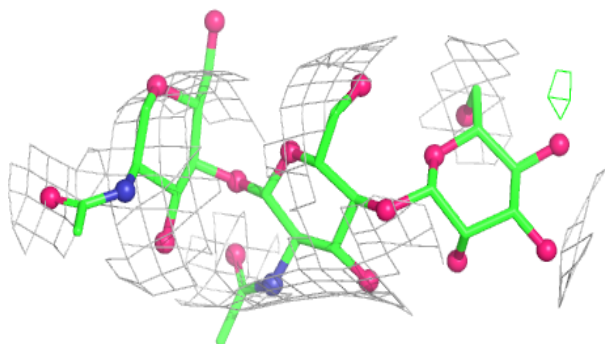
Electron density around Chain Z:

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

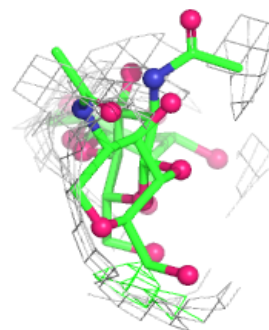
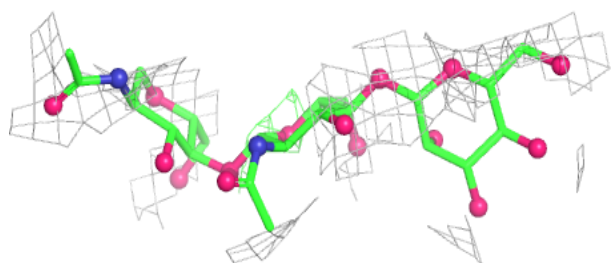
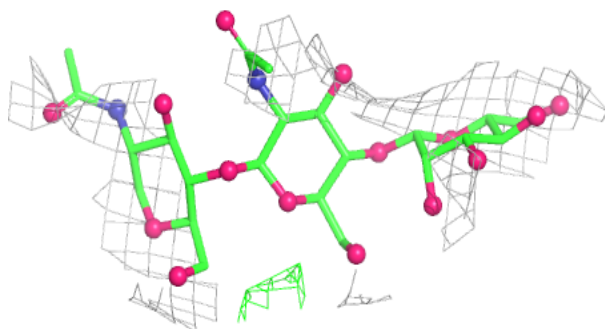


Electron density around Chain F:

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

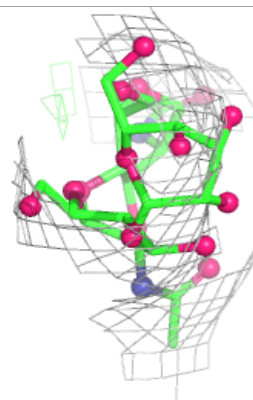
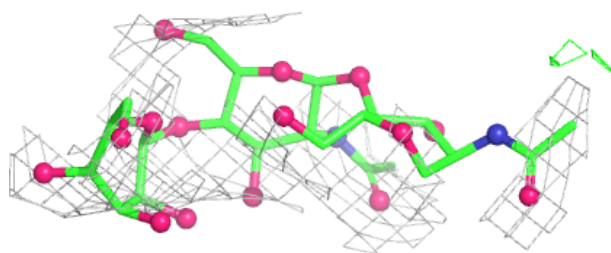
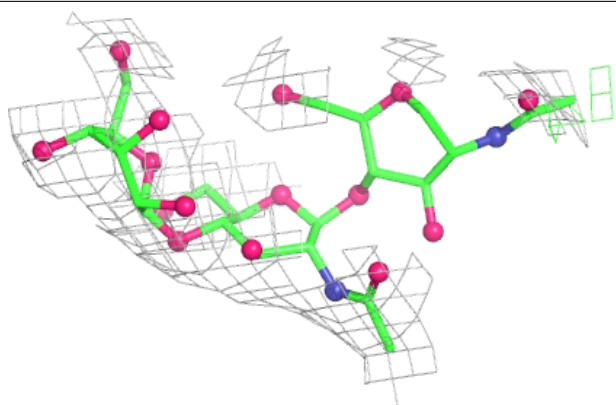
**Electron density around Chain G:**

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

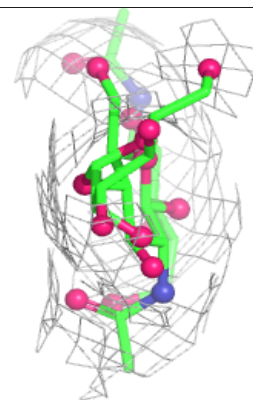
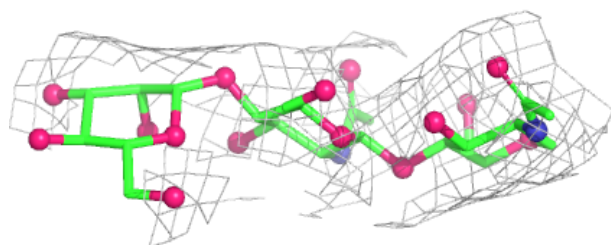
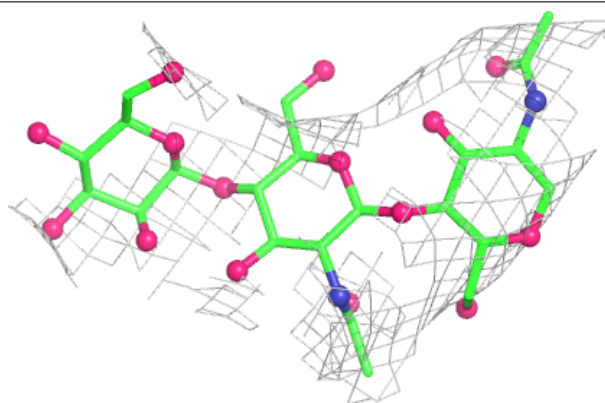


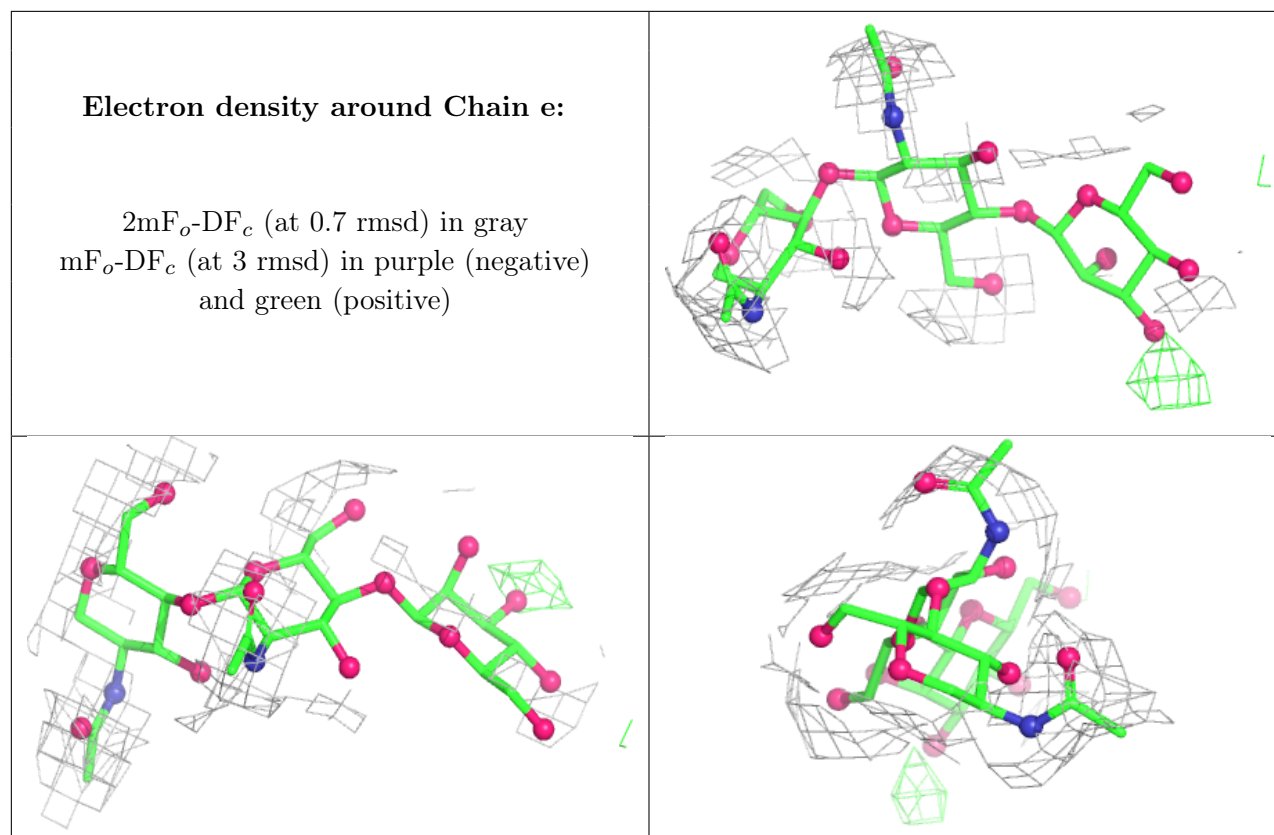
Electron density around Chain O:

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

**Electron density around Chain T:**

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



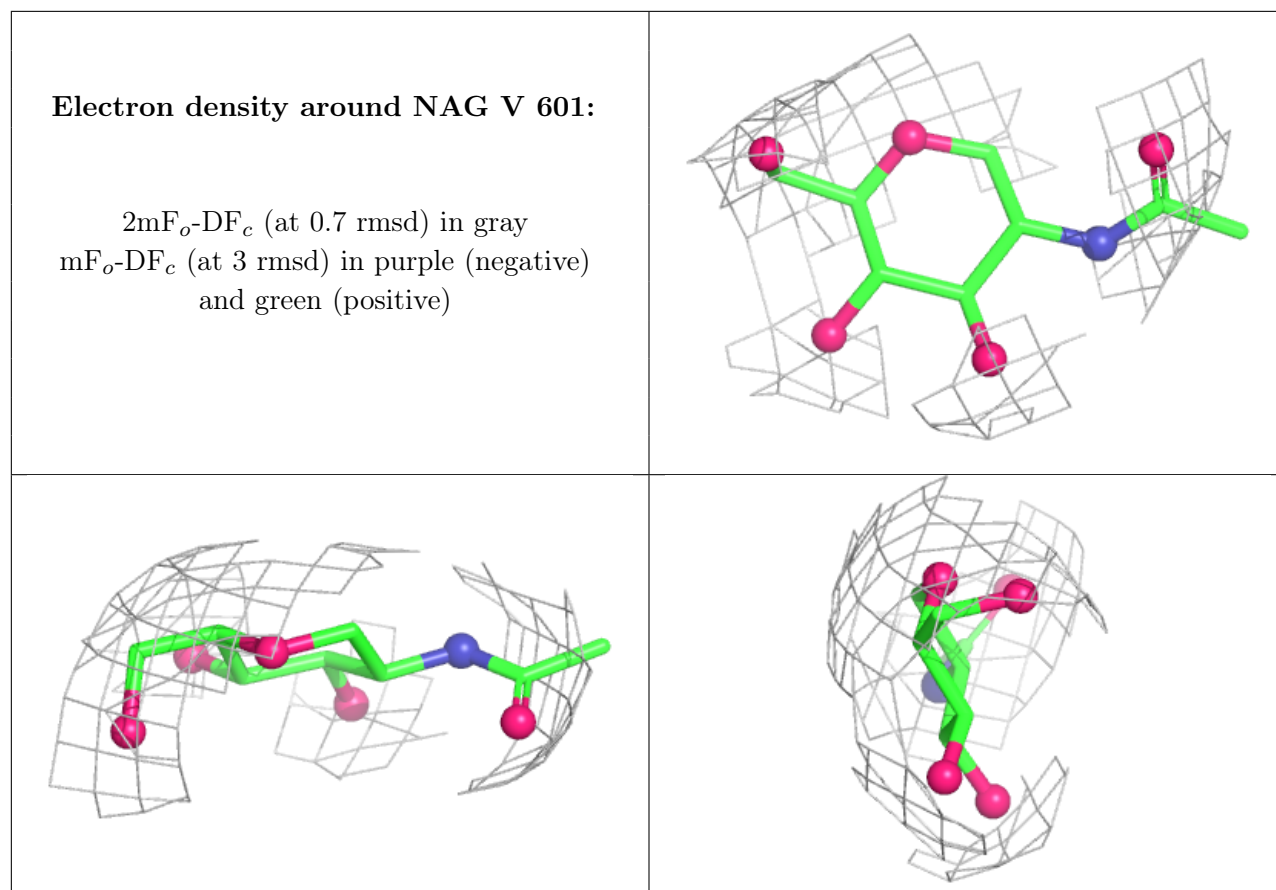


6.4 Ligands [i](#)

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
6	NAG	V	601	14/15	0.89	0.10	160,160,160,160	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.