



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:24 AM UTC

PDB ID : 3QUM / pdb_00003qum
Title : Crystal structure of human prostate specific antigen (PSA) in Fab sandwich with a high affinity and a PCa selective antibody
Authors : Stura, E.A.; Muller, B.H.; Michel, S.; Ducancel, F.
Deposited on : 2011-02-24
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

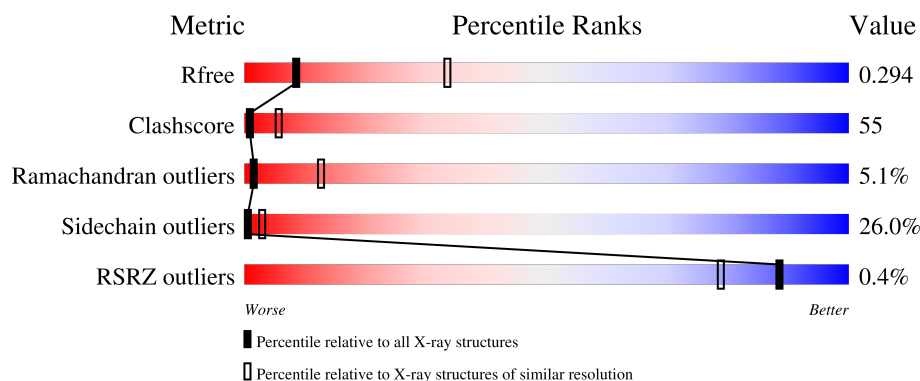
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



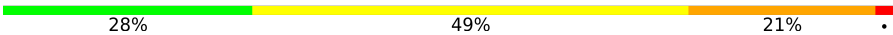
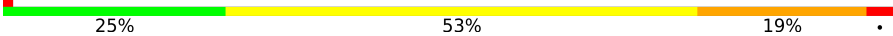
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	P	237	2% 34% 47% 16% .
1	Q	237	26% 51% 21% .
2	L	219	26% 56% 16% .
2	M	219	28% 52% 17% .
3	H	219	29% 47% 21% ..

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Mol	Chain	Length	Quality of chain
3	K	219	
4	A	218	
4	C	218	
5	B	219	
5	D	219	
6	E	15	
7	F	2	
8	G	15	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17606 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 Prostate-specific antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	237	Total	C	N	O	S	4	0	0
			1832	1162	323	333	14			
1	Q	237	Total	C	N	O	S	0	0	0
			1832	1162	323	333	14			

- Molecule 2 is a protein called Fab 5D3D11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			
2	M	219	Total	C	N	O	S	0	0	0
			1704	1063	289	343	9			

- Molecule 3 is a protein called Fab 5D3D11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1637	1040	267	323	7			
3	K	219	Total	C	N	O	S	0	0	0
			1657	1050	272	328	7			

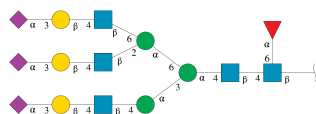
- Molecule 4 is a protein called Fab 5D5A5 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			
4	C	218	Total	C	N	O	S	0	0	0
			1701	1062	287	345	7			

- Molecule 5 is a protein called Fab 5D5A5 Heavy Chain.

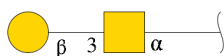
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			
5	D	219	Total	C	N	O	S	0	0	0
			1655	1043	273	330	9			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



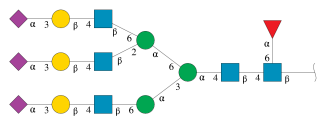
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	E	15	Total	C	N	O	0	0	0
			206	115	8	83			

- Molecule 7 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	F	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	G	15	Total	C	N	O	0	0	0
			206	115	8	83			

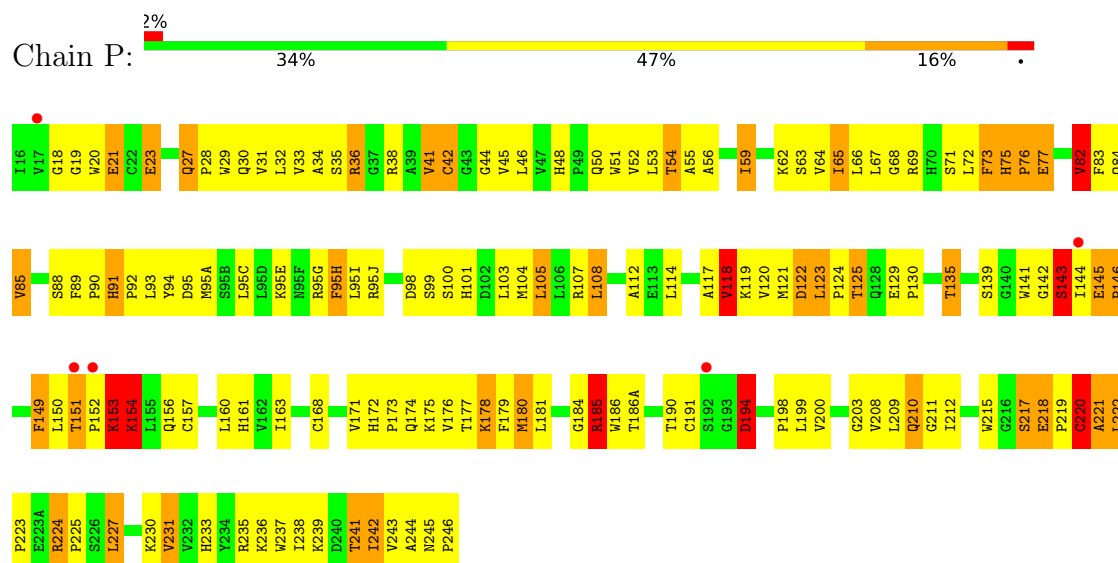
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	26	Total	O	0	0
			26	26		
9	L	4	Total	O	0	0
			4	4		
9	H	10	Total	O	0	0
			10	10		
9	A	4	Total	O	0	0
			4	4		
9	B	4	Total	O	0	0
			4	4		
9	Q	5	Total	O	0	0
			5	5		
9	M	6	Total	O	0	0
			6	6		
9	K	14	Total	O	0	0
			14	14		
9	C	11	Total	O	0	0
			11	11		
9	D	7	Total	O	0	0
			7	7		

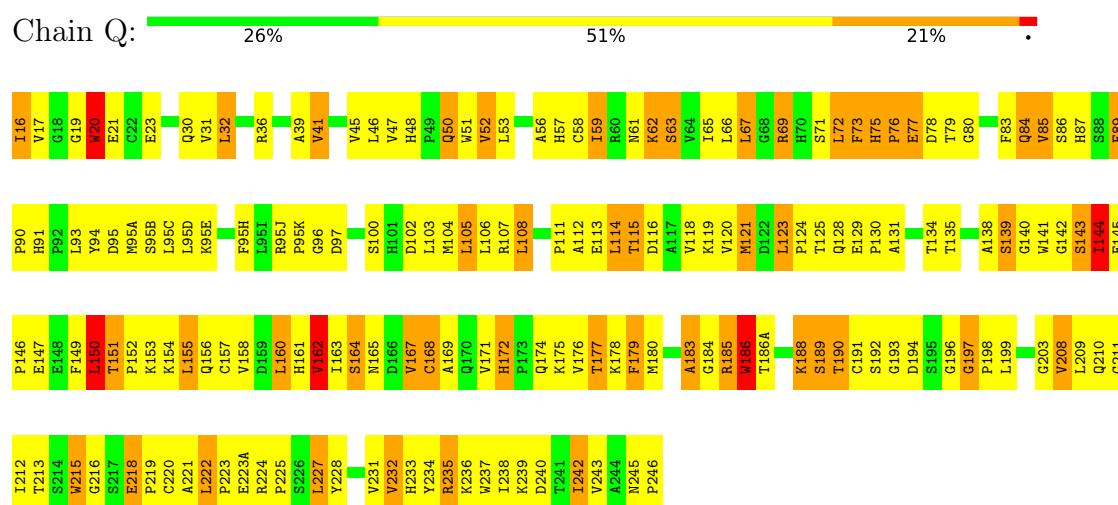
3 Residue-property plots [i](#)

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

• Molecule 1: Prostate-specific antigen

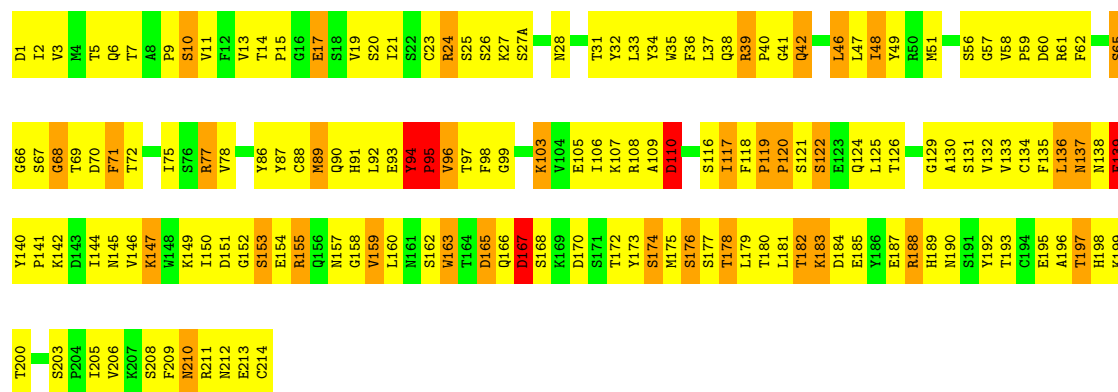


• Molecule 1: Prostate-specific antigen



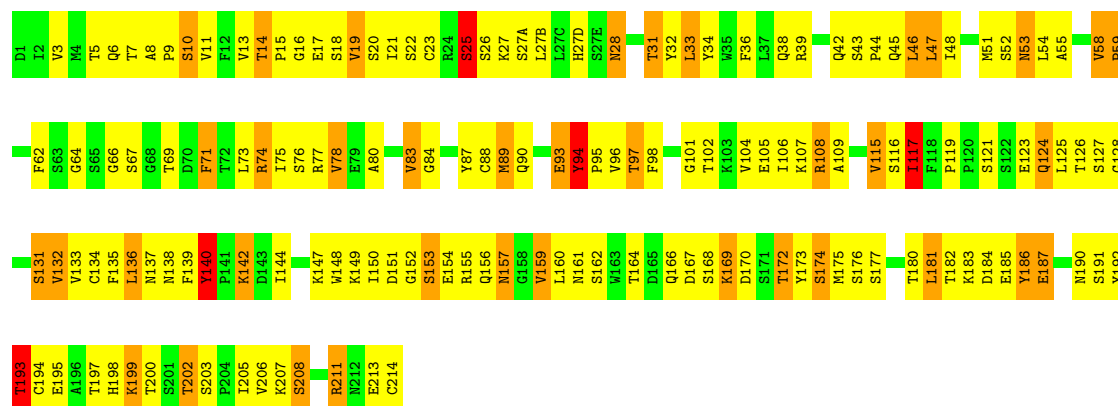
• Molecule 2: Fab 5D3D11 Light Chain





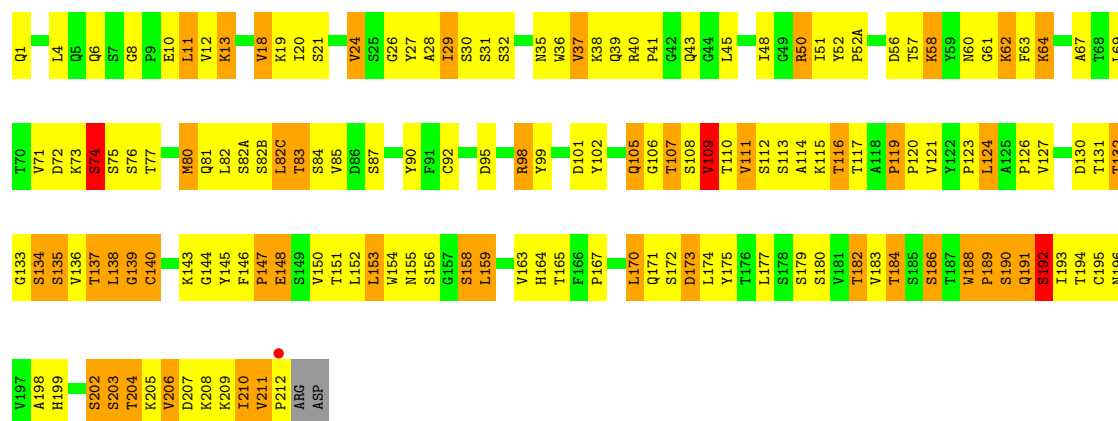
• Molecule 2: Fab 5D3D11 Light Chain

Chain M: 28% 52% 17%



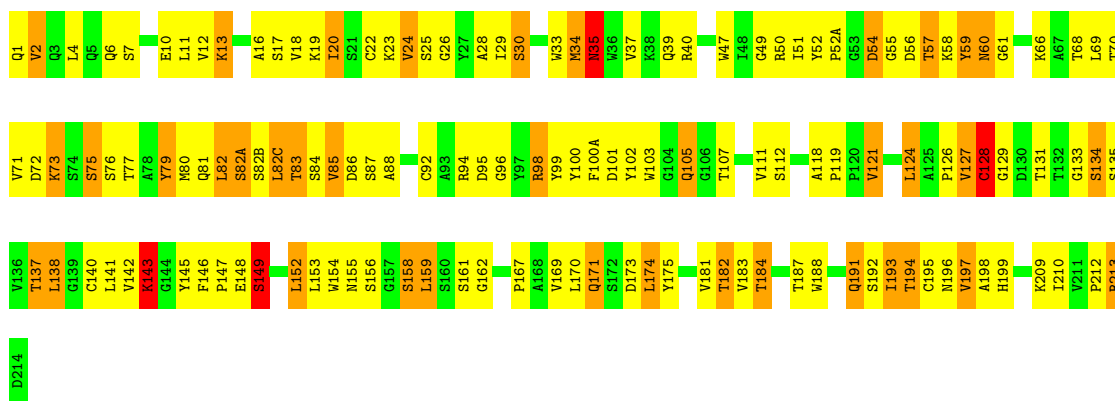
• Molecule 3: Fab 5D3D11 Heavy Chain

Chain H: 29% 47% 21%



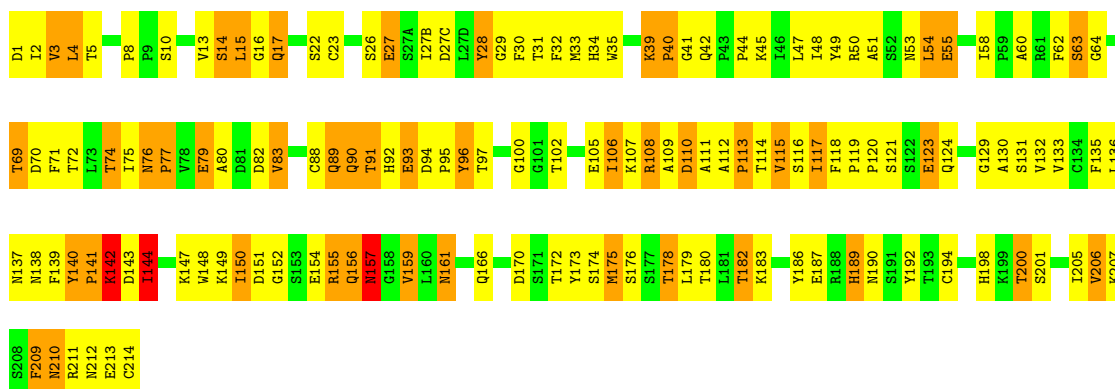
• Molecule 3: Fab 5D3D11 Heavy Chain

Chain K: 37% 44% 17%



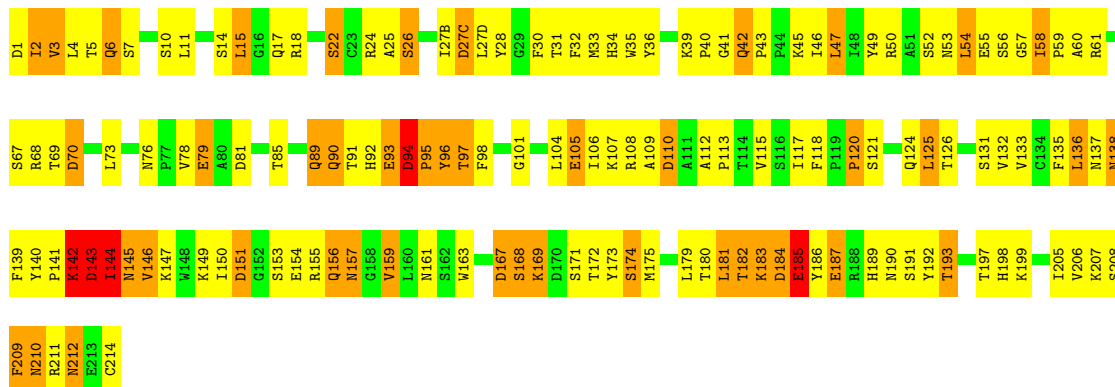
• Molecule 4: Fab 5D5A5 Light Chain

Chain A: 33% 44% 21%



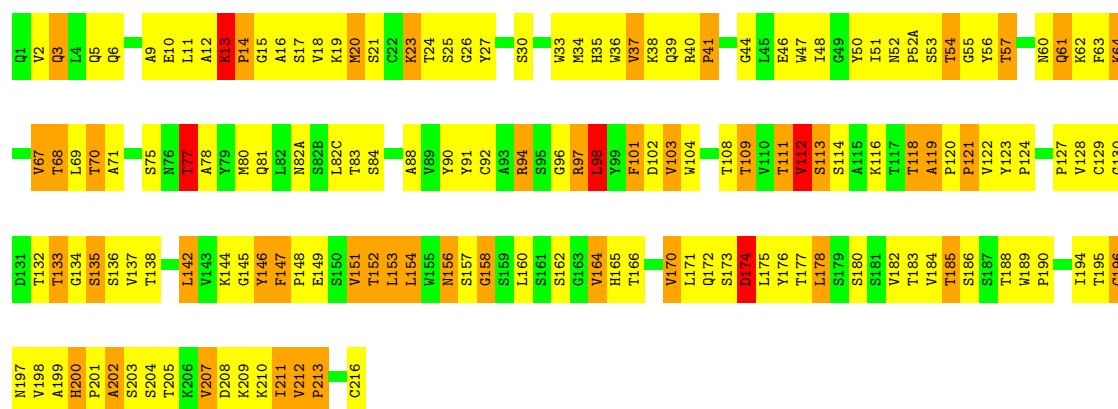
• Molecule 4: Fab 5D5A5 Light Chain

Chain C: 33% 45% 20%

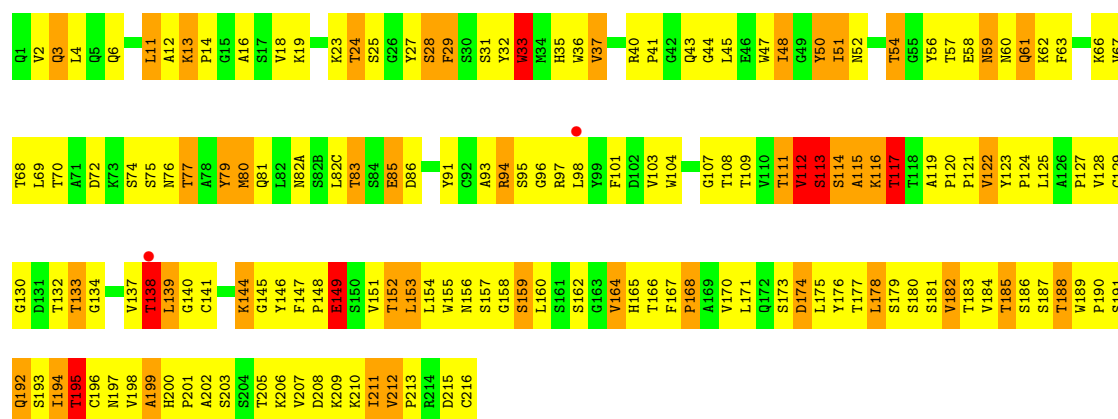


• Molecule 5: Fab 5D5A5 Heavy Chain

Chain B: 28% 49% 21%



• Molecule 5: Fab 5D5A5 Heavy Chain



• Molecule 6: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose



- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	STAA7	MAN8	NAG9	GAL10	STAA11	NAG12	GAL13	STAA14	FUC15
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 226.88Å 118.69Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	58.97 – 3.20 58.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (58.97-3.20) 98.3 (58.97-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.198 , 0.294 0.203 , 0.294	Depositor DCC
R_{free} test set	2370 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	78.1	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17606	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NAG, SIA, MAN, GAL, A2G, FUC

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	P	0.98	2/1883 (0.1%)	1.32	22/2564 (0.9%)
1	Q	0.59	0/1883	1.06	12/2564 (0.5%)
2	L	0.73	0/1743	1.17	10/2366 (0.4%)
2	M	0.74	1/1743 (0.1%)	1.12	13/2366 (0.5%)
3	H	0.85	1/1680 (0.1%)	1.21	13/2294 (0.6%)
3	K	0.89	1/1700 (0.1%)	1.14	8/2319 (0.3%)
4	A	0.68	0/1742	1.10	12/2368 (0.5%)
4	C	0.73	1/1742 (0.1%)	1.03	9/2368 (0.4%)
5	B	0.71	0/1697	1.10	9/2316 (0.4%)
5	D	0.66	0/1697	1.10	10/2316 (0.4%)
All	All	0.76	6/17510 (0.0%)	1.14	118/23841 (0.5%)

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	P	0	2
2	M	0	1
3	H	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	220	CYS	CA-C	-10.20	1.39	1.52
4	C	144	ILE	CA-CB	-6.63	1.45	1.54
3	H	109	VAL	CA-CB	5.75	1.60	1.54
3	K	142	VAL	CA-CB	-5.61	1.47	1.54
2	M	96	VAL	CA-CB	-5.56	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	118	VAL	CA-CB	5.09	1.61	1.54

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	43	GLN	N-CA-C	9.24	120.96	111.07
1	P	154	LYS	N-CA-C	9.09	122.53	110.53
1	P	48	HIS	CA-C-N	-9.06	110.32	119.56
1	P	48	HIS	C-N-CA	-9.06	110.32	119.56
2	L	200	THR	N-CA-C	-8.37	102.08	112.88
3	H	139	GLY	N-CA-C	8.20	122.72	110.75
3	H	8	GLY	CA-C-N	8.10	128.12	119.78
3	H	8	GLY	C-N-CA	8.10	128.12	119.78
5	B	113	SER	N-CA-C	8.04	127.91	110.80
1	P	27	GLN	CA-C-N	7.68	128.08	119.32
1	P	27	GLN	C-N-CA	7.68	128.08	119.32
5	D	195	THR	N-CA-C	7.53	118.21	108.34
2	M	27(A)	SER	N-CA-C	-7.50	100.14	110.35
3	K	143	LYS	N-CA-C	7.49	123.97	114.31
1	P	231	VAL	N-CA-C	7.49	117.61	110.42
2	L	153	SER	N-CA-C	7.22	118.13	108.38
1	Q	143	SER	N-CA-C	7.14	119.15	111.36
5	B	149	GLU	N-CA-C	7.01	119.82	111.33
1	Q	183	ALA	N-CA-C	6.86	116.92	107.73
5	B	158	GLY	N-CA-C	-6.71	105.81	115.27
1	Q	150	LEU	N-CA-C	6.66	118.69	109.29
1	P	91	HIS	CA-C-N	6.59	128.08	119.84
1	P	91	HIS	C-N-CA	6.59	128.08	119.84
5	D	144	LYS	N-CA-C	6.54	119.47	108.02
1	Q	179	PHE	N-CA-C	-6.48	105.37	113.28
3	H	191	GLN	N-CA-C	6.48	119.91	109.02
2	L	94	TYR	N-CA-C	6.40	123.96	109.81
3	H	192	SER	N-CA-C	6.35	118.92	109.59
2	L	32	TYR	N-CA-C	6.33	120.52	110.70
2	L	203	SER	CA-C-N	6.31	127.73	119.84
2	L	203	SER	C-N-CA	6.31	127.73	119.84
1	P	224	ARG	N-CA-C	6.28	117.97	109.24
3	H	108	SER	N-CA-C	6.27	119.18	108.02
1	P	73	PHE	CA-C-N	-6.21	117.13	123.10
1	P	73	PHE	C-N-CA	-6.21	117.13	123.10
3	H	140	CYS	N-CA-C	6.18	119.42	110.28
1	Q	172	HIS	CA-C-N	6.13	125.81	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	172	HIS	C-N-CA	6.13	125.81	119.56
4	A	137	ASN	N-CA-C	6.12	118.88	108.90
2	M	94	TYR	N-CA-C	6.11	123.32	109.81
5	D	103	VAL	N-CA-C	6.11	116.41	108.35
1	P	231	VAL	CB-CA-C	-6.08	104.18	111.97
2	M	22	SER	N-CA-C	6.08	118.87	109.07
1	Q	145	GLU	CA-C-N	6.05	125.60	119.19
1	Q	145	GLU	C-N-CA	6.05	125.60	119.19
4	A	14	SER	CA-C-N	6.02	128.67	120.54
4	A	14	SER	C-N-CA	6.02	128.67	120.54
4	A	76	ASN	CA-C-N	5.97	127.31	119.84
4	A	76	ASN	C-N-CA	5.97	127.31	119.84
4	C	22	SER	N-CA-C	5.97	118.25	109.24
2	M	58	VAL	CA-C-N	5.96	127.29	119.84
2	M	58	VAL	C-N-CA	5.96	127.29	119.84
2	L	139	PHE	N-CA-C	5.94	117.29	107.20
5	D	114	SER	N-CA-C	5.92	117.85	108.79
2	L	95	PRO	N-CA-C	-5.92	100.28	112.47
5	D	113	SER	N-CA-C	5.91	123.39	110.80
2	L	137	ASN	N-CA-C	5.90	123.61	114.64
4	A	159	VAL	N-CA-C	5.89	116.66	108.89
5	B	77	THR	N-CA-C	5.87	117.51	109.18
4	C	94	ASP	N-CA-C	5.86	122.76	109.81
5	D	33	TRP	N-CA-C	-5.82	103.03	110.53
3	H	67	ALA	N-CA-C	5.82	119.04	109.85
2	L	10	SER	N-CA-C	5.81	117.06	108.86
1	P	95(H)	PHE	N-CA-C	5.78	118.32	108.90
3	H	111	VAL	N-CA-C	5.78	116.17	107.80
4	A	206	VAL	N-CA-C	5.77	116.59	108.17
4	C	112	ALA	CA-C-N	5.72	125.72	119.89
4	C	112	ALA	C-N-CA	5.72	125.72	119.89
4	A	115	VAL	N-CA-C	5.72	116.11	108.11
5	D	50	TYR	N-CA-C	5.65	115.75	108.34
1	Q	85	VAL	CB-CA-C	-5.64	104.09	111.81
2	M	152	GLY	N-CA-C	-5.53	108.11	114.69
3	K	2	VAL	N-CA-C	5.50	116.17	109.30
3	K	34	MET	N-CA-C	5.45	116.47	107.20
1	Q	162	VAL	N-CA-C	5.45	116.43	108.58
2	M	10	SER	N-CA-C	5.45	117.54	108.99
4	A	28	TYR	CB-CA-C	-5.43	104.59	111.86
4	C	56	SER	N-CA-C	-5.42	104.17	111.54
1	P	122	ASP	N-CA-C	5.41	117.62	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	193	THR	N-CA-C	5.40	118.23	109.06
5	B	200	HIS	CA-C-N	5.37	126.55	119.84
5	B	200	HIS	C-N-CA	5.37	126.55	119.84
4	A	140	TYR	N-CA-C	5.36	121.66	109.81
2	M	53	ASN	N-CA-C	5.36	118.22	110.28
1	P	21	GLU	N-CA-C	5.36	117.74	110.35
3	K	126	PRO	N-CA-C	-5.35	102.70	111.21
1	Q	75	HIS	CA-C-N	5.32	126.49	119.84
1	Q	75	HIS	C-N-CA	5.32	126.49	119.84
1	P	75	HIS	CA-C-N	5.31	126.47	119.84
1	P	75	HIS	C-N-CA	5.31	126.47	119.84
1	P	85	VAL	CB-CA-C	-5.29	104.89	111.08
2	M	117	ILE	N-CA-C	5.28	115.88	108.17
3	H	148	GLU	N-CA-C	5.26	117.82	111.40
4	C	144	ILE	CB-CA-C	-5.26	102.67	111.29
3	K	118	ALA	CA-C-N	5.25	125.78	120.38
3	K	118	ALA	C-N-CA	5.25	125.78	120.38
1	P	95(I)	LEU	N-CA-C	5.24	118.56	111.17
1	P	82	VAL	N-CA-C	5.24	116.39	108.96
5	B	71	ALA	N-CA-C	5.23	116.79	108.79
3	H	10	GLU	N-CA-C	5.23	117.95	109.06
4	C	185	GLU	N-CA-C	-5.21	107.59	114.31
4	A	62	PHE	N-CA-C	5.20	117.19	107.99
4	A	198	HIS	N-CA-C	5.20	116.42	108.52
3	K	162	GLY	N-CA-C	-5.17	107.41	114.64
4	C	159	VAL	N-CA-C	5.14	116.37	108.71
2	M	124	GLN	N-CA-C	-5.13	105.76	112.23
4	C	93	GLU	N-CA-C	-5.13	103.63	110.55
5	B	13	LYS	CA-C-N	5.12	126.24	119.84
5	B	13	LYS	C-N-CA	5.12	126.24	119.84
5	D	115	ALA	N-CA-C	5.10	117.74	110.24
5	D	117	THR	N-CA-C	5.09	117.47	110.35
1	P	222	LEU	CA-C-N	5.07	124.86	119.28
1	P	222	LEU	C-N-CA	5.07	124.86	119.28
3	K	35	ASN	N-CA-C	5.04	117.90	110.59
5	D	138	THR	N-CA-C	5.04	116.60	108.34
2	M	140	TYR	N-CA-C	5.03	120.92	109.81
3	H	21	SER	N-CA-C	5.02	117.95	110.52
2	M	208	SER	N-CA-C	5.01	115.14	108.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	98	ARG	Sidechain
2	M	93	GLU	Peptide
1	P	153	LYS	Peptide
1	P	95(J)	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1832	0	1802	213	0
1	Q	1832	0	1803	262	0
2	L	1704	0	1636	182	0
2	M	1704	0	1636	165	0
3	H	1637	0	1607	162	0
3	K	1657	0	1624	153	0
4	A	1701	0	1624	193	0
4	C	1701	0	1624	190	0
5	B	1655	0	1612	228	0
5	D	1655	0	1612	215	0
6	E	206	0	172	10	0
7	F	25	0	21	1	0
8	G	206	0	172	13	0
9	A	4	0	0	0	0
9	B	4	0	0	3	0
9	C	11	0	0	0	0
9	D	7	0	0	2	0
9	H	10	0	0	1	0
9	K	14	0	0	1	0
9	L	4	0	0	3	0
9	M	6	0	0	2	0
9	P	26	0	0	5	0
9	Q	5	0	0	2	0
All	All	17606	0	16945	1889	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (1889) 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)
5:D:120:PRO:HG2	5:D:146:TYR:CD1	1.76	1.20
1:P:161:HIS:CE1	1:P:185:ARG:HH21	1.64	1.15
1:Q:73:PHE:HE2	1:Q:153:LYS:HA	1.09	1.14
5:B:111:THR:O	5:B:112:VAL:HG12	1.48	1.14
1:P:237:TRP:O	1:P:241:THR:HG22	1.46	1.12
5:D:111:THR:C	5:D:112:VAL:HG22	1.76	1.08
4:C:140:TYR:CD1	4:C:141:PRO:HA	1.88	1.08
5:D:120:PRO:HG2	5:D:146:TYR:HD1	0.97	1.07
5:B:98:LEU:HD23	5:B:98:LEU:N	1.52	1.07
1:Q:62:LYS:H	1:Q:62:LYS:HD2	1.19	1.06
2:M:131:SER:HB2	2:M:180:THR:HG22	1.38	1.06
2:L:24:ARG:HH21	2:L:70:ASP:HB2	1.11	1.05
4:A:27(B):ILE:HD11	4:A:32:PHE:N	1.71	1.05
5:D:120:PRO:CG	5:D:146:TYR:HD1	1.69	1.05
3:H:13:LYS:H	3:H:13:LYS:HD2	1.22	1.05
4:A:143:ASP:C	4:A:144:ILE:HG22	1.75	1.05
1:Q:72:LEU:HD12	4:C:28:TYR:HB3	1.37	1.04
5:B:111:THR:C	5:B:112:VAL:CG1	2.30	1.03
1:Q:19:GLY:HA3	1:Q:190:THR:OG1	1.58	1.03
5:D:111:THR:O	5:D:112:VAL:HG13	1.57	1.03
1:Q:161:HIS:HD2	1:Q:185:ARG:HB2	1.18	1.02
3:K:119:PRO:HB3	3:K:145:TYR:HB3	1.39	1.01
4:C:31:THR:O	4:C:50:ARG:HG2	1.59	1.01
4:C:125:LEU:HD22	4:C:125:LEU:H	1.21	1.01
5:D:111:THR:O	5:D:112:VAL:HG22	1.58	1.01
1:Q:94:TYR:CE1	1:Q:102:ASP:HB3	1.94	1.01
5:B:153:LEU:HD11	5:B:198:VAL:HG22	1.41	1.00
2:M:193:THR:HB	2:M:208:SER:HB3	1.38	1.00
1:Q:222:LEU:HB2	1:Q:223:PRO:HD2	1.39	0.99
2:M:154:GLU:HG2	2:M:155:ARG:H	1.22	0.99
1:Q:123:LEU:HD12	1:Q:123:LEU:H	1.26	0.99
1:Q:63:SER:O	1:Q:85:VAL:HG23	1.63	0.99
3:H:31:SER:HB2	9:H:220:HOH:O	1.63	0.99
1:P:84:GLN:HE21	5:B:98:LEU:HD23	1.25	0.99
4:A:157:ASN:H	4:A:157:ASN:HD22	1.01	0.98
5:B:111:THR:C	5:B:112:VAL:HG12	1.88	0.98
5:B:120:PRO:HG2	5:B:145:GLY:C	1.88	0.97
1:Q:222:LEU:HB2	1:Q:223:PRO:CD	1.94	0.97
5:D:36:TRP:CE3	5:D:80:MET:HE3	1.99	0.97
4:A:108:ARG:HD2	4:A:140:TYR:HB2	1.46	0.97
4:A:143:ASP:O	4:A:144:ILE:HG22	1.62	0.97
4:A:27(B):ILE:HD11	4:A:32:PHE:H	1.21	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:133:THR:HG22	5:B:134:GLY:H	1.27	0.97
1:Q:144:ILE:HG22	1:Q:194:ASP:HA	1.44	0.97
4:C:47:LEU:O	4:C:54:LEU:HB3	1.65	0.97
2:L:136:LEU:HD12	2:L:136:LEU:N	1.77	0.96
1:Q:59:ILE:HD11	1:Q:104:MET:SD	2.05	0.96
1:P:176:VAL:HA	1:P:180:MET:HE3	1.43	0.96
1:Q:73:PHE:CE2	1:Q:153:LYS:HA	1.99	0.96
2:L:170:ASP:HB3	2:L:172:THR:HG23	1.42	0.96
4:A:148:TRP:O	4:A:154:GLU:HB2	1.66	0.96
1:P:130:PRO:HG3	1:P:210:GLN:HG2	1.44	0.96
4:C:190:ASN:HD21	4:C:212:ASN:HD21	1.05	0.96
5:D:145:GLY:HA2	5:D:175:LEU:HB3	1.48	0.95
5:B:6:GLN:NE2	5:B:92:CYS:H	1.63	0.95
5:B:54:THR:HG22	5:B:56:TYR:H	1.31	0.94
1:Q:186:TRP:CE3	1:Q:224:ARG:HD2	2.01	0.94
1:Q:140:GLY:HA3	1:Q:193:GLY:HA3	1.46	0.94
4:C:54:LEU:H	4:C:54:LEU:HD12	1.31	0.94
1:P:176:VAL:HA	1:P:180:MET:CE	1.97	0.94
5:B:120:PRO:HD3	5:B:146:TYR:HB3	1.45	0.94
3:K:143:LYS:HG3	3:K:143:LYS:O	1.68	0.94
1:P:84:GLN:HE21	5:B:98:LEU:CD2	1.79	0.94
3:H:60:ASN:HD22	3:H:61:GLY:N	1.66	0.94
5:B:61:GLN:HA	5:B:61:GLN:HE21	1.30	0.94
2:M:124:GLN:HE22	2:M:131:SER:HB3	1.32	0.94
1:P:72:LEU:HD21	1:P:141:TRP:CD1	2.02	0.93
3:K:148:GLU:HG3	3:K:149:SER:N	1.83	0.93
2:L:36:PHE:HE1	2:L:89:MET:HE3	1.31	0.93
4:A:39:LYS:HB3	4:A:40:PRO:HD3	1.50	0.93
1:P:221:ALA:C	1:P:222:LEU:HG	1.95	0.93
3:K:75:SER:O	3:K:77:THR:HG23	1.69	0.92
1:P:220:CYS:O	1:P:221:ALA:HB3	1.70	0.92
5:B:146:TYR:CE1	5:B:176:TYR:HB2	2.03	0.92
4:C:90:GLN:HE22	4:C:92:HIS:H	1.16	0.92
5:D:48:ILE:HG23	5:D:63:PHE:CD1	2.04	0.91
2:L:51:MET:HE3	2:L:66:GLY:N	1.85	0.91
1:P:221:ALA:O	1:P:222:LEU:HG	1.71	0.91
2:M:160:LEU:HD21	3:K:171:GLN:HG3	1.52	0.91
3:H:13:LYS:H	3:H:13:LYS:CD	1.84	0.91
1:Q:218:GLU:O	1:Q:222:LEU:HD23	1.71	0.91
4:C:90:GLN:NE2	4:C:92:HIS:H	1.68	0.91
2:L:136:LEU:N	2:L:136:LEU:CD1	2.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:210:ASN:H	4:C:210:ASN:HD22	0.91	0.90
5:D:122:VAL:HG22	5:D:209:LYS:HG3	1.52	0.90
1:P:222:LEU:HB3	1:P:224:ARG:HB2	1.52	0.90
3:H:64:LYS:O	3:H:64:LYS:HD3	1.72	0.90
2:M:128:GLY:O	2:M:183:LYS:HB2	1.71	0.89
4:C:140:TYR:HD1	4:C:141:PRO:HA	1.31	0.89
4:C:27(B):ILE:HD13	4:C:27(B):ILE:H	1.38	0.89
1:Q:94:TYR:CD1	1:Q:102:ASP:HB3	2.08	0.89
5:D:156:ASN:OD1	5:D:194:ILE:HG22	1.73	0.89
2:L:188:ARG:HG3	2:L:188:ARG:O	1.71	0.89
3:K:60:ASN:HD22	3:K:61:GLY:N	1.70	0.88
2:L:36:PHE:CE1	2:L:89:MET:HE3	2.08	0.88
5:D:156:ASN:HD22	5:D:159:SER:HB3	1.35	0.88
2:M:162:SER:OG	3:K:167:PRO:HD2	1.73	0.88
2:L:190:ASN:O	2:L:210:ASN:HA	1.74	0.88
3:H:124:LEU:HB2	3:H:139:GLY:O	1.74	0.87
4:C:210:ASN:HD22	4:C:210:ASN:N	1.70	0.87
1:P:150:LEU:HD23	1:P:152:PRO:HG2	1.56	0.87
5:B:98:LEU:N	5:B:98:LEU:CD2	2.30	0.87
5:D:61:GLN:HA	5:D:61:GLN:HE21	1.38	0.87
1:P:161:HIS:CE1	1:P:185:ARG:NH2	2.42	0.87
2:L:120:PRO:HB3	2:L:130:ALA:HB1	1.57	0.87
5:B:6:GLN:HE22	5:B:92:CYS:H	1.20	0.87
2:M:136:LEU:HD13	2:M:175:MET:HG2	1.56	0.86
4:C:151:ASP:HB2	4:C:189:HIS:HD2	1.37	0.86
4:C:94:ASP:O	4:C:96:TYR:HD1	1.58	0.86
4:A:142:LYS:HD3	4:A:142:LYS:H	1.39	0.86
5:B:12:ALA:O	5:B:112:VAL:HA	1.75	0.86
1:Q:161:HIS:CD2	1:Q:185:ARG:HB2	2.09	0.86
4:A:140:TYR:CG	4:A:140:TYR:O	2.29	0.86
1:P:144:ILE:HD13	1:P:194:ASP:HB3	1.58	0.85
2:L:17:GLU:O	2:L:77:ARG:HA	1.75	0.85
2:L:24:ARG:NH2	2:L:70:ASP:HB2	1.90	0.85
4:A:39:LYS:HB2	4:A:42:GLN:HG3	1.57	0.85
4:A:27(B):ILE:O	4:A:27(B):ILE:HD12	1.77	0.85
4:C:61:ARG:HH12	4:C:79:GLU:HB2	1.40	0.85
2:M:36:PHE:CE2	2:M:46:LEU:HB2	2.12	0.84
5:B:13:LYS:O	5:B:16:ALA:HB3	1.75	0.84
1:Q:47:VAL:HG23	1:Q:48:HIS:H	1.42	0.84
1:Q:119:LYS:HD2	3:K:52:TYR:CE1	2.11	0.84
1:Q:59:ILE:CD1	1:Q:104:MET:SD	2.65	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:155:ARG:HH21	4:A:157:ASN:ND2	1.76	0.84
4:A:140:TYR:O	4:A:140:TYR:CD1	2.30	0.84
4:C:94:ASP:O	4:C:96:TYR:CD1	2.29	0.84
4:C:139:PHE:O	4:C:139:PHE:CD1	2.30	0.84
5:B:128:VAL:HG22	5:B:129:CYS:H	1.41	0.84
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.13	0.83
3:K:148:GLU:HG3	3:K:149:SER:H	1.41	0.83
1:P:150:LEU:HG	1:P:152:PRO:CD	2.08	0.83
5:B:174:ASP:O	5:B:175:LEU:HD12	1.77	0.83
1:P:143:SER:HA	1:P:191:CYS:SG	2.19	0.83
2:M:19:VAL:HG22	2:M:20:SER:H	1.42	0.82
1:P:35:SER:HB3	1:P:62:LYS:O	1.78	0.82
3:K:6:GLN:HE22	3:K:92:CYS:H	1.23	0.82
4:C:67:SER:HB3	4:C:70:ASP:O	1.80	0.82
4:C:144:ILE:HG13	4:C:145:ASN:H	1.45	0.82
3:H:13:LYS:HD2	3:H:13:LYS:N	1.95	0.82
2:M:7:THR:O	2:M:9:PRO:HD3	1.78	0.82
2:L:90:GLN:HE21	2:L:93:GLU:H	1.27	0.82
4:A:14:SER:HA	4:A:107:LYS:HB2	1.60	0.82
2:M:14:THR:OG1	2:M:107:LYS:HE3	1.77	0.82
4:C:61:ARG:NH1	4:C:79:GLU:HB2	1.94	0.82
5:D:156:ASN:ND2	5:D:159:SER:HB3	1.93	0.82
3:K:6:GLN:NE2	3:K:92:CYS:H	1.76	0.82
4:A:79:GLU:HG3	4:A:80:ALA:N	1.94	0.82
4:C:108:ARG:HG3	4:C:140:TYR:CD2	2.14	0.82
2:L:159:VAL:HA	2:L:178:THR:O	1.80	0.81
3:H:188:TRP:CZ2	3:H:210:ILE:HG13	2.14	0.81
5:B:60:ASN:HD22	5:B:61:GLN:N	1.77	0.81
5:D:149:GLU:HA	5:D:149:GLU:OE2	1.79	0.81
1:P:186:TRP:CZ2	1:P:219:PRO:HB3	2.15	0.81
4:A:90:GLN:NE2	4:A:92:HIS:H	1.78	0.81
5:D:120:PRO:CG	5:D:146:TYR:CD1	2.53	0.81
4:C:34:HIS:HD2	4:C:49:TYR:HB2	1.44	0.81
2:L:108:ARG:N	2:L:140:TYR:CE1	2.48	0.81
3:H:57:THR:C	3:H:58:LYS:HG2	2.06	0.81
4:A:91:THR:HG21	5:B:98:LEU:HB3	1.62	0.81
4:A:143:ASP:C	4:A:144:ILE:CG2	2.50	0.81
3:H:188:TRP:HZ2	3:H:210:ILE:HG13	1.44	0.81
4:A:156:GLN:HE21	4:A:156:GLN:H	1.29	0.81
4:A:170:ASP:HB3	4:A:172:THR:HG23	1.60	0.81
5:B:146:TYR:HE1	5:B:176:TYR:HB2	1.41	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:210:ASN:H	4:C:210:ASN:ND2	1.72	0.81
5:D:12:ALA:C	5:D:13:LYS:HD3	2.06	0.81
1:P:56:ALA:O	1:P:59:ILE:HG22	1.81	0.80
5:B:119:ALA:HB3	5:B:205:THR:HG21	1.62	0.80
4:A:157:ASN:HD22	4:A:157:ASN:N	1.79	0.80
1:Q:97:ASP:O	1:Q:175:LYS:HB2	1.82	0.80
5:D:24:THR:HG23	5:D:25:SER:N	1.96	0.80
5:D:111:THR:O	5:D:112:VAL:CG1	2.30	0.80
5:B:156:ASN:HD21	5:B:194:ILE:HA	1.47	0.80
1:Q:87:HIS:HD2	5:D:54:THR:HG22	1.46	0.80
2:M:131:SER:CB	2:M:180:THR:HG22	2.11	0.80
3:K:6:GLN:H	3:K:105:GLN:NE2	1.80	0.80
1:P:71:SER:HB2	1:P:153:LYS:HB2	1.62	0.80
5:B:116:LYS:HB2	5:B:148:PRO:HG3	1.62	0.79
1:Q:21:GLU:HB2	1:Q:155:LEU:O	1.81	0.79
1:P:222:LEU:N	1:P:223:PRO:HD3	1.98	0.79
3:H:4:LEU:CD2	3:H:24:VAL:HG23	2.11	0.79
1:P:221:ALA:O	1:P:222:LEU:CD2	2.31	0.79
4:A:143:ASP:O	4:A:144:ILE:CG2	2.30	0.79
3:H:127:VAL:CG1	3:H:212:PRO:HB3	2.13	0.79
3:H:40:ARG:HH21	3:H:85:VAL:HA	1.48	0.79
1:Q:144:ILE:CG2	1:Q:194:ASP:HA	2.13	0.78
4:C:108:ARG:CG	4:C:140:TYR:CD2	2.67	0.78
5:B:61:GLN:HA	5:B:61:GLN:NE2	1.94	0.78
5:D:111:THR:O	5:D:112:VAL:CG2	2.30	0.78
1:P:161:HIS:CE1	1:P:185:ARG:HD3	2.19	0.78
1:P:168:CYS:HB2	1:P:172:HIS:HD2	1.46	0.78
2:L:137:ASN:O	2:L:138:ASN:CG	2.26	0.78
1:Q:185:ARG:HG3	1:Q:185:ARG:O	1.83	0.78
5:D:16:ALA:O	5:D:82(C):LEU:HD12	1.82	0.78
5:D:112:VAL:O	5:D:113:SER:CB	2.30	0.78
4:A:210:ASN:HB2	4:A:213:GLU:HG3	1.64	0.78
5:D:36:TRP:HE3	5:D:80:MET:HE3	1.49	0.78
2:L:9:PRO:O	2:L:103:LYS:HG2	1.82	0.78
4:A:115:VAL:O	4:A:207:LYS:HE3	1.84	0.78
4:C:192:TYR:HB2	4:C:209:PHE:CE2	2.18	0.78
2:L:170:ASP:HB3	2:L:172:THR:CG2	2.13	0.78
5:B:12:ALA:O	5:B:112:VAL:HB	1.84	0.78
1:P:221:ALA:O	1:P:222:LEU:CG	2.32	0.77
3:K:35:ASN:CG	3:K:100(A):PHE:HE1	1.92	0.77
3:K:170:LEU:HD23	3:K:171:GLN:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:150:LEU:HG	1:P:152:PRO:HD3	1.66	0.77
4:C:144:ILE:CG1	4:C:145:ASN:H	1.97	0.77
1:Q:164:SER:O	1:Q:167:VAL:HG13	1.84	0.77
1:P:145:GLU:H	1:P:146:PRO:HD3	1.50	0.77
4:C:190:ASN:HD21	4:C:212:ASN:ND2	1.82	0.77
1:Q:21:GLU:HA	1:Q:156:GLN:HA	1.65	0.77
3:K:12:VAL:CG1	3:K:16:ALA:HB3	2.15	0.77
1:P:18:GLY:HA2	1:P:190:THR:HG21	1.64	0.77
3:H:51:ILE:O	3:H:52(A):PRO:HD3	1.85	0.77
3:H:153:LEU:HD12	3:H:196:ASN:HB2	1.67	0.77
5:B:133:THR:HG22	5:B:134:GLY:N	2.00	0.77
1:P:35:SER:CB	1:P:62:LYS:O	2.33	0.77
2:M:21:ILE:HD11	2:M:102:THR:HG21	1.66	0.76
5:D:19:LYS:HE2	5:D:79:TYR:HD1	1.50	0.76
3:K:6:GLN:H	3:K:105:GLN:HE22	1.31	0.76
5:D:128:VAL:HG22	5:D:129:CYS:H	1.50	0.76
1:P:130:PRO:HG3	1:P:210:GLN:CG	2.15	0.76
3:H:173:ASP:O	3:H:174:LEU:HD23	1.85	0.76
1:Q:72:LEU:N	1:Q:72:LEU:HD22	1.99	0.76
1:Q:129:GLU:HB2	1:Q:130:PRO:CD	2.15	0.76
3:K:6:GLN:N	3:K:105:GLN:HE22	1.82	0.76
4:A:142:LYS:O	4:A:144:ILE:HG22	1.85	0.76
2:L:6:GLN:HE21	2:L:99:GLY:HA3	1.50	0.76
1:Q:95:ASP:O	1:Q:95(C):LEU:HD13	1.85	0.76
1:Q:162:VAL:HA	1:Q:183:ALA:HB2	1.68	0.76
1:P:186:TRP:HB2	1:P:223:PRO:HA	1.66	0.76
5:B:98:LEU:HD23	5:B:98:LEU:H	1.48	0.76
1:P:20:TRP:HA	1:P:20:TRP:CE3	2.19	0.76
1:P:64:VAL:HG12	1:P:84:GLN:HA	1.67	0.75
2:L:158:GLY:O	2:L:180:THR:HG22	1.86	0.75
4:A:15:LEU:HG	4:A:16:GLY:N	2.01	0.75
2:L:77:ARG:HB3	2:L:77:ARG:HH11	1.50	0.75
2:L:150:ILE:HG12	2:L:153:SER:HB3	1.65	0.75
8:G:12:NAG:H83	8:G:12:NAG:H3	1.68	0.75
2:L:19:VAL:HG12	2:L:75:ILE:HB	1.69	0.75
2:L:173:TYR:O	2:L:174:SER:HB2	1.87	0.75
4:C:118:PHE:HB2	4:C:133:VAL:HG12	1.69	0.75
3:H:165:THR:HG23	3:H:179:SER:HB3	1.69	0.75
1:Q:144:ILE:HD11	1:Q:218:GLU:HA	1.66	0.75
1:Q:168:CYS:HA	1:Q:171:VAL:HG22	1.68	0.75
2:M:136:LEU:HD12	2:M:175:MET:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:125:LEU:HD12	5:D:140:GLY:C	2.12	0.75
5:D:199:ALA:HB1	5:D:206:LYS:HD2	1.67	0.75
1:Q:62:LYS:HD2	1:Q:62:LYS:N	1.97	0.75
2:L:136:LEU:CD1	2:L:136:LEU:H	1.97	0.74
4:A:90:GLN:HE22	4:A:92:HIS:H	1.34	0.74
2:M:87:TYR:HE1	2:M:101:GLY:HA3	1.52	0.74
1:Q:32:LEU:HD23	1:Q:141:TRP:CZ3	2.22	0.74
4:C:34:HIS:HD2	4:C:49:TYR:CB	2.01	0.74
1:Q:211:GLY:HA2	1:Q:231:VAL:HG23	1.67	0.74
1:Q:218:GLU:O	1:Q:222:LEU:CD2	2.35	0.74
4:C:108:ARG:HG3	4:C:140:TYR:HD2	1.52	0.74
5:B:36:TRP:CE3	5:B:80:MET:HE2	2.22	0.74
2:L:213:GLU:HG3	2:L:214:CYS:N	2.02	0.74
6:E:14:SIA:H113	6:E:14:SIA:H4	1.70	0.74
1:P:151:THR:N	1:P:152:PRO:CD	2.50	0.74
8:G:12:NAG:H3	8:G:12:NAG:C8	2.18	0.74
1:Q:50:GLN:NE2	1:Q:111:PRO:HG3	2.03	0.73
1:P:95(G):ARG:H	1:P:95(G):ARG:CD	2.00	0.73
5:B:116:LYS:CE	5:B:202:ALA:HB1	2.17	0.73
1:P:154:LYS:NZ	2:L:28:ASN:O	2.20	0.73
4:A:149:LYS:HE3	4:A:152:GLY:H	1.53	0.73
5:B:123:TYR:HB2	5:B:142:LEU:HD22	1.70	0.73
2:M:150:ILE:HG22	2:M:151:ASP:OD2	1.87	0.73
5:D:11:LEU:HD13	5:D:111:THR:HB	1.70	0.73
5:B:112:VAL:HG23	5:B:113:SER:HB3	1.70	0.73
4:C:144:ILE:CG1	4:C:145:ASN:N	2.51	0.73
5:B:144:LYS:HG3	5:B:177:THR:HG22	1.71	0.73
1:Q:203:GLY:HA3	9:K:222:HOH:O	1.89	0.73
2:M:89:MET:HB3	2:M:98:PHE:CD2	2.24	0.73
1:P:95(G):ARG:H	1:P:95(G):ARG:HD3	1.53	0.73
4:C:125:LEU:HD22	4:C:125:LEU:N	2.00	0.73
5:D:146:TYR:CE2	5:D:176:TYR:HB2	2.23	0.73
4:C:92:HIS:HD2	4:C:93:GLU:HG2	1.53	0.72
4:C:39:LYS:HB2	4:C:42:GLN:HG3	1.70	0.72
5:D:192:GLN:N	5:D:192:GLN:HE21	1.87	0.72
2:M:117:ILE:CD1	2:M:194:CYS:HB2	2.20	0.72
2:M:121:SER:C	2:M:123:GLU:H	1.97	0.72
5:D:112:VAL:O	5:D:113:SER:HB3	1.88	0.72
1:P:208:VAL:HG21	7:F:1:A2G:H14	1.71	0.72
1:Q:95(A):MET:HE3	1:Q:95(D):LEU:HD11	1.70	0.72
1:Q:215:TRP:HE3	1:Q:216:GLY:H	1.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:189:TRP:HD1	5:D:194:ILE:HD11	1.52	0.72
1:Q:65:ILE:HG22	1:Q:67:LEU:HD11	1.72	0.72
2:M:18:SER:HB3	2:M:76:SER:O	1.90	0.71
4:C:54:LEU:HD12	4:C:54:LEU:N	2.03	0.71
1:P:186:TRP:CH2	1:P:219:PRO:HB3	2.24	0.71
1:Q:141:TRP:CD2	1:Q:155:LEU:HD23	2.25	0.71
3:K:153:LEU:CD2	3:K:196:ASN:HB2	2.20	0.71
4:C:34:HIS:CD2	4:C:49:TYR:HB2	2.25	0.71
1:P:149:PHE:N	1:P:149:PHE:CD2	2.58	0.71
4:A:3:VAL:HB	4:A:97:THR:HG21	1.70	0.71
5:D:154:LEU:CB	5:D:197:ASN:HD22	2.02	0.71
1:P:208:VAL:HA	9:P:264:HOH:O	1.90	0.71
1:P:72:LEU:H	1:P:153:LYS:HB3	1.54	0.71
2:L:193:THR:HA	2:L:208:SER:HB3	1.72	0.71
5:B:111:THR:C	5:B:112:VAL:HG13	2.14	0.71
2:L:151:ASP:H	2:L:152:GLY:HA3	1.56	0.71
2:L:213:GLU:O	2:L:214:CYS:HB2	1.88	0.71
4:C:47:LEU:HD23	4:C:47:LEU:N	2.06	0.71
2:M:186:TYR:C	2:M:186:TYR:CD2	2.68	0.71
4:A:190:ASN:HB2	4:A:211:ARG:N	2.06	0.71
5:B:200:HIS:HB3	5:B:205:THR:HB	1.72	0.71
3:K:35:ASN:HD22	3:K:35:ASN:H	1.36	0.71
1:P:150:LEU:CG	1:P:152:PRO:HD2	2.21	0.71
4:A:120:PRO:HD3	4:A:132:VAL:HG22	1.73	0.70
2:M:87:TYR:CE1	2:M:101:GLY:HA3	2.25	0.70
2:L:107:LYS:HA	2:L:140:TYR:HE1	1.55	0.70
2:L:147:LYS:HG2	2:L:195:GLU:HB3	1.73	0.70
5:D:189:TRP:CD1	5:D:194:ILE:HD11	2.26	0.70
5:D:190:PRO:HA	9:D:219:HOH:O	1.91	0.70
1:P:221:ALA:O	1:P:222:LEU:HD23	1.91	0.70
5:B:145:GLY:O	5:B:175:LEU:HD23	1.91	0.70
1:Q:47:VAL:HG23	1:Q:48:HIS:N	2.03	0.70
2:M:27(D):HIS:ND1	2:M:28:ASN:HB3	2.07	0.70
2:M:36:PHE:HE2	2:M:46:LEU:HB2	1.51	0.70
2:M:159:VAL:O	2:M:160:LEU:HD12	1.90	0.70
1:P:84:GLN:NE2	5:B:98:LEU:HD23	2.03	0.70
2:L:39:ARG:HG3	9:L:218:HOH:O	1.90	0.70
1:Q:160:LEU:HG	1:Q:184:GLY:HA2	1.74	0.70
4:C:142:LYS:O	4:C:143:ASP:C	2.34	0.70
2:L:90:GLN:NE2	2:L:93:GLU:H	1.88	0.70
4:A:39:LYS:HB3	4:A:40:PRO:CD	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:136:LEU:HD12	2:M:136:LEU:N	2.05	0.70
3:K:146:PHE:CD2	3:K:147:PRO:CA	2.74	0.70
4:C:47:LEU:HD23	4:C:47:LEU:H	1.57	0.70
3:H:116:THR:HG23	3:H:147:PRO:HD3	1.74	0.70
3:K:55:GLY:O	3:K:57:THR:HG22	1.91	0.70
1:Q:80:GLY:HA3	4:C:30:PHE:HE2	1.57	0.70
3:H:83:THR:CG2	3:H:84:SER:N	2.54	0.70
3:H:152:LEU:HD12	3:H:153:LEU:N	2.05	0.70
2:M:159:VAL:C	2:M:160:LEU:HD12	2.17	0.69
1:P:23:GLU:HG2	3:H:99:TYR:HA	1.72	0.69
5:B:97:ARG:O	5:B:98:LEU:HB2	1.91	0.69
4:C:179:LEU:HD11	4:C:181:LEU:CD2	2.22	0.69
5:D:111:THR:C	5:D:112:VAL:CG2	2.52	0.69
5:D:191:SER:C	5:D:192:GLN:HE21	2.00	0.69
3:H:170:LEU:HD13	3:H:170:LEU:C	2.17	0.69
4:C:96:TYR:HD1	4:C:96:TYR:H	1.40	0.69
3:H:152:LEU:HD12	3:H:152:LEU:C	2.17	0.69
5:B:154:LEU:HD13	5:B:158:GLY:N	2.08	0.69
3:K:146:PHE:CD2	3:K:147:PRO:HA	2.27	0.69
4:A:108:ARG:HG3	4:A:140:TYR:CG	2.27	0.69
2:L:136:LEU:H	2:L:136:LEU:HD13	1.57	0.69
2:L:175:MET:HG2	2:L:176:SER:N	2.07	0.69
1:Q:69:ARG:HA	1:Q:69:ARG:HH21	1.57	0.69
5:D:154:LEU:HD13	5:D:158:GLY:HA3	1.73	0.69
3:K:23:LYS:HG3	3:K:77:THR:HG22	1.75	0.69
3:K:57:THR:O	3:K:58:LYS:HG3	1.93	0.69
9:P:268:HOH:O	6:E:6:GAL:H4	1.93	0.69
3:H:127:VAL:HG12	3:H:212:PRO:HB3	1.74	0.69
3:H:156:SER:H	3:H:196:ASN:ND2	1.90	0.69
1:Q:96:GLY:HA2	1:Q:175:LYS:HZ2	1.58	0.69
2:M:17:GLU:O	2:M:77:ARG:HA	1.92	0.69
4:C:187:GLU:CD	4:C:187:GLU:H	1.99	0.69
5:D:120:PRO:HG3	5:D:146:TYR:HB3	1.75	0.69
3:H:156:SER:H	3:H:196:ASN:HD21	1.40	0.69
3:K:57:THR:HG1	3:K:59:TYR:HE2	1.37	0.69
3:H:60:ASN:HD22	3:H:61:GLY:H	1.38	0.69
1:Q:215:TRP:HE3	1:Q:216:GLY:N	1.90	0.69
4:C:108:ARG:H	4:C:140:TYR:HE2	1.39	0.69
5:D:48:ILE:HG23	5:D:63:PHE:CE1	2.28	0.69
5:D:83:THR:HG23	5:D:86:ASP:OD2	1.93	0.69
5:B:12:ALA:O	5:B:112:VAL:CA	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:186:SER:O	5:D:190:PRO:HD2	1.92	0.68
3:H:188:TRP:CD1	3:H:193:ILE:HD13	2.28	0.68
3:K:82(C):LEU:HD23	3:K:86:ASP:OD2	1.93	0.68
5:D:148:PRO:CB	5:D:202:ALA:HB3	2.23	0.68
5:D:188:THR:O	5:D:192:GLN:HG2	1.92	0.68
2:L:41:GLY:O	2:L:42:GLN:HG2	1.93	0.68
3:H:188:TRP:HB3	3:H:189:PRO:HD3	1.75	0.68
5:D:122:VAL:CG2	5:D:209:LYS:HG3	2.21	0.68
1:Q:188:LYS:HD3	1:Q:221:ALA:CB	2.22	0.68
3:H:170:LEU:O	3:H:170:LEU:HD22	1.94	0.68
4:A:182:THR:HG22	4:A:183:LYS:N	2.09	0.68
5:B:186:SER:O	5:B:190:PRO:HD2	1.93	0.68
2:M:199:LYS:HG3	2:M:200:THR:N	2.08	0.68
1:P:146:PRO:HG2	1:P:149:PHE:HA	1.74	0.68
3:H:12:VAL:HG21	3:H:18:VAL:HG13	1.76	0.68
4:A:155:ARG:NH2	4:A:157:ASN:ND2	2.41	0.68
4:A:143:ASP:O	4:A:144:ILE:CB	2.42	0.68
2:M:183:LYS:O	2:M:186:TYR:HB3	1.94	0.68
5:D:146:TYR:CD2	5:D:176:TYR:HB2	2.29	0.68
4:A:76:ASN:HB2	4:A:77:PRO:HD3	1.76	0.68
5:B:128:VAL:HG13	5:B:130:GLY:H	1.59	0.68
1:Q:47:VAL:CG2	1:Q:48:HIS:H	2.07	0.68
4:C:35:TRP:CD2	4:C:73:LEU:HD22	2.28	0.68
3:H:64:LYS:HD3	3:H:64:LYS:C	2.16	0.68
4:A:33:MET:O	4:A:34:HIS:CD2	2.47	0.68
3:H:4:LEU:HD23	3:H:24:VAL:HG23	1.76	0.67
4:A:8:PRO:O	4:A:102:THR:HG23	1.94	0.67
4:A:174:SER:OG	5:B:165:HIS:CE1	2.47	0.67
3:K:146:PHE:CG	3:K:147:PRO:HA	2.29	0.67
1:Q:108:LEU:H	1:Q:108:LEU:HD23	1.60	0.67
3:K:11:LEU:HD22	3:K:147:PRO:HG3	1.77	0.67
3:K:12:VAL:O	3:K:111:VAL:HA	1.94	0.67
4:A:159:VAL:HA	4:A:178:THR:O	1.95	0.67
4:A:210:ASN:HD21	2:M:74:ARG:HH22	1.43	0.67
5:B:120:PRO:HG2	5:B:145:GLY:CA	2.24	0.67
5:D:212:VAL:HG13	5:D:213:PRO:HD2	1.75	0.67
1:P:119:LYS:HD2	3:H:52:TYR:CD2	2.29	0.67
3:H:171:GLN:OE1	3:H:171:GLN:HA	1.94	0.67
3:K:133:GLY:C	3:K:135:SER:H	2.03	0.67
3:K:188:TRP:HD1	3:K:193:ILE:HG22	1.59	0.67
1:P:82:VAL:HG13	1:P:83:PHE:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:72:ASP:O	3:H:73:LYS:C	2.37	0.67
3:H:192:SER:C	3:H:193:ILE:HD12	2.19	0.67
2:M:38:GLN:HE22	3:K:39:GLN:HE22	1.41	0.67
4:C:144:ILE:HG23	4:C:145:ASN:N	2.09	0.67
5:B:17:SER:HA	5:B:82(C):LEU:HD23	1.76	0.67
4:A:34:HIS:HD2	4:A:49:TYR:HA	1.59	0.67
4:A:182:THR:HG22	4:A:183:LYS:H	1.60	0.67
2:L:34:TYR:HB2	2:L:89:MET:HG2	1.77	0.66
4:A:55:GLU:O	4:A:58:ILE:HD13	1.94	0.66
5:B:212:VAL:HG13	5:B:213:PRO:HD2	1.77	0.66
2:L:210:ASN:HD22	2:L:210:ASN:N	1.92	0.66
3:K:40:ARG:HA	3:K:88:ALA:HB2	1.78	0.66
4:A:14:SER:CA	4:A:107:LYS:HB2	2.26	0.66
3:K:124:LEU:HD21	3:K:141:LEU:HB2	1.75	0.66
3:K:127:VAL:O	3:K:129:GLY:N	2.28	0.66
5:B:101:PHE:N	5:B:101:PHE:HD1	1.93	0.66
1:Q:161:HIS:O	1:Q:183:ALA:HB1	1.95	0.66
2:M:46:LEU:HD22	3:K:99:TYR:CE1	2.30	0.66
4:C:27(C):ASP:OD2	4:C:68:ARG:HA	1.93	0.66
2:L:163:TRP:N	2:L:163:TRP:CE3	2.64	0.66
4:A:135:PHE:C	4:A:136:LEU:HD12	2.20	0.66
5:B:133:THR:CG2	5:B:134:GLY:H	2.07	0.66
5:D:184:VAL:HG22	5:D:185:THR:N	2.11	0.66
5:B:174:ASP:C	5:B:175:LEU:HD12	2.20	0.66
1:Q:176:VAL:O	1:Q:176:VAL:HG12	1.94	0.66
1:P:222:LEU:N	1:P:223:PRO:CD	2.59	0.66
2:L:195:GLU:HG3	2:L:206:VAL:HG22	1.77	0.66
5:B:30:SER:HB3	5:B:53:SER:HB2	1.77	0.66
3:H:36:TRP:CD1	3:H:69:LEU:HD22	2.30	0.66
1:Q:186:TRP:CZ3	1:Q:224:ARG:HD2	2.30	0.66
2:M:54:LEU:HD13	2:M:62:PHE:O	1.96	0.66
4:C:144:ILE:HG13	4:C:145:ASN:N	2.11	0.66
1:P:119:LYS:CD	3:H:52:TYR:CD2	2.79	0.66
1:P:144:ILE:CD1	1:P:194:ASP:HB3	2.24	0.66
2:L:24:ARG:HH21	2:L:70:ASP:CB	1.98	0.66
2:L:140:TYR:CD2	2:L:140:TYR:C	2.74	0.66
1:Q:73:PHE:HE2	1:Q:153:LYS:CA	1.99	0.66
2:M:160:LEU:HD21	3:K:171:GLN:CG	2.24	0.66
1:P:220:CYS:O	1:P:221:ALA:CB	2.39	0.65
3:H:6:GLN:H	3:H:105:GLN:NE2	1.94	0.65
1:Q:67:LEU:HD12	1:Q:67:LEU:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:164:THR:HG23	2:M:174:SER:O	1.96	0.65
2:M:186:TYR:C	2:M:186:TYR:HD2	2.04	0.65
5:B:54:THR:HG22	5:B:56:TYR:N	2.09	0.65
3:K:188:TRP:CD1	3:K:193:ILE:CG2	2.78	0.65
1:Q:65:ILE:HG22	1:Q:67:LEU:CD1	2.25	0.65
1:Q:124:PRO:HG3	1:Q:209:LEU:O	1.96	0.65
2:M:142:LYS:HB2	2:M:173:TYR:CE1	2.32	0.65
4:C:151:ASP:HA	4:C:191:SER:OG	1.95	0.65
5:D:115:ALA:O	5:D:117:THR:N	2.27	0.65
1:P:150:LEU:HG	1:P:152:PRO:HD2	1.77	0.65
2:L:77:ARG:HG3	2:L:77:ARG:O	1.97	0.65
3:K:13:LYS:H	3:K:13:LYS:HD2	1.62	0.65
4:C:94:ASP:O	4:C:96:TYR:N	2.29	0.65
3:H:73:LYS:O	3:H:75:SER:N	2.30	0.65
2:M:93:GLU:CD	2:M:94:TYR:H	2.05	0.65
2:L:41:GLY:C	2:L:42:GLN:HG2	2.21	0.65
4:A:76:ASN:CB	4:A:77:PRO:HD3	2.27	0.65
5:B:6:GLN:HE22	5:B:92:CYS:N	1.93	0.65
3:K:127:VAL:CG2	3:K:128:CYS:N	2.59	0.65
5:D:154:LEU:HB2	5:D:197:ASN:HB2	1.77	0.65
1:P:151:THR:HG23	1:P:152:PRO:HD3	1.77	0.65
2:M:136:LEU:HD13	2:M:175:MET:CG	2.25	0.65
1:P:177:THR:H	1:P:180:MET:HE2	1.62	0.65
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	2.31	0.65
4:A:205:ILE:HA	2:M:67:SER:HB3	1.78	0.65
1:P:84:GLN:NE2	5:B:98:LEU:H	1.94	0.65
3:H:155:ASN:HB2	3:H:158:SER:OG	1.97	0.65
2:M:154:GLU:HG2	2:M:155:ARG:N	2.03	0.65
4:A:48:ILE:HG23	4:A:53:ASN:O	1.96	0.64
2:M:157:ASN:HD22	2:M:157:ASN:C	2.06	0.64
5:D:24:THR:CG2	5:D:25:SER:N	2.59	0.64
1:P:95(G):ARG:HG3	9:P:266:HOH:O	1.96	0.64
1:P:161:HIS:ND1	1:P:185:ARG:NH2	2.44	0.64
3:H:210:ILE:HG12	3:H:211:VAL:N	2.11	0.64
5:B:13:LYS:H	5:B:13:LYS:HD2	1.61	0.64
1:P:101:HIS:HE1	1:P:179:PHE:CE1	2.16	0.64
1:Q:100:SER:HB3	1:Q:177:THR:OG1	1.98	0.64
1:P:75:HIS:N	1:P:76:PRO:HD3	2.12	0.64
2:L:187:GLU:O	2:L:211:ARG:NH1	2.30	0.64
5:B:12:ALA:O	5:B:112:VAL:CB	2.44	0.64
4:C:43:PRO:HB3	5:D:91:TYR:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:155:ARG:NH1	4:C:157:ASN:HB2	2.13	0.64
2:L:146:VAL:HA	2:L:195:GLU:O	1.96	0.64
5:B:121:PRO:HB2	5:B:123:TYR:CZ	2.33	0.64
5:D:171:LEU:HD12	5:D:176:TYR:CZ	2.32	0.64
5:B:39:GLN:HG3	5:B:44:GLY:O	1.97	0.64
2:M:39:ARG:O	2:M:42:GLN:HB2	1.98	0.64
4:A:154:GLU:HG2	4:A:154:GLU:O	1.96	0.64
5:B:147:PHE:O	5:B:147:PHE:CD2	2.51	0.64
1:Q:140:GLY:CA	1:Q:193:GLY:HA3	2.25	0.64
1:P:72:LEU:CD2	1:P:141:TRP:CD1	2.79	0.64
4:A:150:ILE:HD13	4:A:192:TYR:CD1	2.32	0.64
5:D:198:VAL:HG12	5:D:199:ALA:N	2.13	0.64
1:Q:119:LYS:CD	3:K:52:TYR:CE1	2.81	0.64
4:C:108:ARG:HG2	4:C:140:TYR:CD2	2.32	0.64
5:D:148:PRO:HB3	5:D:202:ALA:HB3	1.80	0.64
1:Q:179:PHE:HD2	1:Q:233:HIS:CE1	2.16	0.63
4:C:193:THR:HG22	4:C:208:SER:HB3	1.80	0.63
5:D:48:ILE:HG23	5:D:63:PHE:HD1	1.55	0.63
1:P:125:THR:HG23	1:P:235:ARG:NH1	2.13	0.63
5:B:36:TRP:CD2	5:B:80:MET:HE2	2.33	0.63
5:B:195:THR:HG23	5:B:210:LYS:HB3	1.79	0.63
3:K:12:VAL:HG13	3:K:16:ALA:HB3	1.80	0.63
5:D:215:ASP:O	5:D:216:CYS:HB3	1.98	0.63
5:B:170:VAL:O	5:B:176:TYR:HA	1.97	0.63
3:K:127:VAL:HG23	3:K:128:CYS:N	2.12	0.63
1:P:30:GLN:HE22	1:P:198:PRO:CD	2.10	0.63
1:P:36:ARG:HD3	1:P:36:ARG:N	2.12	0.63
1:P:151:THR:N	1:P:152:PRO:HD3	2.13	0.63
1:Q:143:SER:HB3	1:Q:191:CYS:SG	2.39	0.63
4:A:190:ASN:O	4:A:210:ASN:HA	1.98	0.63
4:A:205:ILE:HA	2:M:67:SER:CB	2.29	0.63
2:M:31:THR:OG1	2:M:51:MET:HE3	1.99	0.63
2:L:38:GLN:HE22	3:H:39:GLN:HE22	1.45	0.63
3:K:69:LEU:O	3:K:70:THR:HG23	1.97	0.63
4:C:39:LYS:HB3	4:C:40:PRO:CD	2.28	0.63
1:P:20:TRP:NE1	2:L:49:TYR:OH	2.28	0.63
4:A:190:ASN:HB2	4:A:211:ARG:H	1.63	0.63
3:K:127:VAL:HG23	3:K:128:CYS:SG	2.38	0.63
2:L:181:LEU:HD23	2:L:182:THR:N	2.14	0.63
3:H:132:THR:HG23	3:H:133:GLY:N	2.13	0.63
4:A:170:ASP:HB3	4:A:172:THR:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:144:LYS:HG3	5:B:177:THR:CG2	2.29	0.63
5:B:153:LEU:CD2	5:B:178:LEU:HD21	2.29	0.63
2:M:126:THR:C	2:M:128:GLY:H	2.06	0.63
4:C:58:ILE:HG22	4:C:59:PRO:HD2	1.81	0.63
1:P:71:SER:HB2	1:P:153:LYS:CB	2.29	0.62
1:P:72:LEU:HD22	1:P:72:LEU:N	2.13	0.62
4:A:91:THR:O	4:A:91:THR:CG2	2.46	0.62
5:D:44:GLY:O	5:D:45:LEU:HD23	1.99	0.62
2:L:110:ASP:HA	2:L:141:PRO:HD3	1.81	0.62
5:B:38:LYS:HD2	5:B:90:TYR:CE1	2.34	0.62
1:Q:66:LEU:HG	4:C:30:PHE:CE1	2.34	0.62
2:M:115:VAL:HG12	2:M:207:LYS:HD2	1.81	0.62
3:K:98:ARG:HG2	3:K:99:TYR:CD2	2.35	0.62
2:M:137:ASN:HA	2:M:174:SER:HB3	1.80	0.62
5:D:36:TRP:O	5:D:48:ILE:HG13	1.99	0.62
4:A:34:HIS:HD2	4:A:49:TYR:CA	2.11	0.62
1:Q:85:VAL:C	5:D:33:TRP:HH2	2.08	0.62
4:C:190:ASN:ND2	4:C:212:ASN:HD21	1.89	0.62
2:M:181:LEU:N	2:M:181:LEU:HD23	2.14	0.62
5:D:154:LEU:HB2	5:D:197:ASN:HD22	1.63	0.62
1:P:46:LEU:HD22	1:P:67:LEU:HD23	1.82	0.62
1:P:150:LEU:CG	1:P:152:PRO:CD	2.78	0.62
4:A:27(B):ILE:CD1	4:A:32:PHE:H	2.04	0.62
1:Q:50:GLN:HG3	1:Q:50:GLN:O	1.99	0.62
1:Q:142:GLY:HA3	1:Q:151:THR:HA	1.81	0.62
2:L:90:GLN:HE21	2:L:93:GLU:N	1.95	0.62
4:C:2:ILE:HD11	4:C:4:LEU:HG	1.82	0.62
5:D:153:LEU:HD22	5:D:180:SER:HB2	1.82	0.62
1:P:144:ILE:HD13	1:P:194:ASP:CB	2.28	0.62
5:B:128:VAL:HG22	5:B:129:CYS:N	2.14	0.62
1:Q:199:LEU:HD13	1:Q:228:TYR:HE1	1.64	0.62
3:K:30:SER:OG	3:K:73:LYS:HE3	2.00	0.62
4:C:140:TYR:CD1	4:C:141:PRO:CA	2.75	0.62
2:M:21:ILE:HG12	2:M:102:THR:OG1	1.99	0.62
3:K:188:TRP:CD1	3:K:193:ILE:HG22	2.35	0.62
2:L:151:ASP:N	2:L:152:GLY:HA3	2.15	0.61
4:C:59:PRO:O	4:C:61:ARG:N	2.33	0.61
1:P:160:LEU:HD23	1:P:185:ARG:O	2.00	0.61
3:H:137:THR:HB	3:H:182:THR:OG1	2.00	0.61
1:Q:72:LEU:HD12	4:C:28:TYR:CB	2.23	0.61
2:L:126:THR:O	2:L:126:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:ASP:HB2	2:L:152:GLY:CA	2.29	0.61
2:L:213:GLU:HG3	2:L:214:CYS:H	1.64	0.61
3:H:6:GLN:H	3:H:105:GLN:HE22	1.46	0.61
5:B:194:ILE:C	5:B:194:ILE:HD12	2.25	0.61
3:K:40:ARG:HA	3:K:88:ALA:CB	2.29	0.61
4:C:61:ARG:HH12	4:C:79:GLU:CB	2.13	0.61
1:P:222:LEU:HD22	1:P:224:ARG:HD3	1.82	0.61
2:L:37:LEU:HB2	2:L:47:LEU:HD11	1.81	0.61
2:L:175:MET:HE2	2:L:177:SER:HB2	1.81	0.61
5:D:111:THR:O	5:D:112:VAL:CB	2.46	0.61
4:A:210:ASN:HD21	2:M:74:ARG:NH2	1.99	0.61
5:D:207:VAL:CG1	5:D:208:ASP:N	2.63	0.61
1:Q:56:ALA:HA	1:Q:104:MET:HE2	1.81	0.61
2:M:33:LEU:C	2:M:33:LEU:HD13	2.26	0.61
4:A:192:TYR:HB2	4:A:209:PHE:HE2	1.65	0.61
3:K:66:LYS:HG3	3:K:66:LYS:O	2.01	0.61
5:D:153:LEU:CD2	5:D:180:SER:HB2	2.30	0.61
3:H:150:VAL:HG23	3:H:198:ALA:O	2.00	0.61
2:L:122:SER:HA	2:L:125:LEU:HD12	1.82	0.61
5:D:171:LEU:HD23	5:D:171:LEU:C	2.25	0.61
2:L:51:MET:HE3	2:L:66:GLY:H	1.63	0.61
5:B:196:CYS:O	5:B:208:ASP:HB2	2.01	0.61
2:M:137:ASN:O	2:M:138:ASN:HB2	2.00	0.61
5:D:215:ASP:O	5:D:216:CYS:CB	2.49	0.61
1:P:19:GLY:HA3	1:P:156:GLN:OE1	2.01	0.60
4:A:192:TYR:HB2	4:A:209:PHE:CE2	2.36	0.60
5:B:120:PRO:HB2	5:B:144:LYS:O	2.01	0.60
1:Q:84:GLN:HB2	5:D:33:TRP:CZ2	2.36	0.60
3:K:82:LEU:N	3:K:82:LEU:HD23	2.15	0.60
4:C:113:PRO:HD3	4:C:198:HIS:CD2	2.36	0.60
1:Q:153:LYS:HD2	9:Q:247:HOH:O	2.01	0.60
1:Q:165:ASN:HD22	1:Q:178:LYS:HD2	1.65	0.60
2:M:46:LEU:O	2:M:46:LEU:HD23	2.02	0.60
2:M:148:TRP:O	2:M:154:GLU:HA	2.01	0.60
3:K:146:PHE:CE2	3:K:147:PRO:HB3	2.36	0.60
5:D:13:LYS:HD3	5:D:13:LYS:N	2.15	0.60
5:D:48:ILE:CG2	5:D:63:PHE:HD1	2.12	0.60
5:D:185:THR:HG22	5:D:187:SER:H	1.66	0.60
1:Q:113:GLU:O	1:Q:115:THR:HG23	2.01	0.60
3:K:137:THR:HB	3:K:182:THR:HB	1.82	0.60
4:C:27(B):ILE:H	4:C:27(B):ILE:CD1	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:148:PRO:HG2	5:D:200:HIS:CE1	2.36	0.60
4:A:27(C):ASP:HA	4:A:31:THR:HG22	1.82	0.60
1:Q:144:ILE:HD13	1:Q:219:PRO:HD2	1.83	0.60
2:L:14:THR:O	2:L:17:GLU:HB2	2.02	0.60
3:H:83:THR:HG23	3:H:84:SER:H	1.65	0.60
5:B:5:GLN:HA	5:B:5:GLN:OE1	2.01	0.60
1:Q:72:LEU:N	1:Q:72:LEU:CD2	2.64	0.60
1:Q:162:VAL:HA	1:Q:183:ALA:CB	2.31	0.60
5:D:194:ILE:HD12	5:D:194:ILE:O	2.01	0.60
1:P:76:PRO:C	1:P:77:GLU:HG3	2.26	0.60
3:H:188:TRP:O	3:H:190:SER:N	2.34	0.60
5:B:185:THR:HB	5:B:188:THR:HG23	1.83	0.60
1:Q:123:LEU:HD12	1:Q:123:LEU:N	2.08	0.60
1:Q:243:VAL:O	1:Q:246:PRO:HG3	2.01	0.60
5:B:171:LEU:HB2	5:B:176:TYR:CD1	2.36	0.60
3:K:12:VAL:HG11	3:K:16:ALA:HB3	1.84	0.60
1:P:221:ALA:C	1:P:222:LEU:CG	2.74	0.60
2:M:149:LYS:HD2	2:M:195:GLU:OE1	2.01	0.60
3:K:35:ASN:N	3:K:35:ASN:ND2	2.49	0.60
1:P:20:TRP:HA	1:P:20:TRP:HE3	1.64	0.60
4:A:118:PHE:HZ	5:B:138:THR:O	1.84	0.60
1:Q:77:GLU:HG2	1:Q:79:THR:H	1.67	0.60
1:Q:130:PRO:HG3	1:Q:210:GLN:CG	2.31	0.60
1:Q:143:SER:O	1:Q:144:ILE:HG12	2.02	0.60
2:M:14:THR:O	2:M:17:GLU:HB2	2.02	0.60
2:M:170:ASP:HB3	9:M:216:HOH:O	2.02	0.60
5:D:146:TYR:CZ	5:D:151:VAL:HG21	2.37	0.60
1:P:161:HIS:HE1	1:P:185:ARG:HH21	1.37	0.60
1:P:186:TRP:HZ2	1:P:219:PRO:HB3	1.66	0.60
1:Q:222:LEU:CB	1:Q:223:PRO:CD	2.73	0.60
2:M:193:THR:CB	2:M:208:SER:HB3	2.24	0.60
4:C:18:ARG:HD3	4:C:76:ASN:ND2	2.17	0.60
4:C:39:LYS:HZ3	4:C:81:ASP:HB2	1.67	0.60
4:C:209:PHE:O	4:C:209:PHE:HD2	1.82	0.60
1:P:114:LEU:H	1:P:114:LEU:HD12	1.66	0.59
2:L:90:GLN:NE2	2:L:93:GLU:N	2.49	0.59
3:H:172:SER:O	3:H:173:ASP:CB	2.49	0.59
1:Q:77:GLU:HG2	1:Q:78:ASP:N	2.17	0.59
5:D:29:PHE:CZ	5:D:77:THR:O	2.55	0.59
1:Q:124:PRO:HB2	1:Q:232:VAL:CG1	2.32	0.59
4:A:22:SER:HB3	4:A:72:THR:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:13:LYS:HD2	5:B:13:LYS:N	2.16	0.59
3:H:6:GLN:NE2	3:H:106:GLY:H	2.01	0.59
5:B:33:TRP:CZ3	5:B:52:ASN:HB2	2.38	0.59
1:Q:129:GLU:HB2	1:Q:130:PRO:HD3	1.85	0.59
4:A:157:ASN:H	4:A:157:ASN:ND2	1.80	0.59
5:B:154:LEU:O	5:B:197:ASN:HB2	2.03	0.59
4:C:96:TYR:CD1	4:C:96:TYR:N	2.70	0.59
5:D:195:THR:OG1	5:D:196:CYS:N	2.35	0.59
4:C:179:LEU:HD11	4:C:181:LEU:HD23	1.84	0.59
1:P:144:ILE:HB	1:P:194:ASP:HA	1.85	0.59
2:L:90:GLN:HG2	2:L:91:HIS:N	2.18	0.59
5:B:145:GLY:O	5:B:175:LEU:CD2	2.51	0.59
1:Q:177:THR:O	1:Q:180:MET:HG3	2.03	0.59
1:Q:188:LYS:HD3	1:Q:221:ALA:HB2	1.85	0.59
3:K:153:LEU:HD21	3:K:196:ASN:HB2	1.83	0.59
4:C:155:ARG:HH11	4:C:157:ASN:HB2	1.67	0.59
5:D:35:HIS:HD2	5:D:47:TRP:HE1	1.50	0.59
5:D:178:LEU:HD23	5:D:179:SER:N	2.18	0.59
1:P:21:GLU:OE1	1:P:154:LYS:HD2	2.02	0.59
1:P:130:PRO:CG	1:P:210:GLN:HG2	2.25	0.59
2:L:163:TRP:HE3	2:L:163:TRP:H	1.49	0.59
5:B:96:GLY:C	5:B:97:ARG:CG	2.75	0.59
3:K:72:ASP:OD2	3:K:75:SER:HB3	2.02	0.59
8:G:1:NAG:H82	8:G:1:NAG:O3	2.03	0.59
4:A:4:LEU:HD12	4:A:4:LEU:O	2.02	0.58
2:L:107:LYS:HA	2:L:140:TYR:CE1	2.38	0.58
4:C:90:GLN:NE2	4:C:92:HIS:N	2.47	0.58
5:D:184:VAL:HG22	5:D:185:THR:H	1.67	0.58
1:P:217:SER:HB3	1:P:227:LEU:HD12	1.85	0.58
5:B:52:ASN:ND2	5:B:52:ASN:C	2.60	0.58
2:M:192:TYR:O	2:M:208:SER:HB2	2.02	0.58
3:K:18:VAL:HG23	3:K:82(C):LEU:HD11	1.85	0.58
3:K:24:VAL:O	3:K:24:VAL:HG12	2.04	0.58
2:M:33:LEU:HD12	2:M:51:MET:HA	1.84	0.58
4:C:4:LEU:HD23	4:C:25:ALA:HA	1.85	0.58
2:L:139:PHE:CD2	2:L:139:PHE:N	2.69	0.58
5:B:196:CYS:HB2	5:B:209:LYS:O	2.03	0.58
4:C:192:TYR:HD2	4:C:209:PHE:HE2	1.51	0.58
5:D:155:TRP:CH2	5:D:196:CYS:SG	2.97	0.58
1:Q:23:GLU:OE1	2:M:34:TYR:OH	2.20	0.58
2:M:55:ALA:O	2:M:58:VAL:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:193:THR:HB	2:M:208:SER:CB	2.23	0.58
1:Q:234:TYR:O	1:Q:237:TRP:N	2.37	0.58
5:D:19:LYS:CE	5:D:79:TYR:HD1	2.16	0.58
5:D:70:THR:OG1	5:D:79:TYR:HB2	2.04	0.58
1:Q:71:SER:OG	1:Q:154:LYS:HG2	2.02	0.58
4:C:168:SER:C	4:C:169:LYS:HG2	2.27	0.58
5:D:94:ARG:HG2	5:D:95:SER:N	2.18	0.58
5:B:16:ALA:O	5:B:82(C):LEU:HD23	2.04	0.58
5:B:201:PRO:O	5:B:202:ALA:O	2.20	0.58
1:Q:80:GLY:HA3	4:C:30:PHE:CE2	2.37	0.58
1:P:65:ILE:HG12	1:P:108:LEU:HD11	1.86	0.58
2:L:196:ALA:HB3	2:L:205:ILE:HB	1.86	0.58
3:H:114:ALA:HB3	3:H:146:PHE:CE2	2.39	0.58
4:A:91:THR:O	4:A:91:THR:HG22	2.03	0.58
1:P:150:LEU:CB	1:P:152:PRO:HD2	2.34	0.57
1:Q:119:LYS:CD	3:K:52:TYR:CD1	2.87	0.57
1:Q:171:VAL:C	1:Q:223(A):GLU:HG3	2.29	0.57
3:K:47:TRP:CH2	3:K:49:GLY:HA2	2.39	0.57
5:D:198:VAL:HG12	5:D:199:ALA:H	1.70	0.57
2:L:106:ILE:HB	2:L:166:GLN:HE22	1.68	0.57
3:H:146:PHE:CG	3:H:147:PRO:HA	2.39	0.57
4:C:47:LEU:O	4:C:54:LEU:CB	2.48	0.57
4:C:54:LEU:HD22	4:C:58:ILE:O	2.04	0.57
1:P:28:PRO:HB3	1:P:119:LYS:H	1.69	0.57
1:Q:121:MET:HG3	1:Q:121:MET:O	2.04	0.57
1:Q:75:HIS:N	1:Q:76:PRO:HD3	2.19	0.57
4:C:108:ARG:HD3	4:C:140:TYR:HB2	1.85	0.57
1:P:145:GLU:N	1:P:146:PRO:HD3	2.17	0.57
2:L:56:SER:O	2:L:58:VAL:N	2.32	0.57
3:H:134:SER:O	3:H:184:THR:HA	2.05	0.57
4:A:175:MET:HG3	4:A:176:SER:N	2.19	0.57
1:Q:188:LYS:HD3	1:Q:221:ALA:HB1	1.85	0.57
4:C:2:ILE:HD13	4:C:26:SER:H	1.70	0.57
4:C:135:PHE:C	4:C:136:LEU:HD12	2.29	0.57
1:P:186:TRP:CB	1:P:223:PRO:HA	2.34	0.57
3:H:199:HIS:ND1	3:H:202:SER:OG	2.38	0.57
5:B:97:ARG:O	5:B:98:LEU:CB	2.52	0.57
5:B:120:PRO:CD	5:B:146:TYR:HB3	2.27	0.57
5:B:142:LEU:O	5:B:142:LEU:HD23	2.04	0.57
5:D:146:TYR:CE2	5:D:176:TYR:CB	2.87	0.57
1:Q:84:GLN:HB2	5:D:33:TRP:CH2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:13:LYS:HB2	5:D:14:PRO:HD2	1.85	0.57
5:D:113:SER:C	5:D:114:SER:OG	2.47	0.57
5:B:60:ASN:HD22	5:B:60:ASN:C	2.09	0.57
5:B:120:PRO:HD3	5:B:146:TYR:CB	2.28	0.57
5:B:154:LEU:HD13	5:B:157:SER:C	2.29	0.57
2:M:136:LEU:HD12	2:M:136:LEU:H	1.68	0.57
2:M:198:HIS:HD2	2:M:200:THR:OG1	1.87	0.57
4:C:151:ASP:HB2	4:C:189:HIS:CD2	2.28	0.57
2:M:107:LYS:HA	2:M:140:TYR:OH	2.05	0.57
3:K:59:TYR:CD2	3:K:59:TYR:N	2.73	0.57
3:K:59:TYR:N	3:K:59:TYR:HD2	2.02	0.57
5:D:193:SER:O	5:D:194:ILE:HG23	2.04	0.57
5:B:137:VAL:HG12	5:B:138:THR:N	2.19	0.57
5:B:189:TRP:CZ2	5:B:211:ILE:HD11	2.39	0.57
3:K:60:ASN:HD22	3:K:60:ASN:C	2.09	0.57
3:K:85:VAL:HG23	3:K:85:VAL:O	2.04	0.57
4:C:49:TYR:OH	4:C:55:GLU:OE1	2.22	0.57
4:C:192:TYR:CD2	4:C:209:PHE:HE2	2.23	0.57
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.87	0.56
5:B:36:TRP:CD1	5:B:69:LEU:CD2	2.88	0.56
5:B:54:THR:HG22	5:B:55:GLY:N	2.20	0.56
5:B:56:TYR:C	5:B:57:THR:HG22	2.30	0.56
1:Q:94:TYR:C	1:Q:94:TYR:CD2	2.82	0.56
1:Q:119:LYS:HD2	3:K:52:TYR:CD1	2.39	0.56
1:P:150:LEU:HG	1:P:151:THR:H	1.71	0.56
2:L:151:ASP:HB2	2:L:152:GLY:HA3	1.86	0.56
4:A:190:ASN:HB2	4:A:212:ASN:H	1.69	0.56
1:Q:142:GLY:HA3	1:Q:151:THR:HB	1.85	0.56
1:P:176:VAL:CA	1:P:180:MET:HE3	2.28	0.56
2:L:159:VAL:C	2:L:160:LEU:HD12	2.30	0.56
4:A:54:LEU:N	4:A:54:LEU:CD1	2.67	0.56
4:A:210:ASN:O	4:A:213:GLU:HB2	2.05	0.56
5:B:11:LEU:HD12	5:B:12:ALA:H	1.69	0.56
5:B:52:ASN:C	5:B:52:ASN:HD22	2.12	0.56
5:B:101:PHE:N	5:B:101:PHE:CD1	2.65	0.56
5:B:152:THR:HG22	5:B:199:ALA:HB3	1.87	0.56
2:M:121:SER:C	2:M:123:GLU:N	2.61	0.56
5:D:51:ILE:O	5:D:51:ILE:HG23	2.05	0.56
5:D:79:TYR:N	5:D:79:TYR:CD2	2.72	0.56
3:H:172:SER:O	3:H:173:ASP:HB3	2.05	0.56
1:Q:77:GLU:CG	1:Q:79:THR:H	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:147:LYS:HD3	2:L:147:LYS:N	2.21	0.56
4:A:108:ARG:HD2	4:A:140:TYR:CB	2.29	0.56
5:B:3:GLN:HB3	9:B:220:HOH:O	2.05	0.56
5:B:111:THR:O	5:B:112:VAL:CG1	2.30	0.56
1:Q:59:ILE:HD13	1:Q:104:MET:SD	2.45	0.56
2:M:108:ARG:HD3	2:M:172:THR:HG22	1.86	0.56
2:M:139:PHE:O	2:M:172:THR:HB	2.06	0.56
1:P:150:LEU:HD23	1:P:152:PRO:CG	2.32	0.56
3:H:184:THR:C	3:H:186:SER:H	2.14	0.56
1:Q:163:ILE:HD12	1:Q:167:VAL:HG21	1.87	0.56
1:Q:179:PHE:CD2	1:Q:233:HIS:CE1	2.94	0.56
4:C:96:TYR:HD1	4:C:96:TYR:N	2.02	0.56
6:E:14:SIA:H4	6:E:14:SIA:C11	2.35	0.56
2:L:71:PHE:N	2:L:71:PHE:CD1	2.73	0.56
1:Q:56:ALA:O	1:Q:95(A):MET:HE1	2.04	0.56
1:P:32:LEU:HD23	1:P:66:LEU:HD22	1.88	0.56
4:C:35:TRP:O	4:C:46:ILE:HD12	2.05	0.56
5:B:142:LEU:HD23	5:B:142:LEU:C	2.30	0.56
1:Q:63:SER:C	1:Q:85:VAL:HG23	2.31	0.56
3:K:145:TYR:HB2	3:K:199:HIS:CE1	2.41	0.56
4:C:27(B):ILE:HD13	4:C:27(C):ASP:OD1	2.04	0.56
4:A:156:GLN:HE21	4:A:156:GLN:N	2.01	0.56
5:D:137:VAL:HG12	5:D:138:THR:N	2.21	0.56
6:E:13:GAL:H4	6:E:14:SIA:O7	2.06	0.56
1:P:45:VAL:CG2	1:P:198:PRO:HG3	2.36	0.55
1:P:95(G):ARG:CD	1:P:95(G):ARG:N	2.69	0.55
4:A:79:GLU:HG3	4:A:80:ALA:H	1.72	0.55
5:B:146:TYR:HE1	5:B:176:TYR:CB	2.16	0.55
5:B:194:ILE:HD12	5:B:194:ILE:O	2.06	0.55
3:K:35:ASN:HD22	3:K:35:ASN:N	2.01	0.55
4:C:179:LEU:HD12	4:C:180:THR:N	2.21	0.55
5:D:75:SER:O	5:D:76:ASN:HB2	2.07	0.55
5:B:6:GLN:NE2	5:B:92:CYS:N	2.45	0.55
5:B:30:SER:HA	5:B:52(A):PRO:HB2	1.88	0.55
2:M:48:ILE:HD11	2:M:54:LEU:HD12	1.88	0.55
5:B:198:VAL:HG12	5:B:199:ALA:N	2.21	0.55
1:P:142:GLY:O	1:P:143:SER:C	2.49	0.55
2:L:37:LEU:HD13	2:L:86:TYR:CZ	2.42	0.55
2:L:106:ILE:CG2	2:L:107:LYS:N	2.69	0.55
2:L:165:ASP:OD2	2:L:165:ASP:N	2.37	0.55
1:Q:141:TRP:CE2	1:Q:155:LEU:HD23	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:48:ILE:HG23	2:M:53:ASN:O	2.06	0.55
3:K:134:SER:O	3:K:184:THR:HA	2.05	0.55
1:P:73:PHE:O	1:P:75:HIS:C	2.49	0.55
2:L:124:GLN:NE2	2:L:130:ALA:HA	2.21	0.55
3:H:83:THR:HG23	3:H:84:SER:N	2.19	0.55
5:B:77:THR:OG1	5:B:78:ALA:N	2.40	0.55
2:M:186:TYR:HD2	2:M:187:GLU:N	2.04	0.55
4:C:27(C):ASP:CG	4:C:68:ARG:HG2	2.31	0.55
4:C:39:LYS:NZ	4:C:81:ASP:HB2	2.22	0.55
3:H:83:THR:HG22	3:H:85:VAL:H	1.72	0.55
4:A:39:LYS:HB2	4:A:42:GLN:CG	2.32	0.55
5:B:165:HIS:O	5:B:166:THR:HB	2.07	0.55
2:M:154:GLU:CG	2:M:155:ARG:H	2.03	0.55
3:K:6:GLN:HE22	3:K:92:CYS:N	2.00	0.55
1:P:95(E):LYS:O	1:P:95(H):PHE:CE1	2.59	0.55
1:Q:50:GLN:O	1:Q:108:LEU:HD23	2.06	0.55
2:M:6:GLN:NE2	2:M:101:GLY:H	2.04	0.55
3:K:121:VAL:O	3:K:121:VAL:HG22	2.07	0.55
4:C:124:GLN:NE2	4:C:131:SER:H	2.04	0.55
4:C:47:LEU:N	4:C:47:LEU:CD2	2.69	0.55
4:C:59:PRO:C	4:C:61:ARG:H	2.14	0.55
5:D:67:VAL:HG12	5:D:68:THR:N	2.22	0.55
4:A:174:SER:OG	5:B:165:HIS:HE1	1.90	0.55
5:B:37:VAL:HG11	5:B:104:TRP:CZ3	2.42	0.55
3:K:98:ARG:HG2	3:K:99:TYR:HD2	1.72	0.55
3:K:153:LEU:HD23	3:K:153:LEU:N	2.21	0.55
5:D:128:VAL:HG13	5:D:129:CYS:N	2.21	0.55
5:D:189:TRP:O	5:D:190:PRO:C	2.46	0.55
3:H:18:VAL:HG21	3:H:109:VAL:HG21	1.89	0.55
3:H:60:ASN:ND2	3:H:61:GLY:N	2.46	0.55
4:A:155:ARG:NH2	4:A:157:ASN:CG	2.64	0.55
5:B:178:LEU:HD23	5:B:178:LEU:C	2.31	0.55
1:Q:134:THR:H	1:Q:162:VAL:HG23	1.72	0.55
4:C:27(D):LEU:HD23	4:C:92:HIS:CE1	2.41	0.55
4:C:154:GLU:HG2	4:C:155:ARG:N	2.21	0.55
4:A:183:LYS:NZ	4:A:187:GLU:HB2	2.22	0.54
3:K:57:THR:OG1	3:K:59:TYR:HE2	1.91	0.54
1:P:238:ILE:O	1:P:239:LYS:C	2.48	0.54
4:A:14:SER:HA	4:A:107:LYS:CB	2.35	0.54
1:Q:141:TRP:N	1:Q:193:GLY:HA2	2.23	0.54
4:C:206:VAL:HG12	4:C:207:LYS:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:96:GLY:HA2	1:Q:175:LYS:NZ	2.22	0.54
2:M:83:VAL:HG22	2:M:84:GLY:N	2.22	0.54
4:C:168:SER:O	4:C:169:LYS:HG2	2.07	0.54
5:D:147:PHE:N	5:D:148:PRO:CD	2.70	0.54
5:B:13:LYS:O	5:B:16:ALA:CB	2.52	0.54
2:M:38:GLN:HG3	2:M:44:PRO:HG3	1.90	0.54
2:L:56:SER:C	2:L:58:VAL:H	2.16	0.54
3:H:105:GLN:HE21	3:H:105:GLN:H	1.54	0.54
4:A:31:THR:O	4:A:50:ARG:HA	2.07	0.54
4:A:166:GLN:HG3	4:A:173:TYR:CE1	2.43	0.54
1:Q:53:LEU:HD11	1:Q:103:LEU:CD1	2.38	0.54
1:Q:91:HIS:HE1	1:Q:93:LEU:HG	1.72	0.54
1:Q:199:LEU:HD22	1:Q:228:TYR:CD1	2.43	0.54
3:K:173:ASP:O	3:K:174:LEU:HD23	2.08	0.54
5:D:29:PHE:HZ	5:D:77:THR:O	1.90	0.54
4:A:149:LYS:HD2	4:A:152:GLY:HA2	1.89	0.54
5:B:24:THR:HG23	5:B:27:TYR:CE2	2.43	0.54
1:Q:65:ILE:O	1:Q:66:LEU:HD12	2.06	0.54
5:D:48:ILE:CG2	5:D:63:PHE:CD1	2.84	0.54
1:Q:95(A):MET:C	1:Q:95(C):LEU:H	2.15	0.54
5:D:119:ALA:HA	5:D:200:HIS:HD1	1.72	0.54
5:D:164:VAL:HG23	5:D:165:HIS:N	2.23	0.54
2:L:162:SER:HA	2:L:163:TRP:CE3	2.42	0.54
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.89	0.54
4:A:117:ILE:HD11	4:A:194:CYS:HB2	1.90	0.54
4:A:141:PRO:O	4:A:143:ASP:N	2.40	0.54
5:B:116:LYS:HG3	5:B:116:LYS:O	2.06	0.54
1:Q:192:SER:HB3	1:Q:219:PRO:O	2.08	0.54
3:K:182:THR:C	3:K:183:VAL:HG13	2.32	0.54
4:C:27(C):ASP:OD2	4:C:68:ARG:HG2	2.08	0.54
5:B:13:LYS:H	5:B:13:LYS:CD	2.21	0.54
1:Q:72:LEU:CD2	1:Q:72:LEU:H	2.20	0.54
5:D:128:VAL:HG13	5:D:130:GLY:H	1.73	0.54
5:D:156:ASN:O	5:D:157:SER:OG	2.23	0.54
5:B:189:TRP:HB3	5:B:190:PRO:HD3	1.90	0.54
1:Q:87:HIS:CD2	5:D:54:THR:HG22	2.37	0.54
1:P:91:HIS:CG	1:P:92:PRO:HD2	2.43	0.53
1:P:237:TRP:C	1:P:241:THR:HG22	2.29	0.53
4:A:39:LYS:CB	4:A:42:GLN:HG3	2.36	0.53
5:B:68:THR:O	5:B:68:THR:HG22	2.07	0.53
2:M:140:TYR:CG	2:M:140:TYR:O	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:114:LEU:HD12	1:P:114:LEU:N	2.23	0.53
1:P:161:HIS:HE1	1:P:185:ARG:NH2	1.97	0.53
3:H:11:LEU:HA	3:H:110:THR:O	2.09	0.53
3:H:101:ASP:OD1	3:H:102:TYR:N	2.42	0.53
4:A:131:SER:HB3	4:A:180:THR:HA	1.89	0.53
5:B:52:ASN:HD22	5:B:52(A):PRO:N	2.05	0.53
1:Q:138:ALA:O	1:Q:157:CYS:HA	2.09	0.53
2:M:80:ALA:O	2:M:83:VAL:HG12	2.07	0.53
3:H:137:THR:C	3:H:138:LEU:HD23	2.33	0.53
4:A:34:HIS:CD2	4:A:49:TYR:HA	2.43	0.53
4:A:210:ASN:ND2	2:M:74:ARG:HH22	2.06	0.53
1:Q:190:THR:OG1	1:Q:190:THR:O	2.26	0.53
5:D:52:ASN:C	5:D:52:ASN:HD22	2.15	0.53
5:D:96:GLY:O	5:D:97:ARG:HG3	2.08	0.53
6:E:4:MAN:H62	6:E:5:NAG:O3	2.08	0.53
4:C:142:LYS:HD3	4:C:173:TYR:OH	2.08	0.53
3:K:2:VAL:HA	3:K:26:GLY:HA3	1.90	0.53
3:K:170:LEU:HD12	3:K:175:TYR:CE1	2.43	0.53
3:H:120:PRO:HD2	3:H:143:LYS:O	2.08	0.53
3:K:94:ARG:HH21	3:K:101:ASP:CG	2.17	0.53
2:L:135:PHE:C	2:L:136:LEU:HD12	2.32	0.53
5:B:120:PRO:HG2	5:B:145:GLY:HA3	1.89	0.53
5:B:154:LEU:C	5:B:154:LEU:HD12	2.34	0.53
1:Q:36:ARG:HG2	1:Q:36:ARG:O	2.08	0.53
1:Q:95(C):LEU:HD12	1:Q:95(C):LEU:N	2.24	0.53
1:P:211:GLY:HA2	1:P:231:VAL:HG23	1.91	0.53
1:Q:150:LEU:HD22	1:Q:151:THR:HG23	1.90	0.53
4:C:120:PRO:HG2	4:C:186:TYR:CE1	2.43	0.53
5:D:144:LYS:HA	5:D:177:THR:HG23	1.90	0.53
2:L:103:LYS:NZ	9:L:216:HOH:O	2.42	0.53
3:H:119:PRO:HD2	3:H:204:THR:HG21	1.91	0.53
2:M:52:SER:HA	2:M:64:GLY:O	2.08	0.53
4:C:35:TRP:CG	4:C:73:LEU:HD22	2.44	0.53
4:C:184:ASP:HA	4:C:187:GLU:CD	2.34	0.53
4:A:150:ILE:HD12	4:A:151:ASP:N	2.24	0.53
5:B:171:LEU:HB2	5:B:176:TYR:CE1	2.44	0.53
1:Q:147:GLU:HA	1:Q:147:GLU:OE1	2.09	0.53
3:K:101:ASP:C	3:K:101:ASP:OD1	2.51	0.53
4:C:43:PRO:HB3	5:D:91:TYR:HE1	1.72	0.53
5:D:124:PRO:HA	5:D:211:ILE:HD11	1.91	0.53
5:D:192:GLN:HE21	5:D:192:GLN:CA	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:PHE:CE2	3:H:180:SER:OG	2.62	0.52
5:B:197:ASN:HA	5:B:208:ASP:HB2	1.91	0.52
4:C:35:TRP:O	4:C:47:LEU:HD23	2.08	0.52
5:D:144:LYS:C	5:D:144:LYS:HD3	2.34	0.52
3:H:13:LYS:CD	3:H:13:LYS:N	2.61	0.52
5:B:102:ASP:O	5:B:103:VAL:HG13	2.10	0.52
1:Q:130:PRO:HG3	1:Q:210:GLN:HG3	1.90	0.52
5:D:171:LEU:HD12	5:D:176:TYR:CE1	2.45	0.52
1:P:30:GLN:HE22	1:P:198:PRO:CG	2.22	0.52
2:L:188:ARG:O	2:L:189:HIS:CG	2.62	0.52
3:H:29:ILE:HG12	3:H:29:ILE:O	2.08	0.52
3:H:146:PHE:HE1	3:H:175:TYR:HE2	1.55	0.52
4:A:212:ASN:O	4:A:213:GLU:HG2	2.09	0.52
5:B:60:ASN:HD22	5:B:61:GLN:H	1.53	0.52
1:P:76:PRO:HG3	4:A:29:GLY:HA2	1.92	0.52
1:P:150:LEU:HB3	1:P:152:PRO:HD2	1.91	0.52
2:L:188:ARG:O	2:L:189:HIS:CD2	2.62	0.52
4:A:16:GLY:O	4:A:17:GLN:O	2.27	0.52
1:Q:23:GLU:HG3	3:K:99:TYR:HA	1.91	0.52
5:D:6:GLN:HE22	5:D:91:TYR:HA	1.74	0.52
5:D:28:SER:HA	9:D:218:HOH:O	2.09	0.52
4:A:142:LYS:O	4:A:144:ILE:CG2	2.57	0.52
2:M:150:ILE:HB	2:M:153:SER:HB3	1.91	0.52
5:D:19:LYS:CE	5:D:79:TYR:CD1	2.93	0.52
2:L:118:PHE:HB2	2:L:133:VAL:HG22	1.92	0.52
1:Q:169:ALA:HA	1:Q:176:VAL:HG21	1.92	0.52
4:C:206:VAL:CG1	4:C:207:LYS:N	2.72	0.52
5:D:153:LEU:HD12	5:D:153:LEU:N	2.25	0.52
3:H:57:THR:O	3:H:58:LYS:HG2	2.09	0.52
1:P:130:PRO:HG3	1:P:210:GLN:CD	2.34	0.52
3:H:48:ILE:O	3:H:48:ILE:HG22	2.09	0.52
3:H:188:TRP:HD1	3:H:193:ILE:HD13	1.72	0.52
4:A:141:PRO:O	4:A:142:LYS:C	2.53	0.52
1:Q:86:SER:OG	1:Q:107:ARG:NE	2.43	0.52
1:Q:233:HIS:HB3	1:Q:234:TYR:CD2	2.44	0.52
3:K:133:GLY:C	3:K:135:SER:N	2.68	0.52
3:K:148:GLU:O	3:K:149:SER:HB2	2.10	0.52
1:P:69:ARG:NH1	4:A:28:TYR:O	2.42	0.52
5:B:35:HIS:HD2	5:B:47:TRP:HE1	1.58	0.52
1:Q:85:VAL:O	5:D:33:TRP:CH2	2.63	0.52
4:C:135:PHE:O	4:C:136:LEU:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:41:VAL:HG12	1:P:42:CYS:HB2	1.92	0.52
1:P:161:HIS:CE1	1:P:185:ARG:CD	2.92	0.52
2:L:183:LYS:HG2	2:L:184:ASP:N	2.25	0.52
1:Q:143:SER:C	1:Q:144:ILE:HG23	2.34	0.52
4:C:180:THR:O	4:C:181:LEU:HD22	2.10	0.52
5:D:153:LEU:HD21	5:D:166:THR:HG23	1.91	0.52
1:P:150:LEU:CD2	1:P:152:PRO:HG2	2.33	0.51
2:L:181:LEU:CD2	2:L:185:GLU:HB2	2.40	0.51
3:H:132:THR:CG2	3:H:133:GLY:N	2.73	0.51
5:D:193:SER:OG	5:D:210:LYS:HE3	2.11	0.51
2:L:38:GLN:HE21	2:L:87:TYR:HE2	1.56	0.51
2:L:116:SER:CB	2:L:118:PHE:HE1	2.24	0.51
4:A:139:PHE:CD1	4:A:139:PHE:O	2.63	0.51
1:Q:72:LEU:HD22	1:Q:72:LEU:H	1.70	0.51
1:Q:172:HIS:N	1:Q:223(A):GLU:HG3	2.24	0.51
2:L:160:LEU:HD21	3:H:171:GLN:HB2	1.92	0.51
1:Q:168:CYS:HA	1:Q:171:VAL:CG2	2.38	0.51
2:M:55:ALA:HB3	2:M:58:VAL:HG21	1.93	0.51
1:P:29:TRP:O	1:P:31:VAL:HG13	2.11	0.51
2:L:13:VAL:CG1	2:L:78:VAL:HG21	2.41	0.51
4:A:3:VAL:O	4:A:26:SER:OG	2.24	0.51
4:C:2:ILE:HD12	4:C:3:VAL:N	2.26	0.51
4:C:3:VAL:O	4:C:3:VAL:HG22	2.11	0.51
2:L:108:ARG:NH2	2:L:140:TYR:HB2	2.26	0.51
3:H:37:VAL:HG23	3:H:38:LYS:N	2.25	0.51
3:H:56:ASP:OD1	3:H:57:THR:N	2.44	0.51
5:D:151:VAL:HG12	5:D:152:THR:N	2.26	0.51
5:D:153:LEU:HD21	5:D:166:THR:CG2	2.41	0.51
8:G:8:MAN:C1	8:G:9:NAG:H2	2.41	0.51
3:H:188:TRP:HZ2	3:H:210:ILE:CG1	2.18	0.51
4:A:90:GLN:HE22	4:A:93:GLU:H	1.57	0.51
4:C:144:ILE:O	4:C:145:ASN:HB2	2.10	0.51
3:H:60:ASN:HD22	3:H:60:ASN:C	2.09	0.51
3:H:153:LEU:CD1	3:H:196:ASN:HB2	2.39	0.51
4:A:135:PHE:O	4:A:136:LEU:HD12	2.11	0.51
5:B:37:VAL:HG23	5:B:46:GLU:O	2.11	0.51
5:B:189:TRP:CE2	5:B:211:ILE:HD11	2.45	0.51
1:Q:65:ILE:CG2	1:Q:67:LEU:HD11	2.39	0.51
3:K:148:GLU:O	3:K:149:SER:CB	2.58	0.51
4:C:27(D):LEU:HD12	4:C:27(D):LEU:O	2.10	0.51
1:P:107:ARG:HH21	1:P:107:ARG:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:ASP:CB	2:L:152:GLY:HA3	2.40	0.51
3:H:40:ARG:NH1	3:H:87:SER:O	2.44	0.51
5:B:17:SER:HA	5:B:82(C):LEU:CD2	2.40	0.51
5:B:146:TYR:CE2	5:B:151:VAL:HG21	2.46	0.51
1:Q:196:GLY:H	1:Q:213:THR:HB	1.76	0.51
2:M:214:CYS:C	3:K:213:ARG:HG3	2.36	0.51
2:L:6:GLN:NE2	2:L:99:GLY:HA3	2.23	0.51
2:L:35:TRP:CE3	2:L:88:CYS:HB3	2.45	0.51
2:L:181:LEU:HD23	2:L:182:THR:H	1.72	0.51
5:B:211:ILE:HD12	5:B:212:VAL:N	2.25	0.51
1:Q:108:LEU:HD23	1:Q:108:LEU:N	2.24	0.51
5:D:6:GLN:NE2	5:D:107:GLY:H	2.09	0.51
5:B:61:GLN:HE21	5:B:61:GLN:CA	2.12	0.51
5:B:120:PRO:O	5:B:121:PRO:C	2.53	0.51
1:Q:75:HIS:CB	2:M:28:ASN:HA	2.41	0.51
2:M:108:ARG:HG3	2:M:109:ALA:O	2.11	0.51
3:K:6:GLN:NE2	3:K:92:CYS:SG	2.84	0.51
4:C:192:TYR:HB2	4:C:209:PHE:HE2	1.71	0.51
5:D:120:PRO:CG	5:D:146:TYR:HB3	2.39	0.51
1:P:98:ASP:HB2	1:P:175:LYS:HD3	1.93	0.50
2:L:147:LYS:N	2:L:147:LYS:CD	2.74	0.50
3:H:74:SER:O	3:H:74:SER:OG	2.30	0.50
1:Q:19:GLY:HA3	1:Q:190:THR:HG1	1.73	0.50
2:M:83:VAL:CG2	2:M:84:GLY:N	2.74	0.50
3:K:99:TYR:CD2	3:K:99:TYR:N	2.78	0.50
5:D:199:ALA:O	5:D:201:PRO:HD3	2.12	0.50
4:A:27(B):ILE:HD11	4:A:32:PHE:CA	2.41	0.50
5:B:195:THR:HG23	5:B:210:LYS:CA	2.42	0.50
1:Q:85:VAL:O	5:D:33:TRP:HH2	1.93	0.50
2:M:8:ALA:O	2:M:102:THR:HG22	2.11	0.50
2:M:83:VAL:HG23	2:M:104:VAL:O	2.10	0.50
1:P:208:VAL:HG12	1:P:209:LEU:O	2.11	0.50
2:L:46:LEU:CD2	3:H:99:TYR:CD1	2.95	0.50
4:A:205:ILE:HG23	2:M:67:SER:HB3	1.93	0.50
1:Q:16:ILE:O	1:Q:16:ILE:HG12	2.11	0.50
5:D:19:LYS:HE2	5:D:79:TYR:CD1	2.39	0.50
5:D:198:VAL:O	5:D:199:ALA:HB2	2.12	0.50
2:M:73:LEU:HG	2:M:74:ARG:N	2.27	0.50
4:C:141:PRO:O	4:C:142:LYS:O	2.30	0.50
4:A:1:ASP:OD2	4:A:95:PRO:HB3	2.12	0.50
4:A:8:PRO:HG2	4:A:10:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:HIS:HD2	4:A:49:TYR:CB	2.22	0.50
4:A:154:GLU:O	4:A:154:GLU:CG	2.60	0.50
5:D:50:TYR:HE1	5:D:58:GLU:HG3	1.76	0.50
1:P:35:SER:HB3	1:P:63:SER:HA	1.93	0.50
4:A:156:GLN:H	4:A:156:GLN:NE2	2.04	0.50
5:B:14:PRO:C	5:B:16:ALA:N	2.68	0.50
1:Q:231:VAL:C	1:Q:233:HIS:N	2.67	0.50
4:C:142:LYS:HD3	4:C:173:TYR:CZ	2.46	0.50
4:C:186:TYR:C	4:C:186:TYR:CD2	2.89	0.50
3:H:40:ARG:HH11	3:H:40:ARG:HG3	1.75	0.50
4:A:58:ILE:HD12	4:A:58:ILE:N	2.26	0.50
5:B:33:TRP:CE3	5:B:52:ASN:HB2	2.47	0.50
1:Q:144:ILE:C	1:Q:146:PRO:HD3	2.37	0.50
2:M:108:ARG:HG2	2:M:140:TYR:CD1	2.46	0.50
5:D:146:TYR:O	5:D:146:TYR:HD2	1.94	0.50
1:P:50:GLN:O	1:P:108:LEU:HD22	2.11	0.50
5:B:37:VAL:HG13	5:B:91:TYR:HB2	1.93	0.50
2:M:46:LEU:HD22	3:K:99:TYR:HE1	1.76	0.50
5:D:40:ARG:CZ	5:D:85:GLU:HG3	2.42	0.50
5:D:125:LEU:HD12	5:D:140:GLY:CA	2.42	0.50
3:H:150:VAL:HG22	3:H:151:THR:N	2.27	0.50
4:A:63:SER:OG	4:A:74:THR:HB	2.12	0.50
2:M:117:ILE:HD13	2:M:194:CYS:HB2	1.93	0.50
2:M:126:THR:C	2:M:128:GLY:N	2.70	0.50
4:C:15:LEU:C	4:C:15:LEU:HD12	2.37	0.50
1:Q:72:LEU:HB3	4:C:28:TYR:HA	1.92	0.49
5:D:125:LEU:HD12	5:D:140:GLY:HA3	1.93	0.49
5:D:178:LEU:HD23	5:D:178:LEU:C	2.37	0.49
2:L:91:HIS:CD2	2:L:91:HIS:O	2.65	0.49
2:L:170:ASP:CB	2:L:172:THR:HG23	2.30	0.49
3:H:138:LEU:HD23	3:H:138:LEU:N	2.27	0.49
1:Q:47:VAL:O	1:Q:120:VAL:HB	2.12	0.49
1:Q:72:LEU:HD21	1:Q:141:TRP:NE1	2.27	0.49
2:M:160:LEU:HB3	3:K:169:VAL:HG11	1.95	0.49
5:D:112:VAL:O	5:D:113:SER:OG	2.30	0.49
2:L:25:SER:C	2:L:27:LYS:H	2.20	0.49
2:L:142:LYS:HG3	2:L:173:TYR:CE1	2.47	0.49
2:L:144:ILE:HB	2:L:197:THR:O	2.12	0.49
2:L:163:TRP:N	2:L:163:TRP:CD2	2.80	0.49
3:H:40:ARG:HG3	3:H:41:PRO:HD2	1.95	0.49
1:Q:139:SER:HA	1:Q:156:GLN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:103:TRP:N	3:K:103:TRP:CD1	2.80	0.49
3:K:127:VAL:O	3:K:128:CYS:C	2.54	0.49
4:C:209:PHE:HD2	4:C:209:PHE:C	2.20	0.49
5:D:13:LYS:O	5:D:16:ALA:HB3	2.12	0.49
5:D:29:PHE:CE2	5:D:76:ASN:C	2.90	0.49
5:D:35:HIS:CD2	5:D:47:TRP:HE1	2.29	0.49
4:A:2:ILE:HG22	4:A:26:SER:HB3	1.95	0.49
5:B:189:TRP:CE3	5:B:190:PRO:HG3	2.48	0.49
1:Q:46:LEU:HD12	1:Q:51:TRP:O	2.13	0.49
1:Q:95(E):LYS:HZ2	8:G:11:SIA:H111	1.77	0.49
5:D:146:TYR:CD2	5:D:146:TYR:O	2.65	0.49
1:P:174:GLN:HG2	1:P:175:LYS:N	2.27	0.49
4:C:155:ARG:HH12	4:C:181:LEU:HD21	1.78	0.49
5:D:157:SER:N	5:D:197:ASN:HD21	2.10	0.49
2:L:77:ARG:O	2:L:77:ARG:CG	2.59	0.49
2:L:95:PRO:O	2:L:96:VAL:C	2.52	0.49
2:L:119:PRO:O	2:L:120:PRO:C	2.56	0.49
3:H:13:LYS:H	3:H:13:LYS:CE	2.25	0.49
4:A:131:SER:HA	4:A:179:LEU:O	2.13	0.49
5:D:114:SER:O	5:D:147:PHE:HD1	1.95	0.49
1:P:65:ILE:HG22	1:P:67:LEU:CD1	2.42	0.49
2:L:2:ILE:HD13	2:L:93:GLU:HB2	1.95	0.49
4:A:206:VAL:O	2:M:66:GLY:HA2	2.13	0.49
1:P:30:GLN:HE22	1:P:198:PRO:HG2	1.78	0.49
1:P:35:SER:HB2	1:P:62:LYS:O	2.11	0.49
1:P:36:ARG:HD3	1:P:36:ARG:H	1.77	0.49
1:P:95(G):ARG:NH2	9:P:267:HOH:O	2.46	0.49
2:L:51:MET:HE1	2:L:66:GLY:O	2.13	0.49
2:L:136:LEU:O	2:L:137:ASN:OD1	2.30	0.49
3:H:146:PHE:CD1	3:H:147:PRO:HA	2.48	0.49
4:A:106:ILE:HG23	4:A:107:LYS:N	2.27	0.49
5:B:173:SER:O	5:B:175:LEU:N	2.46	0.49
1:Q:165:ASN:ND2	1:Q:178:LYS:HD2	2.27	0.49
2:M:62:PHE:CE1	2:M:75:ILE:HG13	2.48	0.49
3:K:13:LYS:HD2	3:K:13:LYS:N	2.27	0.49
5:D:121:PRO:HB2	5:D:123:TYR:CE2	2.48	0.49
5:D:124:PRO:HA	5:D:211:ILE:CD1	2.43	0.49
1:P:28:PRO:CB	1:P:119:LYS:H	2.26	0.49
2:L:195:GLU:HG3	2:L:206:VAL:CG2	2.42	0.49
1:Q:20:TRP:HB2	3:K:98:ARG:NH1	2.28	0.49
1:Q:186:TRP:HE3	1:Q:224:ARG:HD2	1.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:188:LYS:HG2	1:Q:224:ARG:HH12	1.78	0.49
1:Q:231:VAL:O	1:Q:233:HIS:N	2.45	0.49
4:C:209:PHE:C	4:C:209:PHE:CD2	2.91	0.49
8:G:3:MAN:H3	8:G:4:MAN:O2	2.13	0.49
1:P:150:LEU:HG	1:P:151:THR:N	2.28	0.49
2:L:116:SER:HB2	2:L:118:PHE:HE1	1.75	0.49
3:H:20:ILE:HD12	3:H:107:THR:HG21	1.95	0.49
4:A:108:ARG:CG	4:A:140:TYR:CG	2.95	0.49
4:A:157:ASN:ND2	4:A:157:ASN:N	2.48	0.49
5:B:96:GLY:C	5:B:97:ARG:HG2	2.38	0.49
5:B:173:SER:C	5:B:175:LEU:N	2.70	0.49
1:Q:83:PHE:CZ	1:Q:112:ALA:HA	2.48	0.49
1:Q:128:GLN:CG	1:Q:129:GLU:N	2.76	0.49
3:K:154:TRP:CZ3	3:K:195:CYS:HB3	2.48	0.49
4:C:33:MET:O	4:C:50:ARG:N	2.43	0.49
5:D:113:SER:O	5:D:114:SER:OG	2.30	0.49
1:P:153:LYS:HE2	1:P:154:LYS:NZ	2.28	0.48
1:Q:125:THR:HG22	1:Q:128:GLN:N	2.28	0.48
2:M:27:LYS:HB3	2:M:27:LYS:HE3	1.64	0.48
3:K:193:ILE:O	3:K:193:ILE:HG12	2.04	0.48
5:D:154:LEU:HB2	5:D:197:ASN:ND2	2.27	0.48
5:D:173:SER:C	5:D:174:ASP:CG	2.80	0.48
4:A:51:ALA:O	4:A:64:GLY:HA3	2.12	0.48
2:M:38:GLN:NE2	3:K:39:GLN:HE22	2.09	0.48
2:L:178:THR:O	2:L:178:THR:HG22	2.12	0.48
3:H:159:LEU:HD23	3:H:159:LEU:H	1.78	0.48
4:A:123:GLU:OE1	4:A:123:GLU:N	2.46	0.48
5:B:64:LYS:HE3	5:B:64:LYS:HB3	1.47	0.48
1:Q:239:LYS:HG3	1:Q:239:LYS:O	2.12	0.48
4:C:142:LYS:O	4:C:143:ASP:O	2.29	0.48
1:P:238:ILE:O	1:P:242:ILE:HB	2.13	0.48
3:H:50:ARG:NH1	3:H:95:ASP:OD2	2.46	0.48
4:A:205:ILE:CG2	2:M:67:SER:HB3	2.44	0.48
5:B:83:THR:HG22	5:B:84:SER:N	2.27	0.48
5:B:116:LYS:HE3	5:B:202:ALA:HB1	1.95	0.48
1:P:93:LEU:HB2	1:P:101:HIS:CD2	2.47	0.48
1:P:215:TRP:HA	1:P:215:TRP:CE3	2.49	0.48
2:L:133:VAL:HG21	3:H:124:LEU:HD23	1.95	0.48
5:B:35:HIS:CD2	5:B:47:TRP:HE1	2.32	0.48
5:B:60:ASN:O	5:B:61:GLN:C	2.56	0.48
2:M:48:ILE:HD12	2:M:54:LEU:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:33:TRP:CE3	3:K:50:ARG:HG3	2.48	0.48
4:C:11:LEU:HA	4:C:11:LEU:HD12	1.60	0.48
3:H:152:LEU:HD11	3:H:195:CYS:HB2	1.95	0.48
3:H:154:TRP:O	3:H:155:ASN:C	2.56	0.48
3:H:194:THR:HG23	3:H:208:LYS:O	2.13	0.48
4:A:108:ARG:CG	4:A:140:TYR:CD1	2.96	0.48
4:A:156:GLN:O	4:A:159:VAL:HG22	2.13	0.48
4:A:206:VAL:H	2:M:67:SER:H	1.61	0.48
1:Q:84:GLN:NE2	5:D:33:TRP:CD2	2.82	0.48
3:K:124:LEU:HD23	3:K:140:CYS:N	2.29	0.48
4:C:2:ILE:O	4:C:97:THR:HG21	2.13	0.48
4:C:193:THR:HA	4:C:208:SER:HB3	1.96	0.48
5:D:201:PRO:C	5:D:203:SER:H	2.21	0.48
6:E:7:SIA:N5	6:E:7:SIA:H8	2.29	0.48
1:P:124:PRO:HG3	1:P:209:LEU:O	2.14	0.48
1:P:151:THR:H	1:P:152:PRO:HD3	1.79	0.48
2:L:95:PRO:O	2:L:97:THR:HG23	2.14	0.48
1:Q:72:LEU:HD21	1:Q:141:TRP:CD1	2.48	0.48
2:M:34:TYR:CG	2:M:89:MET:HE3	2.49	0.48
3:K:155:ASN:HD22	3:K:159:LEU:CD1	2.27	0.48
2:L:166:GLN:O	2:L:167:ASP:O	2.32	0.48
4:C:125:LEU:H	4:C:125:LEU:CD2	2.02	0.48
8:G:12:NAG:H83	8:G:12:NAG:C3	2.42	0.48
1:P:73:PHE:HD1	1:P:153:LYS:HG2	1.78	0.48
1:P:157:CYS:O	3:H:98:ARG:NH1	2.47	0.48
1:P:244:ALA:C	1:P:246:PRO:HD3	2.39	0.48
2:L:189:HIS:O	2:L:211:ARG:NE	2.47	0.48
3:K:69:LEU:HD23	3:K:80:MET:HG2	1.95	0.48
4:C:167:ASP:CG	4:C:168:SER:N	2.72	0.48
1:P:71:SER:O	1:P:72:LEU:HD13	2.14	0.48
1:P:123:LEU:N	1:P:123:LEU:CD1	2.76	0.48
1:P:218:GLU:HA	1:P:219:PRO:HD3	1.43	0.48
2:L:56:SER:C	2:L:58:VAL:N	2.72	0.48
2:L:183:LYS:H	2:L:183:LYS:HD2	1.78	0.48
4:A:3:VAL:C	4:A:26:SER:OG	2.57	0.48
4:A:90:GLN:HE22	4:A:92:HIS:N	2.09	0.48
4:A:156:GLN:N	4:A:156:GLN:NE2	2.61	0.48
5:B:40:ARG:O	5:B:41:PRO:C	2.56	0.48
5:B:189:TRP:O	5:B:190:PRO:C	2.57	0.48
5:B:195:THR:CG2	5:B:210:LYS:HB3	2.43	0.48
2:M:27(B):LEU:HD21	2:M:90:GLN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:183:LYS:H	2:L:183:LYS:CD	2.27	0.47
3:H:105:GLN:HE21	3:H:105:GLN:N	2.12	0.47
4:A:33:MET:C	4:A:34:HIS:CG	2.92	0.47
4:A:150:ILE:HD13	4:A:192:TYR:CE1	2.49	0.47
4:A:205:ILE:HG23	2:M:67:SER:CB	2.44	0.47
5:B:24:THR:CG2	5:B:25:SER:N	2.76	0.47
1:Q:67:LEU:N	1:Q:67:LEU:CD1	2.77	0.47
2:M:47:LEU:O	2:M:48:ILE:HD13	2.15	0.47
3:K:83:THR:OG1	3:K:84:SER:N	2.45	0.47
4:C:146:VAL:CG1	4:C:147:LYS:N	2.76	0.47
5:D:66:LYS:HD3	5:D:82(A):ASN:O	2.14	0.47
4:A:94:ASP:HA	4:A:96:TYR:CE1	2.49	0.47
5:B:14:PRO:O	5:B:16:ALA:N	2.46	0.47
1:Q:124:PRO:HB2	1:Q:232:VAL:HG12	1.95	0.47
2:M:206:VAL:O	2:M:206:VAL:HG12	2.13	0.47
3:K:98:ARG:CG	3:K:99:TYR:HD2	2.26	0.47
3:K:153:LEU:O	3:K:153:LEU:HG	2.14	0.47
3:H:73:LYS:C	3:H:75:SER:H	2.22	0.47
3:H:170:LEU:C	3:H:170:LEU:CD1	2.86	0.47
4:A:23:CYS:HB2	4:A:35:TRP:CH2	2.49	0.47
5:B:60:ASN:ND2	5:B:62:LYS:HG2	2.29	0.47
5:D:75:SER:CB	5:D:77:THR:HG23	2.45	0.47
5:D:207:VAL:HG12	5:D:208:ASP:N	2.29	0.47
1:P:75:HIS:N	1:P:76:PRO:CD	2.77	0.47
2:L:108:ARG:HG2	2:L:109:ALA:H	1.78	0.47
4:A:112:ALA:O	4:A:113:PRO:O	2.32	0.47
1:Q:234:TYR:O	1:Q:236:LYS:N	2.47	0.47
5:D:184:VAL:CG2	5:D:185:THR:N	2.77	0.47
5:D:198:VAL:CG1	5:D:199:ALA:N	2.78	0.47
1:P:76:PRO:CG	4:A:29:GLY:HA2	2.44	0.47
2:L:117:ILE:C	2:L:118:PHE:CD1	2.93	0.47
2:L:131:SER:HB3	2:L:180:THR:CB	2.44	0.47
4:A:142:LYS:H	4:A:142:LYS:CD	2.15	0.47
5:B:195:THR:HG23	5:B:210:LYS:CB	2.45	0.47
2:M:167:ASP:CG	2:M:170:ASP:HB2	2.39	0.47
4:C:89:GLN:NE2	4:C:98:PHE:CZ	2.82	0.47
4:C:157:ASN:H	4:C:157:ASN:HD22	1.62	0.47
8:G:8:MAN:H4	8:G:9:NAG:H4	1.97	0.47
1:P:231:VAL:C	1:P:233:HIS:N	2.71	0.47
2:L:135:PHE:CE2	3:H:180:SER:HB3	2.49	0.47
3:H:147:PRO:HB2	3:H:148:GLU:H	1.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:161:ASN:HB2	4:A:175:MET:HE3	1.95	0.47
1:Q:119:LYS:HE3	3:K:52:TYR:HD1	1.79	0.47
4:C:54:LEU:H	4:C:54:LEU:CD1	2.03	0.47
4:C:121:SER:HB3	4:C:124:GLN:HB2	1.96	0.47
4:C:136:LEU:HD21	4:C:146:VAL:CG2	2.45	0.47
5:D:157:SER:CA	5:D:197:ASN:HD21	2.27	0.47
5:D:196:CYS:O	5:D:208:ASP:HA	2.14	0.47
1:P:95(E):LYS:H	1:P:95(H):PHE:HE1	1.63	0.47
2:L:137:ASN:O	2:L:138:ASN:OD1	2.32	0.47
3:H:146:PHE:CE1	3:H:175:TYR:HE2	2.32	0.47
4:A:27(B):ILE:HA	4:A:92:HIS:ND1	2.29	0.47
4:A:89:GLN:HG2	4:A:90:GLN:N	2.30	0.47
4:A:151:ASP:OD2	4:A:189:HIS:CB	2.62	0.47
4:A:192:TYR:HD2	4:A:209:PHE:CE2	2.32	0.47
5:B:97:ARG:C	5:B:98:LEU:HD23	2.33	0.47
5:B:120:PRO:O	5:B:121:PRO:O	2.33	0.47
1:Q:66:LEU:HG	4:C:30:PHE:CD1	2.50	0.47
2:M:15:PRO:C	2:M:17:GLU:H	2.22	0.47
2:M:48:ILE:CD1	2:M:54:LEU:HA	2.44	0.47
3:K:13:LYS:HA	3:K:112:SER:O	2.15	0.47
3:K:29:ILE:O	3:K:29:ILE:HG12	2.14	0.47
3:K:56:ASP:C	3:K:57:THR:HG22	2.40	0.47
3:K:96:GLY:HA3	3:K:101:ASP:OD2	2.14	0.47
4:C:7:SER:O	4:C:22:SER:N	2.41	0.47
4:C:137:ASN:HA	4:C:174:SER:HB3	1.97	0.47
4:C:190:ASN:O	4:C:211:ARG:N	2.39	0.47
4:C:193:THR:HG22	4:C:208:SER:CB	2.44	0.47
5:D:50:TYR:CD1	5:D:58:GLU:HB2	2.50	0.47
1:P:242:ILE:HG22	1:P:243:VAL:N	2.30	0.47
2:L:173:TYR:O	2:L:174:SER:CB	2.60	0.47
4:A:109:ALA:O	4:A:110:ASP:C	2.58	0.47
5:B:60:ASN:HB3	5:B:63:PHE:CD1	2.50	0.47
5:B:75:SER:O	5:B:77:THR:HG22	2.15	0.47
5:B:118:THR:O	5:B:120:PRO:CD	2.63	0.47
1:Q:91:HIS:CE1	1:Q:93:LEU:HG	2.48	0.47
4:C:27(B):ILE:CD1	4:C:27(B):ILE:N	2.78	0.47
4:C:156:GLN:O	4:C:159:VAL:HG12	2.15	0.47
1:P:71:SER:C	1:P:72:LEU:HD13	2.39	0.47
2:L:67:SER:O	2:L:69:THR:N	2.48	0.47
2:L:94:TYR:OH	3:H:50:ARG:HD3	2.15	0.47
2:L:155:ARG:HG2	2:L:155:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:153:LEU:HD12	5:B:153:LEU:HA	1.63	0.47
2:M:19:VAL:HG22	2:M:20:SER:N	2.20	0.47
3:K:13:LYS:H	3:K:13:LYS:CD	2.26	0.47
4:C:157:ASN:HD22	4:C:157:ASN:N	2.13	0.47
5:D:75:SER:HB2	5:D:77:THR:HG23	1.97	0.47
5:B:60:ASN:HB3	5:B:63:PHE:HD1	1.80	0.47
5:B:197:ASN:HA	5:B:208:ASP:CB	2.45	0.47
2:M:140:TYR:CD2	2:M:140:TYR:C	2.92	0.47
2:M:167:ASP:OD1	2:M:170:ASP:HB2	2.14	0.47
5:D:33:TRP:N	5:D:33:TRP:HE3	2.13	0.47
5:D:114:SER:O	5:D:147:PHE:CD1	2.68	0.47
3:H:18:VAL:HG22	3:H:82(C):LEU:HD11	1.98	0.46
3:H:111:VAL:O	3:H:112:SER:HB3	2.15	0.46
4:A:70:ASP:C	4:A:71:PHE:CD1	2.94	0.46
5:B:69:LEU:O	5:B:70:THR:HG23	2.15	0.46
2:M:38:GLN:HE22	3:K:39:GLN:NE2	2.10	0.46
2:M:182:THR:OG1	2:M:185:GLU:OE1	2.29	0.46
2:L:10:SER:OG	2:L:11:VAL:N	2.48	0.46
3:H:83:THR:HG22	3:H:84:SER:N	2.29	0.46
4:A:47:LEU:HA	4:A:58:ILE:HG12	1.96	0.46
4:A:170:ASP:CB	4:A:172:THR:HG23	2.40	0.46
1:Q:61:ASN:OD1	8:G:1:NAG:N2	2.48	0.46
4:C:113:PRO:HD3	4:C:198:HIS:HD2	1.77	0.46
4:C:155:ARG:HB3	4:C:155:ARG:CZ	2.45	0.46
1:P:33:VAL:HG12	1:P:34:ALA:N	2.30	0.46
3:H:48:ILE:O	3:H:48:ILE:CG2	2.63	0.46
4:A:143:ASP:O	4:A:144:ILE:HB	2.13	0.46
4:A:190:ASN:HB3	4:A:212:ASN:OD1	2.15	0.46
5:B:208:ASP:O	5:B:208:ASP:OD2	2.33	0.46
5:B:211:ILE:O	5:B:212:VAL:HG23	2.16	0.46
2:M:132:VAL:CG1	2:M:133:VAL:N	2.78	0.46
3:K:152:LEU:HD23	3:K:152:LEU:O	2.15	0.46
4:C:117:ILE:HG12	4:C:118:PHE:H	1.79	0.46
4:C:141:PRO:O	4:C:142:LYS:C	2.56	0.46
2:L:2:ILE:HD11	2:L:93:GLU:HG3	1.97	0.46
5:B:33:TRP:HZ3	5:B:52:ASN:CG	2.24	0.46
5:B:63:PHE:CD1	5:B:63:PHE:N	2.84	0.46
2:M:47:LEU:O	2:M:55:ALA:CB	2.64	0.46
2:M:160:LEU:HD23	3:K:169:VAL:CG1	2.45	0.46
3:K:194:THR:HB	3:K:209:LYS:HA	1.97	0.46
5:D:148:PRO:HB3	5:D:202:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:164:VAL:CG2	5:D:165:HIS:N	2.76	0.46
1:P:52:VAL:CG1	1:P:53:LEU:N	2.78	0.46
3:H:12:VAL:CG2	3:H:18:VAL:HG13	2.46	0.46
3:H:24:VAL:HG12	3:H:76:SER:HB3	1.97	0.46
3:H:51:ILE:HA	3:H:56:ASP:O	2.16	0.46
5:B:36:TRP:CE3	5:B:80:MET:CE	2.95	0.46
1:Q:95(H):PHE:HA	9:Q:251:HOH:O	2.16	0.46
1:Q:196:GLY:O	1:Q:197:GLY:C	2.58	0.46
2:M:135:PHE:C	2:M:136:LEU:HG	2.40	0.46
3:K:54:ASP:C	3:K:54:ASP:OD1	2.59	0.46
5:D:212:VAL:HG13	5:D:213:PRO:CD	2.43	0.46
1:P:72:LEU:HD21	1:P:141:TRP:NE1	2.29	0.46
3:H:194:THR:HG23	3:H:208:LYS:C	2.41	0.46
4:A:132:VAL:HG12	4:A:148:TRP:CH2	2.50	0.46
5:B:112:VAL:CG2	5:B:113:SER:HB3	2.43	0.46
1:Q:208:VAL:HG23	1:Q:209:LEU:N	2.28	0.46
4:C:109:ALA:O	4:C:110:ASP:C	2.58	0.46
4:C:179:LEU:HD12	4:C:180:THR:H	1.81	0.46
5:D:97:ARG:O	5:D:98:LEU:HB2	2.14	0.46
3:H:75:SER:O	3:H:77:THR:HG23	2.16	0.46
5:B:38:LYS:HB2	5:B:90:TYR:CE1	2.51	0.46
5:B:112:VAL:HG23	5:B:113:SER:N	2.30	0.46
5:B:164:VAL:CG2	5:B:165:HIS:N	2.78	0.46
1:Q:86:SER:HB2	5:D:31:SER:HA	1.97	0.46
1:Q:95(C):LEU:N	1:Q:95(C):LEU:CD1	2.79	0.46
1:Q:199:LEU:HD22	1:Q:228:TYR:HD1	1.80	0.46
2:M:25:SER:HB2	2:M:26:SER:H	1.36	0.46
4:C:2:ILE:HD11	4:C:4:LEU:CG	2.45	0.46
4:C:146:VAL:HG13	4:C:147:LYS:N	2.31	0.46
2:L:106:ILE:HG23	2:L:107:LYS:H	1.79	0.46
3:H:36:TRP:CE3	3:H:80:MET:HE2	2.51	0.46
3:H:188:TRP:CB	3:H:189:PRO:HD3	2.43	0.46
4:A:27(C):ASP:CA	4:A:31:THR:HG22	2.46	0.46
5:B:23:LYS:HD3	5:B:24:THR:N	2.31	0.46
5:B:63:PHE:HB3	5:B:67:VAL:CG2	2.45	0.46
1:Q:169:ALA:HA	1:Q:176:VAL:CG2	2.46	0.46
4:C:118:PHE:O	4:C:132:VAL:HG13	2.16	0.46
3:H:40:ARG:NH1	3:H:40:ARG:HG3	2.31	0.46
5:B:121:PRO:CB	5:B:123:TYR:CZ	2.98	0.46
2:M:162:SER:OG	3:K:167:PRO:CD	2.55	0.46
4:C:135:PHE:C	4:C:136:LEU:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:184:VAL:CG2	5:D:185:THR:H	2.29	0.46
5:D:199:ALA:CB	5:D:206:LYS:HD2	2.41	0.46
1:P:68:GLY:HA2	1:P:117:ALA:O	2.16	0.46
4:A:55:GLU:O	4:A:58:ILE:CD1	2.63	0.46
1:Q:85:VAL:C	5:D:33:TRP:CH2	2.93	0.46
1:Q:144:ILE:CD1	1:Q:219:PRO:HD2	2.45	0.46
4:C:104:LEU:HD23	4:C:105:GLU:O	2.15	0.46
1:P:98:ASP:C	1:P:98:ASP:OD1	2.57	0.45
5:B:84:SER:HA	9:B:218:HOH:O	2.16	0.45
1:Q:46:LEU:HD13	1:Q:52:VAL:HG23	1.98	0.45
1:Q:174:GLN:HE22	1:Q:227:LEU:HD11	1.80	0.45
1:Q:234:TYR:C	1:Q:236:LYS:N	2.74	0.45
2:M:47:LEU:O	2:M:55:ALA:HB2	2.16	0.45
2:M:93:GLU:CG	2:M:94:TYR:H	2.28	0.45
5:D:144:LYS:HD3	5:D:144:LYS:O	2.16	0.45
1:P:186:TRP:HB2	1:P:223:PRO:CA	2.43	0.45
3:H:60:ASN:ND2	3:H:60:ASN:C	2.72	0.45
5:B:182:VAL:HG13	5:B:183:THR:N	2.32	0.45
1:Q:65:ILE:C	1:Q:66:LEU:HD12	2.40	0.45
1:Q:222:LEU:HD11	1:Q:223(A):GLU:O	2.17	0.45
1:P:52:VAL:HG12	1:P:53:LEU:N	2.31	0.45
1:P:84:GLN:CD	5:B:33:TRP:CD1	2.95	0.45
5:B:23:LYS:HD3	5:B:23:LYS:C	2.41	0.45
5:B:134:GLY:O	5:B:135:SER:C	2.58	0.45
1:Q:129:GLU:HB2	1:Q:130:PRO:HD2	1.98	0.45
1:Q:199:LEU:HD13	1:Q:228:TYR:CE1	2.49	0.45
1:Q:222:LEU:HD12	1:Q:223(A):GLU:H	1.80	0.45
3:K:20:ILE:N	3:K:20:ILE:HD13	2.31	0.45
4:C:187:GLU:CD	4:C:187:GLU:N	2.73	0.45
5:D:194:ILE:O	5:D:194:ILE:CD1	2.64	0.45
5:D:198:VAL:CG1	5:D:199:ALA:H	2.29	0.45
1:P:217:SER:O	1:P:217:SER:OG	2.30	0.45
2:L:27(A):SER:HA	2:L:68:GLY:O	2.16	0.45
2:L:124:GLN:HG2	2:L:129:GLY:O	2.16	0.45
2:L:129:GLY:HA2	2:L:183:LYS:N	2.31	0.45
3:H:26:GLY:O	3:H:27:TYR:HB3	2.16	0.45
5:B:182:VAL:HG22	5:B:183:THR:H	1.81	0.45
1:Q:105:LEU:HD23	1:Q:105:LEU:HA	1.60	0.45
1:Q:119:LYS:HE3	3:K:52:TYR:CD1	2.51	0.45
2:M:186:TYR:HD2	2:M:187:GLU:HA	1.82	0.45
3:H:199:HIS:HD1	3:H:202:SER:HG	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:40:PRO:HD2	4:A:41:GLY:H	1.82	0.45
5:B:14:PRO:C	5:B:16:ALA:H	2.24	0.45
5:B:156:ASN:O	5:B:197:ASN:ND2	2.50	0.45
1:Q:94:TYR:HE1	1:Q:102:ASP:HB3	1.69	0.45
1:Q:231:VAL:O	1:Q:232:VAL:C	2.58	0.45
5:D:2:VAL:HA	5:D:25:SER:O	2.17	0.45
5:D:51:ILE:HA	5:D:56:TYR:O	2.17	0.45
6:E:7:SIA:H8	6:E:7:SIA:C10	2.47	0.45
4:A:91:THR:CG2	5:B:98:LEU:HD13	2.46	0.45
2:M:88:CYS:O	2:M:98:PHE:HA	2.16	0.45
2:M:211:ARG:NE	9:M:218:HOH:O	2.34	0.45
4:C:121:SER:OG	5:D:124:PRO:HD2	2.17	0.45
4:C:149:LYS:HA	4:C:154:GLU:HA	1.99	0.45
4:C:173:TYR:N	4:C:173:TYR:CD1	2.84	0.45
1:P:95(E):LYS:HD3	1:P:95(G):ARG:O	2.16	0.45
1:P:121:MET:HG3	1:P:122:ASP:N	2.31	0.45
3:H:69:LEU:CD2	3:H:80:MET:HG3	2.45	0.45
1:Q:17:VAL:HG22	1:Q:20:TRP:HA	1.98	0.45
1:Q:66:LEU:HG	4:C:30:PHE:HE1	1.81	0.45
1:Q:160:LEU:HA	1:Q:185:ARG:HB3	1.98	0.45
3:K:155:ASN:HD22	3:K:159:LEU:HD12	1.82	0.45
5:D:3:GLN:C	5:D:4:LEU:HD23	2.41	0.45
5:D:32:TYR:N	5:D:32:TYR:CD1	2.84	0.45
8:G:12:NAG:C8	8:G:12:NAG:C3	2.90	0.45
1:P:101:HIS:HE1	1:P:179:PHE:CD1	2.34	0.45
4:A:178:THR:O	4:A:178:THR:HG22	2.16	0.45
5:B:52:ASN:O	5:B:55:GLY:N	2.48	0.45
3:H:136:VAL:HG22	3:H:138:LEU:HD22	1.99	0.45
1:Q:234:TYR:CD2	1:Q:234:TYR:N	2.84	0.45
2:M:166:GLN:HA	2:M:173:TYR:CE2	2.52	0.45
2:M:198:HIS:CD2	2:M:200:THR:OG1	2.69	0.45
4:C:41:GLY:C	4:C:42:GLN:HG2	2.42	0.45
4:C:183:LYS:O	4:C:183:LYS:HG2	2.15	0.45
1:P:31:VAL:HG23	1:P:32:LEU:N	2.32	0.45
1:P:63:SER:O	1:P:85:VAL:HG23	2.17	0.45
4:A:33:MET:O	4:A:34:HIS:CG	2.69	0.45
4:A:108:ARG:HG3	4:A:140:TYR:CD1	2.52	0.45
1:Q:95(B):SER:HB3	1:Q:95(C):LEU:HD12	1.97	0.45
2:M:134:CYS:HB2	2:M:148:TRP:CH2	2.52	0.45
3:H:170:LEU:HB3	3:H:175:TYR:CD1	2.52	0.44
4:A:22:SER:CB	4:A:72:THR:HG22	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:33:TRP:HZ3	5:B:52:ASN:OD1	2.00	0.44
1:Q:94:TYR:CD2	1:Q:95:ASP:N	2.85	0.44
2:M:106:ILE:CG2	2:M:107:LYS:N	2.80	0.44
4:C:192:TYR:O	4:C:208:SER:HB2	2.17	0.44
5:D:13:LYS:CB	5:D:14:PRO:HD2	2.46	0.44
6:E:2:NAG:O3	6:E:3:MAN:H5	2.17	0.44
1:P:59:ILE:HD12	1:P:90:PRO:HG3	1.98	0.44
1:P:215:TRP:HA	1:P:215:TRP:HE3	1.82	0.44
2:L:124:GLN:CD	2:L:130:ALA:HA	2.43	0.44
4:A:4:LEU:HD13	4:A:88:CYS:SG	2.56	0.44
4:A:14:SER:N	4:A:107:LYS:HB2	2.33	0.44
1:Q:103:LEU:HD12	1:Q:212:ILE:HD11	1.99	0.44
1:Q:131:ALA:HB3	1:Q:134:THR:OG1	2.17	0.44
2:M:161:ASN:OD1	2:M:177:SER:HA	2.17	0.44
3:K:146:PHE:CD2	3:K:147:PRO:N	2.85	0.44
5:D:23:LYS:HA	5:D:77:THR:HA	1.99	0.44
3:H:170:LEU:HB3	3:H:175:TYR:CE1	2.53	0.44
2:M:23:CYS:O	2:M:71:PHE:HD1	1.99	0.44
3:K:81:GLN:C	3:K:82:LEU:HD23	2.42	0.44
3:K:105:GLN:H	3:K:105:GLN:HG3	1.49	0.44
4:C:167:ASP:OD1	4:C:168:SER:N	2.50	0.44
1:P:56:ALA:HA	1:P:104:MET:HB2	2.00	0.44
1:P:89:PHE:N	1:P:89:PHE:CD1	2.86	0.44
2:L:60:ASP:C	2:L:62:PHE:N	2.75	0.44
4:A:39:LYS:CB	4:A:40:PRO:CD	2.93	0.44
4:A:124:GLN:HG2	4:A:129:GLY:O	2.17	0.44
4:A:132:VAL:HG12	4:A:148:TRP:HH2	1.82	0.44
1:Q:143:SER:O	1:Q:144:ILE:HG23	2.18	0.44
3:K:28:ALA:C	3:K:30:SER:H	2.26	0.44
4:C:14:SER:HA	4:C:107:LYS:HB2	2.00	0.44
4:C:121:SER:HB2	5:D:124:PRO:HD2	2.00	0.44
4:C:139:PHE:CD1	4:C:139:PHE:C	2.95	0.44
5:D:122:VAL:HG11	5:D:198:VAL:HG21	2.00	0.44
5:D:199:ALA:HA	5:D:205:THR:O	2.17	0.44
1:P:181:LEU:HG	1:P:230:LYS:HB2	1.99	0.44
5:B:98:LEU:HD22	5:B:98:LEU:HA	1.61	0.44
5:B:146:TYR:CD1	5:B:176:TYR:HB2	2.50	0.44
2:M:197:THR:HG22	2:M:198:HIS:H	1.83	0.44
4:C:149:LYS:HG2	4:C:154:GLU:CA	2.48	0.44
2:L:13:VAL:HG12	2:L:78:VAL:HG21	1.98	0.44
3:H:164:HIS:O	3:H:179:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:36:TRP:CD1	5:B:69:LEU:HD21	2.52	0.44
5:B:146:TYR:HD1	5:B:146:TYR:C	2.26	0.44
1:Q:46:LEU:HD12	1:Q:46:LEU:HA	1.78	0.44
3:K:79:TYR:CD2	3:K:79:TYR:N	2.84	0.44
5:D:133:THR:O	5:D:133:THR:CG2	2.66	0.44
5:D:148:PRO:HD2	5:D:200:HIS:CE1	2.52	0.44
2:L:5:THR:HA	9:L:217:HOH:O	2.17	0.44
2:L:21:ILE:O	2:L:72:THR:HG23	2.17	0.44
2:L:106:ILE:CG2	2:L:107:LYS:H	2.31	0.44
4:A:48:ILE:HG12	4:A:53:ASN:O	2.18	0.44
4:A:49:TYR:CD2	4:A:49:TYR:O	2.71	0.44
5:B:52:ASN:HD22	5:B:52(A):PRO:CD	2.31	0.44
1:Q:95(J):ARG:HA	1:Q:95(K):PRO:HD3	1.82	0.44
3:K:4:LEU:CD2	3:K:24:VAL:HG22	2.47	0.44
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.52	0.44
3:K:66:LYS:HE3	3:K:86:ASP:OD1	2.17	0.44
4:C:27(B):ILE:HD13	4:C:27(C):ASP:H	1.82	0.44
4:C:90:GLN:NE2	4:C:90:GLN:C	2.76	0.44
5:D:93:ALA:HB2	5:D:104:TRP:HA	1.98	0.44
1:P:84:GLN:HE21	5:B:98:LEU:H	1.64	0.44
1:P:145:GLU:N	1:P:146:PRO:CD	2.80	0.44
1:P:185:ARG:HG2	1:P:186(A):THR:HG23	2.00	0.44
2:L:135:PHE:CE2	3:H:180:SER:CB	3.01	0.44
5:B:112:VAL:HG11	9:B:218:HOH:O	2.18	0.44
4:C:32:PHE:HB3	4:C:91:THR:OG1	2.18	0.44
1:P:59:ILE:HB	1:P:104:MET:HE1	2.00	0.44
1:P:83:PHE:CZ	1:P:112:ALA:HA	2.52	0.44
5:B:60:ASN:C	5:B:60:ASN:ND2	2.76	0.44
1:Q:50:GLN:HE21	1:Q:111:PRO:HG3	1.79	0.44
1:Q:234:TYR:O	1:Q:235:ARG:C	2.59	0.44
1:P:75:HIS:N	1:P:75:HIS:CD2	2.85	0.43
2:L:48:ILE:HD13	2:L:48:ILE:N	2.33	0.43
3:H:193:ILE:HD12	3:H:193:ILE:N	2.32	0.43
3:H:206:VAL:HG23	3:H:207:ASP:N	2.33	0.43
5:B:36:TRP:CZ3	5:B:92:CYS:HB3	2.53	0.43
1:Q:114:LEU:HD12	1:Q:114:LEU:HA	1.70	0.43
1:Q:242:ILE:HG22	1:Q:243:VAL:N	2.33	0.43
2:M:186:TYR:HD2	2:M:187:GLU:CA	2.31	0.43
1:P:129:GLU:OE1	1:P:230:LYS:HD2	2.18	0.43
2:L:36:PHE:CE2	2:L:46:LEU:HB2	2.54	0.43
4:A:80:ALA:C	4:A:82:ASP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:210:ASN:ND2	2:M:74:ARG:NH2	2.63	0.43
1:Q:45:VAL:HG21	1:Q:198:PRO:HB3	1.99	0.43
1:Q:51:TRP:CZ3	1:Q:107:ARG:HB2	2.53	0.43
2:M:17:GLU:HB3	2:M:18:SER:H	1.73	0.43
2:M:58:VAL:CG1	2:M:59:PRO:HD2	2.48	0.43
4:C:46:ILE:HD12	4:C:47:LEU:H	1.83	0.43
5:D:171:LEU:HD12	5:D:176:TYR:OH	2.18	0.43
2:L:181:LEU:HD22	2:L:185:GLU:HB2	2.00	0.43
3:H:153:LEU:HD13	3:H:196:ASN:HD22	1.82	0.43
3:H:170:LEU:O	3:H:171:GLN:C	2.61	0.43
5:B:9:ALA:HB2	5:B:109:THR:HG23	2.00	0.43
5:B:194:ILE:C	5:B:194:ILE:CD1	2.91	0.43
5:D:153:LEU:HA	5:D:197:ASN:O	2.17	0.43
1:P:30:GLN:NE2	1:P:198:PRO:HG2	2.33	0.43
1:P:44:GLY:CA	1:P:54:THR:HG23	2.49	0.43
1:P:154:LYS:H	1:P:154:LYS:HG3	1.48	0.43
3:H:202:SER:HB2	3:H:204:THR:OG1	2.18	0.43
4:A:48:ILE:HD13	4:A:64:GLY:CA	2.48	0.43
5:B:96:GLY:O	5:B:97:ARG:HG2	2.18	0.43
5:B:118:THR:O	5:B:120:PRO:N	2.52	0.43
5:B:146:TYR:CD1	5:B:146:TYR:C	2.96	0.43
1:Q:131:ALA:HB3	1:Q:134:THR:HG1	1.83	0.43
1:Q:139:SER:HB3	1:Q:157:CYS:SG	2.58	0.43
1:Q:142:GLY:HA3	1:Q:151:THR:CA	2.47	0.43
5:D:77:THR:OG1	5:D:79:TYR:CE2	2.71	0.43
2:L:199:LYS:HD2	2:L:199:LYS:HA	1.60	0.43
4:A:111:ALA:C	4:A:200:THR:HG21	2.43	0.43
1:Q:95(A):MET:C	1:Q:95(C):LEU:N	2.74	0.43
1:Q:174:GLN:NE2	1:Q:227:LEU:HD11	2.34	0.43
2:M:27(B):LEU:CD2	2:M:90:GLN:HB2	2.48	0.43
4:C:47:LEU:HB3	4:C:58:ILE:HG13	2.01	0.43
5:D:59:ASN:O	5:D:60:ASN:C	2.60	0.43
2:L:89:MET:CE	2:L:98:PHE:CZ	3.01	0.43
2:L:144:ILE:HD12	2:L:145:ASN:N	2.33	0.43
4:A:150:ILE:HD12	4:A:150:ILE:C	2.43	0.43
5:B:20:MET:HE1	5:B:90:TYR:CB	2.49	0.43
5:B:134:GLY:C	5:B:136:SER:N	2.73	0.43
5:D:66:LYS:HE2	5:D:66:LYS:HB2	1.86	0.43
5:D:139:LEU:HD12	5:D:139:LEU:N	2.32	0.43
1:P:178:LYS:HD3	1:P:178:LYS:HA	1.71	0.43
2:L:149:LYS:HB2	2:L:149:LYS:HE3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:THR:CA	2:L:208:SER:HB3	2.45	0.43
3:H:61:GLY:C	3:H:63:PHE:N	2.76	0.43
4:A:119:PRO:HB3	4:A:209:PHE:CE1	2.54	0.43
4:A:209:PHE:CD2	4:A:209:PHE:C	2.96	0.43
5:B:124:PRO:HB3	5:B:211:ILE:HG22	2.00	0.43
1:Q:46:LEU:CD1	1:Q:52:VAL:HG23	2.48	0.43
3:K:1:GLN:CD	3:K:1:GLN:N	2.75	0.43
1:P:71:SER:HB2	1:P:153:LYS:HD2	2.00	0.43
2:L:19:VAL:HG22	2:L:20:SER:H	1.83	0.43
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.70	0.43
3:H:193:ILE:O	3:H:210:ILE:HG22	2.19	0.43
5:B:202:ALA:O	5:B:203:SER:C	2.61	0.43
1:Q:94:TYR:CE2	1:Q:95:ASP:O	2.71	0.43
2:M:169:LYS:HE3	2:M:169:LYS:HB2	1.74	0.43
1:P:144:ILE:O	1:P:144:ILE:HG23	2.19	0.43
4:A:130:ALA:HB3	4:A:182:THR:O	2.19	0.43
5:B:189:TRP:CZ2	5:B:211:ILE:CD1	3.02	0.43
1:Q:167:VAL:O	1:Q:167:VAL:HG23	2.19	0.43
2:M:124:GLN:NE2	2:M:131:SER:HB3	2.14	0.43
3:K:33:TRP:HB2	3:K:95:ASP:HB2	2.00	0.43
3:K:138:LEU:CD2	3:K:193:ILE:HD13	2.48	0.43
4:C:34:HIS:HD2	4:C:49:TYR:CA	2.31	0.43
5:D:27:TYR:CD1	5:D:28:SER:N	2.87	0.43
1:P:94:TYR:HD2	1:P:95(A):MET:HE2	1.83	0.43
1:P:135:THR:HA	1:P:161:HIS:HB3	2.01	0.43
3:H:188:TRP:C	3:H:190:SER:N	2.77	0.43
4:A:108:ARG:HG2	4:A:140:TYR:CD1	2.53	0.43
1:Q:50:GLN:HE22	1:Q:111:PRO:HG3	1.80	0.43
1:Q:53:LEU:HD12	1:Q:104:MET:O	2.19	0.43
3:K:212:PRO:O	3:K:213:ARG:C	2.62	0.43
4:C:32:PHE:O	4:C:90:GLN:HA	2.19	0.43
5:D:160:LEU:HG	5:D:162:SER:OG	2.19	0.43
1:P:139:SER:HA	1:P:156:GLN:O	2.18	0.42
2:L:89:MET:HE2	2:L:98:PHE:CZ	2.53	0.42
3:H:123:PRO:HG3	3:H:208:LYS:CG	2.48	0.42
3:H:153:LEU:CD1	3:H:196:ASN:HD22	2.32	0.42
5:B:116:LYS:HZ1	5:B:202:ALA:HB1	1.83	0.42
1:Q:95(H):PHE:CD2	8:G:11:SIA:H91	2.54	0.42
1:Q:171:VAL:HB	1:Q:223(A):GLU:HB3	2.01	0.42
2:M:36:PHE:HD2	2:M:46:LEU:HA	1.84	0.42
1:P:82:VAL:O	1:P:83:PHE:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:95(C):LEU:HD13	1:P:99:SER:HB3	2.01	0.42
2:L:172:THR:C	2:L:173:TYR:CD2	2.97	0.42
3:H:80:MET:HE1	3:H:90:TYR:HD2	1.84	0.42
3:H:195:CYS:O	3:H:207:ASP:HA	2.19	0.42
4:A:131:SER:CB	4:A:180:THR:HA	2.49	0.42
1:Q:168:CYS:O	1:Q:172:HIS:HB2	2.19	0.42
2:M:90:GLN:CD	2:M:90:GLN:C	2.87	0.42
4:C:121:SER:CB	5:D:124:PRO:HD2	2.49	0.42
5:D:120:PRO:HB3	5:D:144:LYS:O	2.19	0.42
6:E:3:MAN:O2	6:E:4:MAN:C1	2.67	0.42
1:P:119:LYS:HD2	3:H:52:TYR:CE2	2.54	0.42
1:P:119:LYS:HD3	3:H:52:TYR:CD2	2.54	0.42
2:L:47:LEU:C	2:L:48:ILE:HD13	2.44	0.42
5:B:116:LYS:O	5:B:116:LYS:CG	2.67	0.42
1:Q:20:TRP:HB2	3:K:98:ARG:CZ	2.49	0.42
1:Q:140:GLY:O	1:Q:155:LEU:HD22	2.20	0.42
2:M:13:VAL:HG11	2:M:78:VAL:HG11	2.02	0.42
4:C:139:PHE:O	4:C:139:PHE:CG	2.68	0.42
1:P:105:LEU:HD21	1:P:238:ILE:HG23	2.01	0.42
1:P:231:VAL:O	1:P:233:HIS:N	2.52	0.42
2:L:39:ARG:HB3	2:L:40:PRO:CD	2.49	0.42
2:L:121:SER:OG	3:H:123:PRO:HD2	2.20	0.42
2:L:153:SER:OG	2:L:154:GLU:N	2.53	0.42
5:B:56:TYR:C	5:B:57:THR:CG2	2.91	0.42
1:Q:95(A):MET:HG3	1:Q:95(D):LEU:CD1	2.50	0.42
1:Q:130:PRO:HG3	1:Q:210:GLN:HG2	1.98	0.42
1:Q:144:ILE:O	1:Q:146:PRO:HD3	2.19	0.42
1:Q:188:LYS:HE2	1:Q:224:ARG:CZ	2.50	0.42
2:M:32:TYR:CD2	2:M:32:TYR:N	2.87	0.42
2:M:131:SER:HB2	2:M:180:THR:CG2	2.28	0.42
3:K:87:SER:O	3:K:88:ALA:HB2	2.20	0.42
4:C:1:ASP:HB3	4:C:95:PRO:HB2	2.00	0.42
1:P:64:VAL:C	1:P:65:ILE:HD13	2.44	0.42
1:P:124:PRO:HB3	1:P:208:VAL:HG11	2.00	0.42
1:P:179:PHE:C	1:P:180:MET:HG2	2.44	0.42
2:L:106:ILE:HG22	2:L:107:LYS:N	2.35	0.42
2:L:118:PHE:CD1	2:L:118:PHE:N	2.87	0.42
2:L:170:ASP:C	2:L:172:THR:N	2.75	0.42
2:L:181:LEU:HD21	2:L:185:GLU:OE2	2.18	0.42
2:L:210:ASN:N	2:L:210:ASN:ND2	2.62	0.42
3:H:144:GLY:C	3:H:174:LEU:HD13	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:116:LYS:NZ	5:B:202:ALA:HB1	2.35	0.42
1:Q:75:HIS:HB3	2:M:28:ASN:HA	2.01	0.42
2:M:142:LYS:HA	2:M:173:TYR:HD1	1.84	0.42
4:C:136:LEU:CD1	4:C:136:LEU:N	2.82	0.42
5:D:205:THR:C	5:D:206:LYS:HD3	2.44	0.42
1:P:184:GLY:O	1:P:185:ARG:CB	2.67	0.42
1:Q:134:THR:O	1:Q:161:HIS:HB2	2.19	0.42
1:Q:213:THR:HA	1:Q:228:TYR:CD2	2.54	0.42
3:K:18:VAL:HG23	3:K:82(C):LEU:CD1	2.49	0.42
3:K:75:SER:O	3:K:76:SER:C	2.62	0.42
4:C:141:PRO:HD2	4:C:198:HIS:HE1	1.84	0.42
5:D:33:TRP:N	5:D:33:TRP:CE3	2.88	0.42
1:P:95(G):ARG:CD	9:P:266:HOH:O	2.68	0.42
1:P:231:VAL:C	1:P:233:HIS:H	2.26	0.42
2:L:120:PRO:O	2:L:121:SER:C	2.60	0.42
2:L:131:SER:HB3	2:L:180:THR:HA	2.01	0.42
4:A:141:PRO:O	4:A:143:ASP:O	2.38	0.42
5:B:133:THR:CG2	5:B:134:GLY:N	2.70	0.42
5:B:195:THR:HG23	5:B:210:LYS:N	2.35	0.42
1:Q:69:ARG:NH1	1:Q:77:GLU:OE1	2.52	0.42
2:M:132:VAL:HG13	2:M:133:VAL:N	2.34	0.42
3:K:83:THR:OG1	3:K:85:VAL:HG13	2.20	0.42
4:C:190:ASN:ND2	4:C:212:ASN:ND2	2.59	0.42
5:D:72:ASP:OD1	5:D:74:SER:HB3	2.19	0.42
2:L:91:HIS:O	2:L:91:HIS:HD2	2.03	0.42
1:Q:86:SER:HA	5:D:33:TRP:HZ3	1.85	0.42
1:Q:153:LYS:HB3	1:Q:154:LYS:H	1.64	0.42
4:C:138:ASN:HD22	4:C:172:THR:HG21	1.84	0.42
1:P:153:LYS:H	1:P:153:LYS:HG3	1.67	0.42
3:H:12:VAL:O	3:H:111:VAL:HA	2.20	0.42
3:H:51:ILE:HD13	3:H:71:VAL:HG13	2.01	0.42
3:H:80:MET:HE1	3:H:90:TYR:CD2	2.55	0.42
5:B:17:SER:HB2	5:B:82(A):ASN:HA	2.01	0.42
5:B:19:LYS:HB2	5:B:81:GLN:HG3	2.02	0.42
1:Q:238:ILE:O	1:Q:240:ASP:N	2.53	0.42
2:M:115:VAL:HG12	2:M:207:LYS:CD	2.48	0.42
5:D:101:PHE:N	5:D:101:PHE:CD1	2.83	0.42
2:L:15:PRO:C	2:L:17:GLU:H	2.27	0.42
3:H:62:LYS:HE2	3:H:62:LYS:HB3	1.93	0.42
3:H:211:VAL:HA	3:H:212:PRO:HD3	1.78	0.42
4:A:34:HIS:CD2	4:A:49:TYR:CB	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:213:GLU:O	4:A:214:CYS:HB3	2.20	0.42
1:Q:215:TRP:CE3	1:Q:216:GLY:N	2.80	0.42
2:M:150:ILE:N	2:M:150:ILE:HD12	2.35	0.42
5:D:51:ILE:O	5:D:51:ILE:CG2	2.67	0.42
2:L:13:VAL:CG1	2:L:14:THR:N	2.83	0.41
2:L:77:ARG:HB3	2:L:77:ARG:NH1	2.25	0.41
2:L:159:VAL:HG12	2:L:179:LEU:HA	2.01	0.41
5:B:188:THR:OG1	5:B:189:TRP:N	2.53	0.41
1:Q:94:TYR:CD1	1:Q:102:ASP:CB	2.92	0.41
2:M:18:SER:HB2	2:M:75:ILE:O	2.20	0.41
2:M:182:THR:O	2:M:185:GLU:OE1	2.38	0.41
3:K:22:CYS:SG	3:K:34:MET:HE1	2.60	0.41
3:K:181:VAL:HG22	3:K:182:THR:N	2.34	0.41
3:H:188:TRP:O	3:H:189:PRO:C	2.63	0.41
4:A:26:SER:O	4:A:27:GLU:HB3	2.20	0.41
5:B:147:PHE:H	5:B:148:PRO:CD	2.33	0.41
1:Q:45:VAL:CG2	1:Q:198:PRO:HB3	2.49	0.41
1:Q:163:ILE:HG12	1:Q:183:ALA:HA	2.03	0.41
1:Q:224:ARG:HB3	1:Q:225:PRO:HD3	2.02	0.41
3:K:18:VAL:HG12	3:K:19:LYS:N	2.34	0.41
3:K:153:LEU:HD23	3:K:153:LEU:H	1.84	0.41
3:H:136:VAL:N	3:H:183:VAL:O	2.50	0.41
4:A:27(C):ASP:HA	4:A:30:PHE:O	2.20	0.41
4:A:149:LYS:CE	4:A:152:GLY:H	2.28	0.41
1:Q:58:CYS:O	1:Q:59:ILE:HG12	2.19	0.41
4:C:124:GLN:NE2	4:C:131:SER:N	2.67	0.41
4:C:161:ASN:HB3	4:C:175:MET:HE2	2.01	0.41
5:D:4:LEU:HD23	5:D:4:LEU:N	2.35	0.41
5:D:6:GLN:HE21	5:D:107:GLY:H	1.66	0.41
5:D:155:TRP:CG	5:D:182:VAL:HG21	2.55	0.41
5:D:167:PHE:HA	5:D:168:PRO:HD2	1.71	0.41
2:L:2:ILE:CD1	2:L:2:ILE:H	2.33	0.41
2:L:110:ASP:OD1	2:L:110:ASP:N	2.53	0.41
5:B:148:PRO:HD2	5:B:200:HIS:CE1	2.55	0.41
1:Q:165:ASN:CB	1:Q:178:LYS:HD2	2.50	0.41
1:Q:185:ARG:O	1:Q:186:TRP:C	2.63	0.41
1:Q:228:TYR:HD2	1:Q:228:TYR:HA	1.69	0.41
2:M:142:LYS:HA	2:M:173:TYR:CD1	2.56	0.41
2:M:166:GLN:OE1	2:M:173:TYR:CZ	2.72	0.41
3:K:82:LEU:C	3:K:82(A):SER:HG	2.27	0.41
5:D:18:VAL:HG12	5:D:19:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:121:PRO:HB2	5:D:123:TYR:CZ	2.55	0.41
1:P:45:VAL:HG22	1:P:198:PRO:HG3	2.02	0.41
3:H:133:GLY:C	3:H:135:SER:H	2.28	0.41
1:Q:89:PHE:HA	1:Q:90:PRO:HD3	1.90	0.41
2:M:89:MET:HA	2:M:97:THR:O	2.21	0.41
5:D:60:ASN:C	5:D:62:LYS:N	2.79	0.41
5:B:134:GLY:O	5:B:186:SER:HB3	2.20	0.41
1:Q:32:LEU:HD23	1:Q:141:TRP:CE3	2.55	0.41
1:Q:123:LEU:HD21	1:Q:238:ILE:HG21	2.02	0.41
4:C:149:LYS:HG2	4:C:154:GLU:N	2.36	0.41
5:D:115:ALA:O	5:D:117:THR:HG22	2.21	0.41
1:P:54:THR:HB	1:P:55:ALA:H	1.64	0.41
2:L:192:TYR:HB2	2:L:209:PHE:CE2	2.55	0.41
4:A:69:THR:HG22	4:A:70:ASP:OD2	2.21	0.41
4:A:132:VAL:N	4:A:179:LEU:O	2.48	0.41
4:A:141:PRO:C	4:A:143:ASP:N	2.79	0.41
4:A:182:THR:CG2	4:A:183:LYS:N	2.79	0.41
5:B:118:THR:HG23	5:B:119:ALA:N	2.33	0.41
5:B:198:VAL:CG1	5:B:199:ALA:N	2.84	0.41
1:Q:53:LEU:HD11	1:Q:103:LEU:HG	2.03	0.41
2:M:46:LEU:CD2	3:K:99:TYR:CE1	3.03	0.41
2:M:138:ASN:HA	2:M:172:THR:OG1	2.20	0.41
2:M:211:ARG:HD3	2:M:211:ARG:HA	1.87	0.41
3:K:156:SER:C	3:K:158:SER:H	2.28	0.41
1:P:69:ARG:NH2	1:P:76:PRO:HA	2.36	0.41
2:L:89:MET:HE2	2:L:89:MET:HB2	1.82	0.41
3:H:202:SER:C	3:H:203:SER:OG	2.64	0.41
4:A:123:GLU:CD	4:A:123:GLU:H	2.29	0.41
4:A:142:LYS:HD3	4:A:142:LYS:N	2.21	0.41
4:A:201:SER:CB	4:A:205:ILE:HD11	2.49	0.41
5:B:94:ARG:HD2	5:B:103:VAL:CG2	2.50	0.41
2:M:33:LEU:C	2:M:33:LEU:CD1	2.93	0.41
3:K:60:ASN:HD22	3:K:61:GLY:H	1.59	0.41
3:K:187:THR:HB	3:K:191:GLN:NE2	2.36	0.41
4:C:179:LEU:HD11	4:C:181:LEU:HD22	2.00	0.41
1:P:51:TRP:CZ3	1:P:107:ARG:HB2	2.56	0.41
1:P:53:LEU:HA	1:P:53:LEU:HD12	1.90	0.41
1:P:56:ALA:O	1:P:59:ILE:CG2	2.61	0.41
1:P:59:ILE:HD13	1:P:59:ILE:HG21	1.79	0.41
1:P:65:ILE:HG12	1:P:108:LEU:CD1	2.49	0.41
1:P:95:ASP:HB3	1:P:95(C):LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:144:ILE:HD12	1:P:144:ILE:HA	1.98	0.41
1:P:224:ARG:HA	1:P:225:PRO:HD2	1.70	0.41
1:P:245:ASN:N	1:P:246:PRO:HD3	2.35	0.41
2:L:2:ILE:HD12	2:L:2:ILE:N	2.35	0.41
3:H:133:GLY:O	3:H:135:SER:N	2.53	0.41
4:A:47:LEU:O	4:A:54:LEU:HA	2.21	0.41
5:B:13:LYS:HA	5:B:14:PRO:HD3	1.93	0.41
1:Q:46:LEU:HD22	1:Q:67:LEU:HD23	2.02	0.41
1:Q:50:GLN:HE21	1:Q:50:GLN:HB2	1.49	0.41
1:Q:58:CYS:O	1:Q:104:MET:HE1	2.20	0.41
1:Q:128:GLN:HG2	1:Q:129:GLU:N	2.35	0.41
3:K:19:LYS:O	3:K:19:LYS:HG2	2.21	0.41
3:K:51:ILE:O	3:K:52(A):PRO:HD3	2.20	0.41
3:K:138:LEU:HD23	3:K:193:ILE:HD13	2.02	0.41
3:K:197:VAL:HG12	3:K:198:ALA:H	1.86	0.41
4:C:181:LEU:HD13	4:C:181:LEU:HA	1.59	0.41
4:C:184:ASP:C	4:C:187:GLU:OE2	2.64	0.41
4:C:185:GLU:O	4:C:185:GLU:HG3	2.21	0.41
2:L:58:VAL:HA	2:L:59:PRO:HD3	1.70	0.41
2:L:182:THR:OG1	2:L:183:LYS:N	2.53	0.41
4:A:33:MET:O	4:A:50:ARG:N	2.44	0.41
5:B:26:GLY:O	5:B:27:TYR:HB3	2.22	0.41
5:B:94:ARG:HB3	5:B:103:VAL:HG23	2.02	0.41
5:B:128:VAL:C	5:B:130:GLY:N	2.78	0.41
1:Q:32:LEU:HD11	1:Q:39:ALA:CB	2.51	0.41
1:Q:57:HIS:CD2	1:Q:57:HIS:C	2.99	0.41
2:M:202:THR:H	2:M:202:THR:HG22	1.56	0.41
4:C:163:TRP:CZ2	4:C:175:MET:HE3	2.56	0.41
5:D:167:PHE:O	5:D:168:PRO:C	2.64	0.41
6:E:2:NAG:H4	6:E:3:MAN:H2	1.74	0.41
1:P:123:LEU:HA	1:P:124:PRO:HD3	1.80	0.40
1:P:203:GLY:HA3	3:H:28:ALA:HB3	2.02	0.40
1:P:236:LYS:HD3	1:P:236:LYS:HA	1.84	0.40
3:H:184:THR:C	3:H:186:SER:N	2.79	0.40
4:A:148:TRP:CD1	4:A:159:VAL:HG11	2.55	0.40
4:A:186:TYR:HD1	4:A:192:TYR:HH	1.65	0.40
4:A:209:PHE:CD2	4:A:209:PHE:O	2.74	0.40
5:B:116:LYS:HE2	5:B:202:ALA:HB1	2.02	0.40
1:Q:47:VAL:CG2	1:Q:48:HIS:N	2.68	0.40
2:M:138:ASN:N	2:M:173:TYR:O	2.52	0.40
4:C:36:TYR:CE1	4:C:46:ILE:HB	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:37:VAL:HA	5:D:48:ILE:HG13	2.03	0.40
8:G:5:NAG:H4	8:G:6:GAL:H2	1.80	0.40
1:P:172:HIS:HA	1:P:173:PRO:HD3	1.89	0.40
2:L:193:THR:CG2	2:L:206:VAL:HG13	2.50	0.40
4:A:117:ILE:O	4:A:117:ILE:CG2	2.67	0.40
5:B:173:SER:O	5:B:174:ASP:C	2.63	0.40
1:Q:89:PHE:CD1	1:Q:89:PHE:N	2.89	0.40
1:Q:91:HIS:HE1	1:Q:93:LEU:CG	2.31	0.40
1:Q:95(H):PHE:HD2	8:G:11:SIA:H91	1.87	0.40
1:Q:208:VAL:CG2	1:Q:209:LEU:N	2.81	0.40
3:K:20:ILE:HD12	3:K:107:THR:HG21	2.02	0.40
3:K:80:MET:SD	3:K:82:LEU:HD21	2.62	0.40
3:K:182:THR:C	3:K:183:VAL:CG1	2.94	0.40
5:D:134:GLY:O	5:D:186:SER:HB3	2.21	0.40
1:P:103:LEU:HA	1:P:103:LEU:HD12	1.86	0.40
3:H:19:LYS:HG3	3:H:81:GLN:HG3	2.04	0.40
3:H:36:TRP:CZ3	3:H:92:CYS:HB3	2.56	0.40
5:B:52:ASN:HD22	5:B:52(A):PRO:HD2	1.86	0.40
2:M:51:MET:HE2	2:M:71:PHE:CE2	2.56	0.40
5:D:36:TRP:C	5:D:48:ILE:HG13	2.46	0.40
5:D:139:LEU:HD21	5:D:189:TRP:CD2	2.56	0.40
1:P:83:PHE:CE2	1:P:112:ALA:HB2	2.57	0.40
2:L:136:LEU:CD2	2:L:144:ILE:HD11	2.51	0.40
4:A:83:VAL:O	4:A:83:VAL:HG13	2.21	0.40
5:B:203:SER:O	5:B:205:THR:N	2.48	0.40
5:B:207:VAL:HG23	5:B:208:ASP:N	2.36	0.40
1:Q:32:LEU:HD11	1:Q:39:ALA:HB1	2.04	0.40
1:Q:119:LYS:CD	3:K:52:TYR:HE1	2.30	0.40
1:Q:174:GLN:NE2	1:Q:227:LEU:HD21	2.37	0.40
3:K:170:LEU:HD23	3:K:170:LEU:C	2.46	0.40
1:P:44:GLY:HA2	1:P:54:THR:HG23	2.02	0.40
2:L:60:ASP:O	2:L:61:ARG:C	2.64	0.40
2:L:198:HIS:CG	2:L:199:LYS:H	2.39	0.40
3:H:135:SER:HA	3:H:184:THR:HA	2.02	0.40
3:H:170:LEU:H	3:H:170:LEU:HD12	1.87	0.40
4:A:106:ILE:CG2	4:A:107:LYS:N	2.83	0.40
4:A:111:ALA:HB3	4:A:140:TYR:H	1.87	0.40
4:A:149:LYS:HA	4:A:154:GLU:HA	2.04	0.40
5:B:174:ASP:OD2	5:B:174:ASP:N	2.52	0.40
4:C:6:GLN:HE22	4:C:101:GLY:HA2	1.87	0.40
5:D:48:ILE:HD12	5:D:80:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:113:SER:C	5:D:114:SER:HG	2.23	0.40
5:D:119:ALA:HA	5:D:120:PRO:HD3	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	235/237 (99%)	195 (83%)	31 (13%)	9 (4%)	2	18
1	Q	235/237 (99%)	186 (79%)	39 (17%)	10 (4%)	2	16
2	L	217/219 (99%)	166 (76%)	39 (18%)	12 (6%)	1	11
2	M	217/219 (99%)	177 (82%)	31 (14%)	9 (4%)	2	17
3	H	215/219 (98%)	186 (86%)	18 (8%)	11 (5%)	1	13
3	K	217/219 (99%)	181 (83%)	32 (15%)	4 (2%)	6	34
4	A	216/218 (99%)	177 (82%)	22 (10%)	17 (8%)	1	5
4	C	216/218 (99%)	173 (80%)	30 (14%)	13 (6%)	1	10
5	B	217/219 (99%)	166 (76%)	35 (16%)	16 (7%)	1	6
5	D	217/219 (99%)	163 (75%)	42 (19%)	12 (6%)	1	11
All	All	2202/2224 (99%)	1770 (80%)	319 (14%)	113 (5%)	1	13

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	PRO
2	L	167	ASP
2	L	174	SER
3	H	173	ASP
4	A	17	GLN

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Mol	Chain	Res	Type
4	A	39	LYS
4	A	40	PRO
4	A	113	PRO
4	A	144	ILE
5	B	41	PRO
5	B	127	PRO
5	B	202	ALA
5	B	213	PRO
1	Q	144	ILE
2	M	59	PRO
2	M	153	SER
3	K	128	CYS
3	K	149	SER
4	C	17	GLN
4	C	142	LYS
5	D	112	VAL
5	D	116	LYS
1	P	118	VAL
1	P	143	SER
1	P	146	PRO
1	P	194	ASP
2	L	68	GLY
2	L	110	ASP
3	H	74	SER
3	H	190	SER
4	A	142	LYS
5	B	48	ILE
5	B	98	LEU
5	B	112	VAL
5	B	133	THR
1	Q	20	TRP
2	M	16	GLY
4	C	57	GLY
4	C	60	ALA
4	C	110	ASP
4	C	143	ASP
5	D	29	PHE
5	D	113	SER
5	D	149	GLU
5	D	159	SER
5	D	199	ALA
1	P	76	PRO

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Mol	Chain	Res	Type
1	P	220	CYS
1	P	221	ALA
2	L	188	ARG
3	H	62	LYS
4	A	96	TYR
4	A	100	GLY
4	A	182	THR
5	B	15	GLY
5	B	88	ALA
5	B	121	PRO
5	B	204	SER
1	Q	41	VAL
1	Q	76	PRO
1	Q	152	PRO
1	Q	189	SER
1	Q	235	ARG
2	M	95	PRO
3	K	54	ASP
3	K	100	TYR
4	C	27(C)	ASP
4	C	53	ASN
4	C	138	ASN
5	D	168	PRO
1	P	185	ARG
2	L	119	PRO
2	L	157	ASN
3	H	134	SER
4	A	60	ALA
4	A	157	ASN
5	B	147	PHE
5	B	174	ASP
1	Q	186	TRP
1	Q	197	GLY
2	M	25	SER
4	C	144	ILE
4	C	182	THR
2	L	39	ARG
2	L	57	GLY
2	L	65	SER
2	L	120	PRO
3	H	126	PRO
4	A	27	GLU

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Mol	Chain	Res	Type
4	A	110	ASP
4	A	138	ASN
5	B	119	ALA
2	M	19	VAL
2	M	94	TYR
5	D	41	PRO
1	P	145	GLU
3	H	188	TRP
4	A	141	PRO
5	D	127	PRO
5	D	185	THR
4	A	77	PRO
4	C	95	PRO
3	H	167	PRO
5	B	14	PRO
1	Q	232	VAL
2	M	119	PRO
3	H	119	PRO
2	M	140	TYR
5	D	51	ILE
3	H	189	PRO
4	A	44	PRO
4	C	120	PRO
3	H	147	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	P	205/205 (100%)	165 (80%)	40 (20%)	1	8
1	Q	205/205 (100%)	150 (73%)	55 (27%)	0	2
2	L	196/196 (100%)	154 (79%)	42 (21%)	1	6
2	M	196/196 (100%)	141 (72%)	55 (28%)	0	2
3	H	187/189 (99%)	131 (70%)	56 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	189/189 (100%)	137 (72%)	52 (28%)	0	2
4	A	193/193 (100%)	152 (79%)	41 (21%)	1	6
4	C	193/193 (100%)	134 (69%)	59 (31%)	0	1
5	B	189/189 (100%)	133 (70%)	56 (30%)	0	1
5	D	189/189 (100%)	140 (74%)	49 (26%)	0	3
All	All	1942/1944 (100%)	1437 (74%)	505 (26%)	0	3

All (505) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	23	GLU
1	P	27	GLN
1	P	36	ARG
1	P	38	ARG
1	P	41	VAL
1	P	42	CYS
1	P	54	THR
1	P	59	ILE
1	P	65	ILE
1	P	77	GLU
1	P	82	VAL
1	P	88	SER
1	P	100	SER
1	P	105	LEU
1	P	108	LEU
1	P	118	VAL
1	P	120	VAL
1	P	123	LEU
1	P	125	THR
1	P	135	THR
1	P	143	SER
1	P	149	PHE
1	P	151	THR
1	P	153	LYS
1	P	154	LYS
1	P	163	ILE
1	P	171	VAL
1	P	178	LYS
1	P	180	MET
1	P	185	ARG

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Mol	Chain	Res	Type
1	P	194	ASP
1	P	199	LEU
1	P	200	VAL
1	P	210	GLN
1	P	212	ILE
1	P	217	SER
1	P	218	GLU
1	P	227	LEU
1	P	241	THR
1	P	242	ILE
2	L	1	ASP
2	L	3	VAL
2	L	7	THR
2	L	17	GLU
2	L	23	CYS
2	L	24	ARG
2	L	26	SER
2	L	31	THR
2	L	33	LEU
2	L	42	GLN
2	L	46	LEU
2	L	48	ILE
2	L	65	SER
2	L	71	PHE
2	L	77	ARG
2	L	89	MET
2	L	92	LEU
2	L	94	TYR
2	L	96	VAL
2	L	103	LYS
2	L	105	GLU
2	L	110	ASP
2	L	117	ILE
2	L	122	SER
2	L	132	VAL
2	L	134	CYS
2	L	136	LEU
2	L	139	PHE
2	L	147	LYS
2	L	155	ARG
2	L	159	VAL
2	L	163	TRP

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Mol	Chain	Res	Type
2	L	165	ASP
2	L	167	ASP
2	L	168	SER
2	L	176	SER
2	L	178	THR
2	L	182	THR
2	L	183	LYS
2	L	197	THR
2	L	210	ASN
2	L	212	ASN
3	H	1	GLN
3	H	11	LEU
3	H	13	LYS
3	H	18	VAL
3	H	24	VAL
3	H	29	ILE
3	H	30	SER
3	H	32	SER
3	H	35	ASN
3	H	37	VAL
3	H	45	LEU
3	H	50	ARG
3	H	58	LYS
3	H	64	LYS
3	H	74	SER
3	H	80	MET
3	H	82	LEU
3	H	82(A)	SER
3	H	82(B)	SER
3	H	82(C)	LEU
3	H	83	THR
3	H	105	GLN
3	H	107	THR
3	H	109	VAL
3	H	113	SER
3	H	115	LYS
3	H	116	THR
3	H	117	THR
3	H	121	VAL
3	H	124	LEU
3	H	130	ASP
3	H	131	THR

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Mol	Chain	Res	Type
3	H	132	THR
3	H	135	SER
3	H	137	THR
3	H	138	LEU
3	H	140	CYS
3	H	153	LEU
3	H	158	SER
3	H	159	LEU
3	H	163	VAL
3	H	170	LEU
3	H	177	LEU
3	H	182	THR
3	H	184	THR
3	H	186	SER
3	H	191	GLN
3	H	192	SER
3	H	202	SER
3	H	203	SER
3	H	204	THR
3	H	205	LYS
3	H	206	VAL
3	H	209	LYS
3	H	210	ILE
3	H	211	VAL
4	A	3	VAL
4	A	4	LEU
4	A	5	THR
4	A	13	VAL
4	A	15	LEU
4	A	45	LYS
4	A	54	LEU
4	A	55	GLU
4	A	63	SER
4	A	69	THR
4	A	74	THR
4	A	75	ILE
4	A	79	GLU
4	A	83	VAL
4	A	89	GLN
4	A	90	GLN
4	A	91	THR
4	A	93	GLU

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Mol	Chain	Res	Type
4	A	105	GLU
4	A	106	ILE
4	A	108	ARG
4	A	114	THR
4	A	116	SER
4	A	117	ILE
4	A	121	SER
4	A	123	GLU
4	A	133	VAL
4	A	142	LYS
4	A	144	ILE
4	A	147	LYS
4	A	150	ILE
4	A	155	ARG
4	A	156	GLN
4	A	157	ASN
4	A	161	ASN
4	A	175	MET
4	A	178	THR
4	A	189	HIS
4	A	200	THR
4	A	209	PHE
4	A	210	ASN
5	B	2	VAL
5	B	3	GLN
5	B	10	GLU
5	B	13	LYS
5	B	18	VAL
5	B	20	MET
5	B	21	SER
5	B	23	LYS
5	B	34	MET
5	B	37	VAL
5	B	50	TYR
5	B	51	ILE
5	B	54	THR
5	B	57	THR
5	B	61	GLN
5	B	64	LYS
5	B	67	VAL
5	B	68	THR
5	B	70	THR

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Mol	Chain	Res	Type
5	B	77	THR
5	B	94	ARG
5	B	97	ARG
5	B	98	LEU
5	B	101	PHE
5	B	103	VAL
5	B	108	THR
5	B	109	THR
5	B	111	THR
5	B	112	VAL
5	B	114	SER
5	B	118	THR
5	B	122	VAL
5	B	132	THR
5	B	135	SER
5	B	142	LEU
5	B	146	TYR
5	B	151	VAL
5	B	152	THR
5	B	153	LEU
5	B	154	LEU
5	B	156	ASN
5	B	160	LEU
5	B	162	SER
5	B	164	VAL
5	B	170	VAL
5	B	172	GLN
5	B	174	ASP
5	B	178	LEU
5	B	180	SER
5	B	184	VAL
5	B	185	THR
5	B	196	CYS
5	B	207	VAL
5	B	211	ILE
5	B	212	VAL
5	B	216	CYS
1	Q	16	ILE
1	Q	20	TRP
1	Q	30	GLN
1	Q	31	VAL
1	Q	32	LEU

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Mol	Chain	Res	Type
1	Q	41	VAL
1	Q	50	GLN
1	Q	52	VAL
1	Q	59	ILE
1	Q	62	LYS
1	Q	63	SER
1	Q	67	LEU
1	Q	69	ARG
1	Q	72	LEU
1	Q	73	PHE
1	Q	77	GLU
1	Q	84	GLN
1	Q	89	PHE
1	Q	105	LEU
1	Q	106	LEU
1	Q	108	LEU
1	Q	114	LEU
1	Q	115	THR
1	Q	116	ASP
1	Q	118	VAL
1	Q	121	MET
1	Q	123	LEU
1	Q	135	THR
1	Q	139	SER
1	Q	144	ILE
1	Q	149	PHE
1	Q	150	LEU
1	Q	151	THR
1	Q	155	LEU
1	Q	158	VAL
1	Q	160	LEU
1	Q	162	VAL
1	Q	164	SER
1	Q	167	VAL
1	Q	168	CYS
1	Q	177	THR
1	Q	185	ARG
1	Q	186	TRP
1	Q	186(A)	THR
1	Q	188	LYS
1	Q	189	SER
1	Q	190	THR

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Mol	Chain	Res	Type
1	Q	208	VAL
1	Q	215	TRP
1	Q	218	GLU
1	Q	220	CYS
1	Q	222	LEU
1	Q	227	LEU
1	Q	242	ILE
1	Q	245	ASN
2	M	3	VAL
2	M	5	THR
2	M	10	SER
2	M	11	VAL
2	M	14	THR
2	M	25	SER
2	M	28	ASN
2	M	31	THR
2	M	33	LEU
2	M	43	SER
2	M	45	GLN
2	M	46	LEU
2	M	47	LEU
2	M	69	THR
2	M	71	PHE
2	M	74	ARG
2	M	78	VAL
2	M	83	VAL
2	M	89	MET
2	M	94	TYR
2	M	97	THR
2	M	105	GLU
2	M	108	ARG
2	M	115	VAL
2	M	116	SER
2	M	117	ILE
2	M	125	LEU
2	M	127	SER
2	M	131	SER
2	M	132	VAL
2	M	136	LEU
2	M	142	LYS
2	M	144	ILE
2	M	147	LYS

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Mol	Chain	Res	Type
2	M	156	GLN
2	M	157	ASN
2	M	159	VAL
2	M	168	SER
2	M	169	LYS
2	M	172	THR
2	M	174	SER
2	M	176	SER
2	M	181	LEU
2	M	184	ASP
2	M	186	TYR
2	M	187	GLU
2	M	190	ASN
2	M	191	SER
2	M	193	THR
2	M	199	LYS
2	M	202	THR
2	M	203	SER
2	M	205	ILE
2	M	211	ARG
2	M	213	GLU
3	K	7	SER
3	K	10	GLU
3	K	13	LYS
3	K	17	SER
3	K	20	ILE
3	K	24	VAL
3	K	25	SER
3	K	30	SER
3	K	35	ASN
3	K	37	VAL
3	K	57	THR
3	K	59	TYR
3	K	60	ASN
3	K	68	THR
3	K	71	VAL
3	K	73	LYS
3	K	75	SER
3	K	79	TYR
3	K	82	LEU
3	K	82(A)	SER
3	K	82(B)	SER

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Mol	Chain	Res	Type
3	K	82(C)	LEU
3	K	83	THR
3	K	85	VAL
3	K	98	ARG
3	K	102	TYR
3	K	105	GLN
3	K	121	VAL
3	K	124	LEU
3	K	127	VAL
3	K	128	CYS
3	K	131	THR
3	K	134	SER
3	K	137	THR
3	K	138	LEU
3	K	143	LYS
3	K	149	SER
3	K	152	LEU
3	K	158	SER
3	K	159	LEU
3	K	161	SER
3	K	171	GLN
3	K	174	LEU
3	K	182	THR
3	K	184	THR
3	K	191	GLN
3	K	192	SER
3	K	193	ILE
3	K	194	THR
3	K	197	VAL
3	K	210	ILE
3	K	213	ARG
4	C	2	ILE
4	C	3	VAL
4	C	5	THR
4	C	6	GLN
4	C	10	SER
4	C	15	LEU
4	C	24	ARG
4	C	26	SER
4	C	42	GLN
4	C	45	LYS
4	C	47	LEU

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Mol	Chain	Res	Type
4	C	52	SER
4	C	54	LEU
4	C	58	ILE
4	C	69	THR
4	C	70	ASP
4	C	78	VAL
4	C	79	GLU
4	C	85	THR
4	C	89	GLN
4	C	90	GLN
4	C	94	ASP
4	C	96	TYR
4	C	97	THR
4	C	105	GLU
4	C	106	ILE
4	C	115	VAL
4	C	125	LEU
4	C	126	THR
4	C	136	LEU
4	C	142	LYS
4	C	143	ASP
4	C	144	ILE
4	C	145	ASN
4	C	146	VAL
4	C	150	ILE
4	C	151	ASP
4	C	153	SER
4	C	156	GLN
4	C	157	ASN
4	C	167	ASP
4	C	168	SER
4	C	169	LYS
4	C	171	SER
4	C	174	SER
4	C	181	LEU
4	C	182	THR
4	C	183	LYS
4	C	184	ASP
4	C	185	GLU
4	C	187	GLU
4	C	193	THR
4	C	197	THR

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Mol	Chain	Res	Type
4	C	199	LYS
4	C	205	ILE
4	C	209	PHE
4	C	210	ASN
4	C	212	ASN
4	C	214	CYS
5	D	3	GLN
5	D	11	LEU
5	D	13	LYS
5	D	24	THR
5	D	28	SER
5	D	33	TRP
5	D	37	VAL
5	D	43	GLN
5	D	48	ILE
5	D	54	THR
5	D	57	THR
5	D	59	ASN
5	D	61	GLN
5	D	69	LEU
5	D	77	THR
5	D	79	TYR
5	D	80	MET
5	D	81	GLN
5	D	83	THR
5	D	85	GLU
5	D	94	ARG
5	D	108	THR
5	D	109	THR
5	D	111	THR
5	D	112	VAL
5	D	116	LYS
5	D	117	THR
5	D	122	VAL
5	D	132	THR
5	D	133	THR
5	D	138	THR
5	D	139	LEU
5	D	141	CYS
5	D	149	GLU
5	D	152	THR
5	D	153	LEU

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Mol	Chain	Res	Type
5	D	164	VAL
5	D	170	VAL
5	D	174	ASP
5	D	178	LEU
5	D	181	SER
5	D	182	VAL
5	D	183	THR
5	D	188	THR
5	D	192	GLN
5	D	194	ILE
5	D	195	THR
5	D	211	ILE
5	D	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	27	GLN
1	P	30	GLN
1	P	84	GLN
1	P	101	HIS
1	P	210	GLN
2	L	6	GLN
2	L	28	ASN
2	L	38	GLN
2	L	90	GLN
2	L	91	HIS
2	L	124	GLN
2	L	166	GLN
2	L	189	HIS
2	L	210	ASN
2	L	212	ASN
3	H	3	GLN
3	H	6	GLN
3	H	60	ASN
3	H	81	GLN
3	H	105	GLN
3	H	196	ASN
4	A	34	HIS
4	A	38	GLN
4	A	89	GLN
4	A	90	GLN

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Mol	Chain	Res	Type
4	A	124	GLN
4	A	156	GLN
4	A	157	ASN
4	A	189	HIS
4	A	198	HIS
4	A	210	ASN
5	B	6	GLN
5	B	35	HIS
5	B	39	GLN
5	B	52	ASN
5	B	60	ASN
5	B	61	GLN
5	B	156	ASN
5	B	165	HIS
5	B	197	ASN
1	Q	25	HIS
1	Q	30	GLN
1	Q	50	GLN
1	Q	70	HIS
1	Q	128	GLN
1	Q	161	HIS
1	Q	174	GLN
1	Q	202	ASN
1	Q	210	GLN
1	Q	233	HIS
2	M	6	GLN
2	M	30	ASN
2	M	38	GLN
2	M	124	GLN
2	M	138	ASN
2	M	145	ASN
2	M	156	GLN
2	M	157	ASN
2	M	190	ASN
2	M	198	HIS
3	K	6	GLN
3	K	35	ASN
3	K	39	GLN
3	K	60	ASN
3	K	105	GLN
3	K	191	GLN
4	C	17	GLN

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Mol	Chain	Res	Type
4	C	34	HIS
4	C	38	GLN
4	C	90	GLN
4	C	92	HIS
4	C	124	GLN
4	C	138	ASN
4	C	145	ASN
4	C	156	GLN
4	C	157	ASN
4	C	189	HIS
4	C	190	ASN
4	C	198	HIS
4	C	210	ASN
5	D	6	GLN
5	D	35	HIS
5	D	52	ASN
5	D	60	ASN
5	D	61	GLN
5	D	76	ASN
5	D	156	ASN
5	D	172	GLN
5	D	192	GLN
5	D	197	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

32 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	$\# Z > 2$
6	NAG	E	1	1,6	14,14,15	1.14	1 (7%)	17,19,21	1.86	4 (23%)
6	GAL	E	10	6	11,11,12	1.22	1 (9%)	15,15,17	0.55	0
6	SIA	E	11	6	20,20,21	2.09	5 (25%)	21,28,31	1.48	2 (9%)
6	NAG	E	12	6	14,14,15	0.55	0	17,19,21	0.90	0
6	GAL	E	13	6	11,11,12	0.55	0	15,15,17	1.73	4 (26%)
6	SIA	E	14	6	20,20,21	0.76	0	21,28,31	1.65	5 (23%)
6	FUC	E	15	6	10,10,11	0.66	0	14,14,16	0.66	0
6	NAG	E	2	6	14,14,15	0.59	0	17,19,21	1.16	2 (11%)
6	MAN	E	3	6	11,11,12	1.10	1 (9%)	15,15,17	1.91	3 (20%)
6	MAN	E	4	6	11,11,12	0.71	0	15,15,17	1.48	3 (20%)
6	NAG	E	5	6	14,14,15	0.85	1 (7%)	17,19,21	1.93	3 (17%)
6	GAL	E	6	6	11,11,12	0.65	0	15,15,17	1.17	1 (6%)
6	SIA	E	7	6	20,20,21	0.89	0	21,28,31	1.35	4 (19%)
6	MAN	E	8	6	11,11,12	0.67	0	15,15,17	2.48	4 (26%)
6	NAG	E	9	6	14,14,15	0.72	0	17,19,21	1.60	2 (11%)
7	A2G	F	1	7,1	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
7	GAL	F	2	7	11,11,12	0.73	0	15,15,17	1.30	3 (20%)
8	NAG	G	1	1,8	14,14,15	0.58	0	17,19,21	2.09	5 (29%)
8	GAL	G	10	8	11,11,12	0.80	0	15,15,17	1.77	5 (33%)
8	SIA	G	11	8	20,20,21	0.65	0	21,28,31	1.07	2 (9%)
8	NAG	G	12	8	14,14,15	0.56	0	17,19,21	2.69	7 (41%)
8	GAL	G	13	8	11,11,12	0.91	1 (9%)	15,15,17	1.14	1 (6%)
8	SIA	G	14	8	20,20,21	0.78	0	21,28,31	1.02	2 (9%)
8	FUC	G	15	8	10,10,11	0.64	0	14,14,16	1.71	3 (21%)
8	NAG	G	2	8	14,14,15	0.56	0	17,19,21	1.75	5 (29%)
8	MAN	G	3	8	11,11,12	0.71	0	15,15,17	2.42	6 (40%)
8	MAN	G	4	8	11,11,12	0.66	0	15,15,17	1.48	3 (20%)
8	NAG	G	5	8	14,14,15	0.66	0	17,19,21	1.69	6 (35%)
8	GAL	G	6	8	11,11,12	0.72	0	15,15,17	1.04	1 (6%)
8	SIA	G	7	8	20,20,21	0.84	0	21,28,31	0.95	1 (4%)
8	MAN	G	8	8	11,11,12	0.72	0	15,15,17	2.07	3 (20%)
8	NAG	G	9	8	14,14,15	1.31	1 (7%)	17,19,21	1.67	4 (23%)

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	E	1	1,6	-	0/6/23/26	0/1/1/1
6	GAL	E	10	6	-	2/2/19/22	0/1/1/1
6	SIA	E	11	6	-	13/18/34/38	0/1/1/1
6	NAG	E	12	6	-	0/6/23/26	0/1/1/1
6	GAL	E	13	6	-	1/2/19/22	0/1/1/1
6	SIA	E	14	6	-	8/18/34/38	0/1/1/1
6	FUC	E	15	6	-	-	0/1/1/1
6	NAG	E	2	6	-	1/6/23/26	0/1/1/1
6	MAN	E	3	6	-	1/2/19/22	0/1/1/1
6	MAN	E	4	6	-	1/2/19/22	1/1/1/1
6	NAG	E	5	6	-	1/6/23/26	0/1/1/1
6	GAL	E	6	6	-	2/2/19/22	0/1/1/1
6	SIA	E	7	6	-	10/18/34/38	0/1/1/1
6	MAN	E	8	6	-	2/2/19/22	0/1/1/1
6	NAG	E	9	6	-	2/6/23/26	0/1/1/1
7	A2G	F	1	7,1	-	2/6/23/26	0/1/1/1
7	GAL	F	2	7	-	1/2/19/22	0/1/1/1
8	NAG	G	1	1,8	-	2/6/23/26	0/1/1/1
8	GAL	G	10	8	-	1/2/19/22	0/1/1/1
8	SIA	G	11	8	-	9/18/34/38	0/1/1/1
8	NAG	G	12	8	-	3/6/23/26	0/1/1/1
8	GAL	G	13	8	-	1/2/19/22	0/1/1/1
8	SIA	G	14	8	-	4/18/34/38	0/1/1/1
8	FUC	G	15	8	-	-	0/1/1/1
8	NAG	G	2	8	-	2/6/23/26	0/1/1/1
8	MAN	G	3	8	-	0/2/19/22	0/1/1/1
8	MAN	G	4	8	-	1/2/19/22	0/1/1/1
8	NAG	G	5	8	-	2/6/23/26	0/1/1/1
8	GAL	G	6	8	-	2/2/19/22	0/1/1/1
8	SIA	G	7	8	-	2/18/34/38	0/1/1/1
8	MAN	G	8	8	-	2/2/19/22	0/1/1/1
8	NAG	G	9	8	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	11	SIA	C11-C10	-4.92	1.40	1.50
6	E	11	SIA	O10-C10	-4.66	1.12	1.23
8	G	9	NAG	O5-C1	-4.29	1.36	1.43
6	E	11	SIA	C10-N5	4.01	1.47	1.34
6	E	10	GAL	O3-C3	2.81	1.49	1.43
6	E	5	NAG	C1-C2	2.67	1.56	1.52
6	E	3	MAN	C2-C3	2.54	1.56	1.52
6	E	11	SIA	C9-C8	2.37	1.58	1.52
8	G	13	GAL	C2-C3	2.16	1.55	1.52
6	E	11	SIA	C7-C6	2.16	1.55	1.52
6	E	1	NAG	O5-C5	-2.14	1.39	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	8	MAN	C1-O5-C5	7.67	122.47	112.19
8	G	3	MAN	C1-O5-C5	6.15	120.43	112.19
8	G	12	NAG	C1-O5-C5	5.84	120.01	112.19
6	E	5	NAG	C1-O5-C5	5.76	119.91	112.19
8	G	12	NAG	C2-N2-C7	5.42	130.16	122.90
8	G	8	MAN	O2-C2-C1	5.14	121.00	109.22
6	E	1	NAG	O5-C1-C2	-5.08	103.43	111.29
8	G	1	NAG	C4-C3-C2	4.82	118.08	111.02
8	G	8	MAN	C1-O5-C5	4.71	118.50	112.19
6	E	3	MAN	C1-O5-C5	4.37	118.05	112.19
8	G	12	NAG	O4-C4-C5	4.07	119.36	109.32
8	G	2	NAG	C2-N2-C7	3.98	128.24	122.90
8	G	3	MAN	C3-C4-C5	3.81	117.14	110.23
8	G	9	NAG	C4-C3-C2	3.79	116.58	111.02
6	E	13	GAL	C1-O5-C5	3.72	117.17	112.19
8	G	1	NAG	C2-N2-C7	-3.68	117.97	122.90
6	E	9	NAG	C1-O5-C5	3.65	117.07	112.19
6	E	3	MAN	C1-C2-C3	3.59	114.88	109.64
8	G	10	GAL	C3-C4-C5	3.55	116.67	110.23
8	G	1	NAG	C1-O5-C5	3.50	116.87	112.19
6	E	9	NAG	C4-C3-C2	3.40	116.00	111.02
8	G	12	NAG	C8-C7-N2	3.37	121.71	116.12
8	G	5	NAG	C4-C3-C2	3.35	115.93	111.02
6	E	4	MAN	C3-C4-C5	-3.35	104.16	110.23
8	G	15	FUC	C1-O5-C5	3.34	120.85	112.97
8	G	15	FUC	O5-C5-C4	3.32	115.54	109.55
6	E	5	NAG	C2-N2-C7	3.32	127.35	122.90
6	E	13	GAL	O3-C3-C2	3.28	116.75	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	3	MAN	C1-C2-C3	3.25	114.38	109.64
8	G	4	MAN	C1-O5-C5	3.24	116.53	112.19
8	G	12	NAG	C4-C3-C2	3.21	115.72	111.02
8	G	13	GAL	O3-C3-C2	3.21	116.61	110.05
8	G	12	NAG	O4-C4-C3	-3.20	102.83	110.38
6	E	14	SIA	C11-C10-N5	3.17	121.37	116.12
6	E	14	SIA	C5-N5-C10	3.16	130.50	123.11
6	E	6	GAL	C1-C2-C3	3.13	114.20	109.64
8	G	15	FUC	C3-C4-C5	3.13	114.57	109.81
8	G	9	NAG	C2-N2-C7	3.05	126.99	122.90
6	E	8	MAN	C1-C2-C3	-2.97	105.32	109.64
6	E	7	SIA	C8-C7-C6	2.94	118.58	113.05
6	E	11	SIA	O1B-C1-C2	2.94	120.35	112.71
8	G	10	GAL	C1-O5-C5	2.89	116.06	112.19
8	G	4	MAN	O5-C5-C6	2.88	113.26	107.66
8	G	5	NAG	C1-O5-C5	2.85	116.01	112.19
6	E	13	GAL	C3-C4-C5	-2.83	105.09	110.23
6	E	8	MAN	C3-C4-C5	2.82	115.34	110.23
6	E	7	SIA	O6-C2-C1	2.78	112.97	107.72
6	E	3	MAN	O3-C3-C2	2.77	115.71	110.05
8	G	11	SIA	O1B-C1-C2	2.75	119.87	112.71
8	G	4	MAN	C1-C2-C3	2.69	113.56	109.64
8	G	14	SIA	O1B-C1-C2	2.68	119.67	112.71
8	G	9	NAG	C1-C2-N2	-2.67	106.23	110.43
8	G	3	MAN	O3-C3-C2	2.65	115.46	110.05
8	G	10	GAL	C1-C2-C3	-2.65	105.78	109.64
8	G	5	NAG	O5-C1-C2	2.64	115.37	111.29
6	E	11	SIA	C6-C5-N5	2.62	115.09	110.91
8	G	3	MAN	C6-C5-C4	-2.62	106.58	113.02
8	G	1	NAG	C1-C2-N2	-2.61	106.33	110.43
7	F	2	GAL	C2-C3-C4	2.60	115.44	110.86
6	E	7	SIA	O1B-C1-C2	2.56	119.36	112.71
6	E	8	MAN	O5-C5-C4	2.55	117.02	110.83
8	G	7	SIA	O1B-C1-C2	2.52	119.28	112.71
8	G	2	NAG	C4-C3-C2	2.52	114.71	111.02
8	G	6	GAL	C1-C2-C3	2.50	113.28	109.64
8	G	10	GAL	O3-C3-C2	2.47	115.10	110.05
7	F	2	GAL	C3-C4-C5	2.47	114.72	110.23
8	G	1	NAG	O5-C1-C2	-2.44	107.52	111.29
6	E	14	SIA	O1B-C1-C2	2.38	118.91	112.71
6	E	1	NAG	C1-C2-N2	-2.36	106.71	110.43
6	E	13	GAL	O5-C5-C6	2.36	112.25	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2	NAG	C4-C3-C2	2.31	114.40	111.02
8	G	5	NAG	C8-C7-N2	2.24	119.84	116.12
8	G	2	NAG	O5-C1-C2	-2.24	107.83	111.29
6	E	5	NAG	O4-C4-C3	2.21	115.59	110.38
8	G	9	NAG	C1-O5-C5	2.18	115.11	112.19
8	G	3	MAN	O5-C5-C4	2.18	116.13	110.83
6	E	1	NAG	C1-O5-C5	2.17	115.10	112.19
8	G	8	MAN	O5-C5-C6	2.16	111.87	107.66
8	G	14	SIA	O1A-C1-C2	-2.16	118.19	122.85
7	F	2	GAL	C1-C2-C3	2.15	112.77	109.64
8	G	10	GAL	O5-C1-C2	-2.13	105.70	110.79
8	G	2	NAG	C1-C2-N2	2.13	113.78	110.43
6	E	2	NAG	O3-C3-C2	-2.12	104.99	109.40
8	G	5	NAG	C2-N2-C7	2.11	125.72	122.90
6	E	14	SIA	O6-C2-C1	2.10	111.69	107.72
8	G	5	NAG	C3-C4-C5	-2.09	106.44	110.23
7	F	1	A2G	O4-C4-C5	2.09	114.47	109.32
8	G	11	SIA	O1A-C1-C2	-2.09	118.34	122.85
6	E	4	MAN	O5-C5-C6	2.08	111.71	107.66
6	E	4	MAN	C6-C5-C4	2.07	118.11	113.02
6	E	14	SIA	C6-C5-N5	-2.07	107.60	110.91
8	G	2	NAG	C1-O5-C5	2.07	114.96	112.19
7	F	1	A2G	C1-O5-C5	2.06	114.94	112.19
6	E	7	SIA	O6-C2-C3	-2.05	107.80	110.56
8	G	12	NAG	O7-C7-C8	-2.05	118.41	122.05
6	E	1	NAG	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	7	SIA	C5-C6-C7-C8
6	E	7	SIA	C5-C6-C7-O7
6	E	7	SIA	O6-C6-C7-C8
6	E	7	SIA	O6-C6-C7-O7
6	E	7	SIA	O7-C7-C8-C9
6	E	7	SIA	C7-C8-C9-O9
6	E	7	SIA	O8-C8-C9-O9
6	E	11	SIA	C5-C6-C7-C8
6	E	11	SIA	C5-C6-C7-O7
6	E	11	SIA	O6-C6-C7-C8
6	E	11	SIA	O6-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
6	E	11	SIA	C6-C7-C8-O8
6	E	11	SIA	O7-C7-C8-C9
6	E	11	SIA	O7-C7-C8-O8
6	E	11	SIA	O8-C8-C9-O9
6	E	14	SIA	C5-C6-C7-C8
6	E	14	SIA	C5-C6-C7-O7
6	E	14	SIA	O6-C6-C7-C8
6	E	14	SIA	O6-C6-C7-O7
8	G	11	SIA	O8-C8-C9-O9
8	G	12	NAG	C3-C2-N2-C7
8	G	7	SIA	O8-C8-C9-O9
8	G	14	SIA	O8-C8-C9-O9
6	E	11	SIA	C7-C8-C9-O9
8	G	11	SIA	C7-C8-C9-O9
6	E	7	SIA	C6-C7-C8-C9
6	E	11	SIA	C6-C7-C8-C9
7	F	1	A2G	O5-C5-C6-O6
8	G	8	MAN	O5-C5-C6-O6
8	G	6	GAL	C4-C5-C6-O6
6	E	8	MAN	O5-C5-C6-O6
6	E	9	NAG	O5-C5-C6-O6
8	G	8	MAN	C4-C5-C6-O6
6	E	7	SIA	O7-C7-C8-O8
6	E	9	NAG	C4-C5-C6-O6
6	E	7	SIA	C6-C7-C8-O8
6	E	11	SIA	C11-C10-N5-C5
6	E	11	SIA	O10-C10-N5-C5
6	E	14	SIA	C11-C10-N5-C5
6	E	14	SIA	O10-C10-N5-C5
8	G	1	NAG	C8-C7-N2-C2
8	G	1	NAG	O7-C7-N2-C2
8	G	5	NAG	C8-C7-N2-C2
8	G	5	NAG	O7-C7-N2-C2
8	G	11	SIA	C11-C10-N5-C5
8	G	11	SIA	O10-C10-N5-C5
8	G	12	NAG	C8-C7-N2-C2
8	G	12	NAG	O7-C7-N2-C2
6	E	8	MAN	C4-C5-C6-O6
8	G	6	GAL	O5-C5-C6-O6
6	E	10	GAL	C4-C5-C6-O6
8	G	7	SIA	C7-C8-C9-O9
8	G	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	E	10	GAL	O5-C5-C6-O6
8	G	11	SIA	C6-C7-C8-O8
6	E	6	GAL	C4-C5-C6-O6
6	E	14	SIA	C4-C5-N5-C10
6	E	13	GAL	O5-C5-C6-O6
6	E	4	MAN	O5-C5-C6-O6
6	E	6	GAL	O5-C5-C6-O6
7	F	2	GAL	O5-C5-C6-O6
8	G	11	SIA	O1A-C1-C2-O6
6	E	3	MAN	O5-C5-C6-O6
8	G	2	NAG	C4-C5-C6-O6
7	F	1	A2G	C4-C5-C6-O6
8	G	14	SIA	C7-C8-C9-O9
8	G	11	SIA	C6-C7-C8-C9
8	G	13	GAL	C4-C5-C6-O6
8	G	10	GAL	C4-C5-C6-O6
8	G	11	SIA	O7-C7-C8-O8
6	E	2	NAG	O5-C5-C6-O6
6	E	5	NAG	C3-C2-N2-C7
8	G	2	NAG	C3-C2-N2-C7
8	G	14	SIA	O1A-C1-C2-O6
8	G	11	SIA	O7-C7-C8-C9
6	E	11	SIA	O1A-C1-C2-O6
8	G	14	SIA	C4-C5-N5-C10
6	E	14	SIA	C6-C5-N5-C10

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	4	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 24 short contacts:

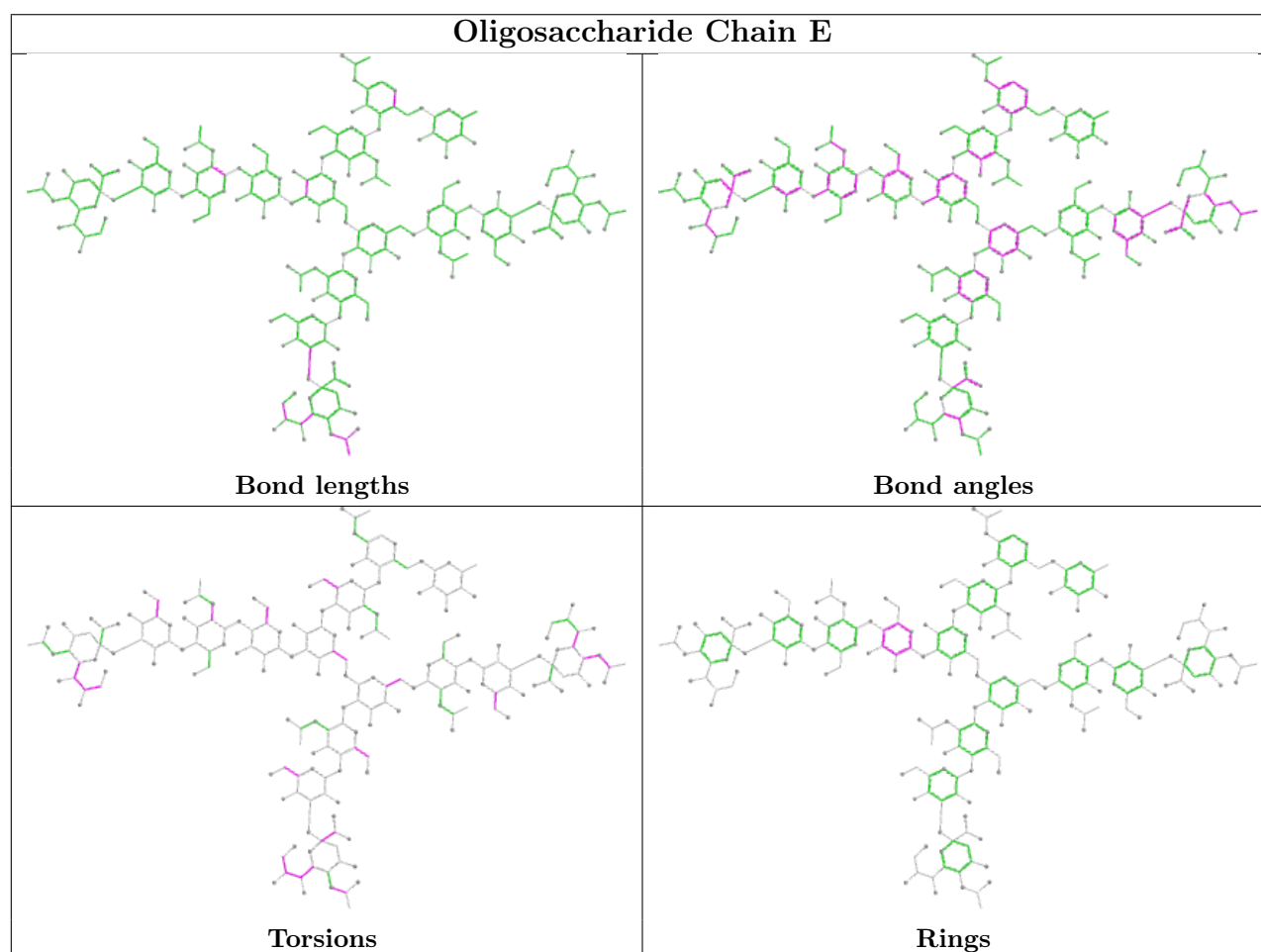
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	3	MAN	1	0
8	G	11	SIA	3	0
6	E	2	NAG	2	0
6	E	14	SIA	3	0
6	E	5	NAG	1	0
7	F	1	A2G	1	0
6	E	6	GAL	1	0
8	G	5	NAG	1	0

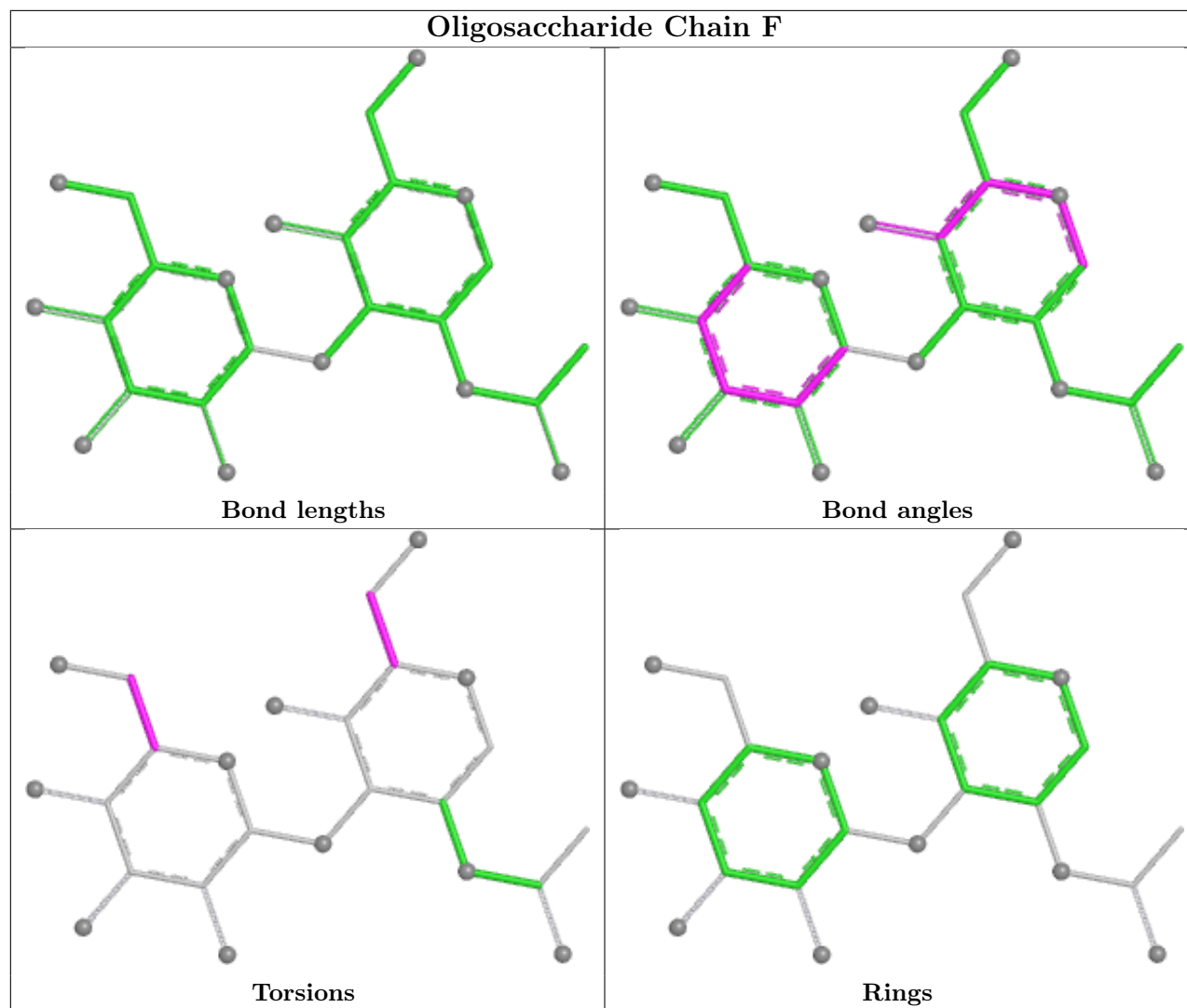
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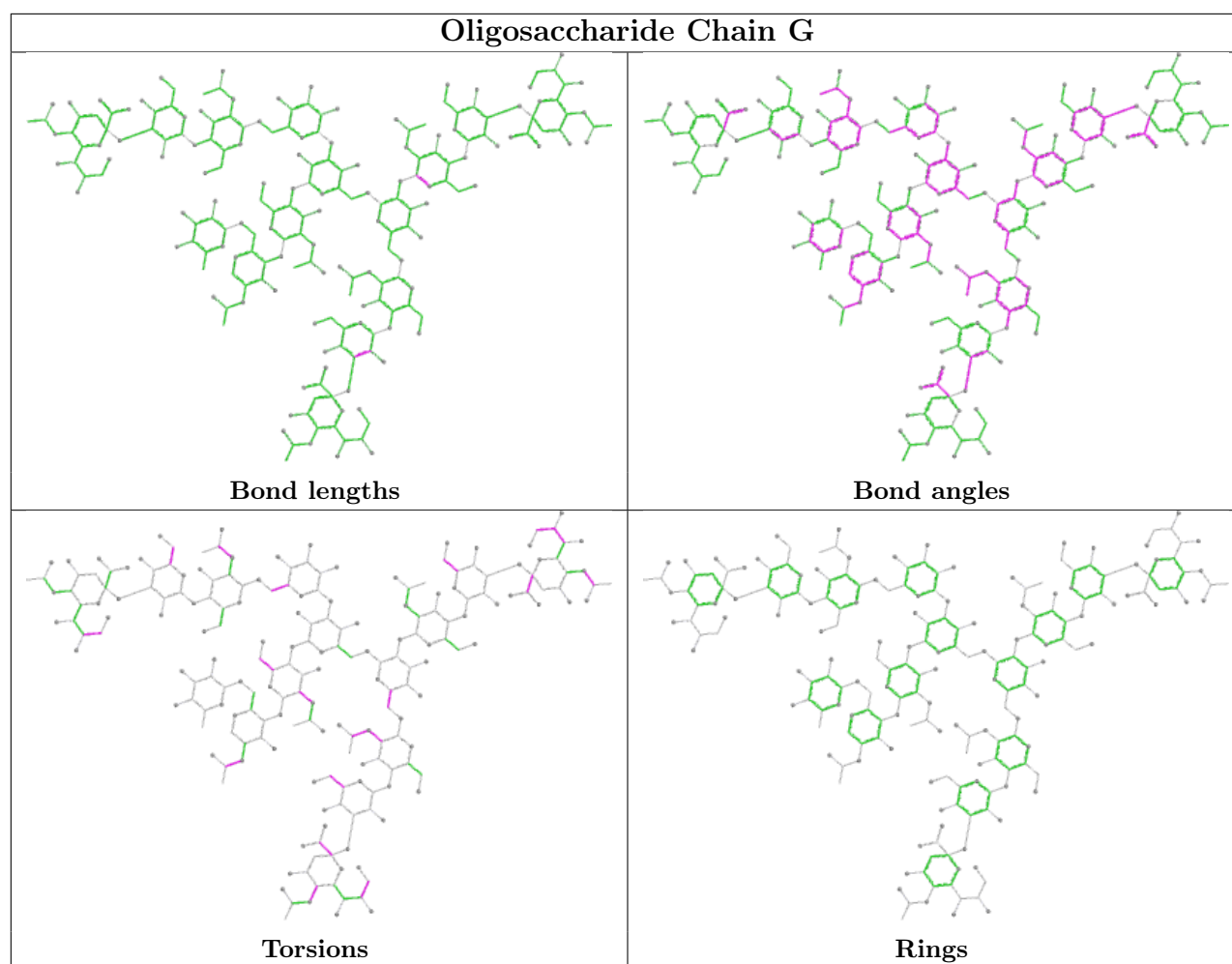
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	4	MAN	2	0
8	G	4	MAN	1	0
6	E	7	SIA	2	0
8	G	6	GAL	1	0
8	G	8	MAN	2	0
8	G	12	NAG	4	0
6	E	13	GAL	1	0
6	E	3	MAN	3	0
8	G	9	NAG	2	0
8	G	1	NAG	2	0

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







5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	237/237 (100%)	-0.29	5 (2%) 63 43	28, 49, 121, 155	4 (1%)
1	Q	237/237 (100%)	0.08	0 100 100	58, 94, 155, 193	0
2	L	219/219 (100%)	-0.28	0 100 100	36, 76, 123, 155	0
2	M	219/219 (100%)	-0.29	0 100 100	46, 71, 104, 154	0
3	H	217/219 (99%)	-0.43	1 (0%) 87 76	27, 52, 139, 172	0
3	K	219/219 (100%)	-0.48	0 100 100	33, 56, 83, 142	0
4	A	218/218 (100%)	-0.28	0 100 100	51, 79, 104, 141	0
4	C	218/218 (100%)	-0.20	0 100 100	50, 76, 108, 150	0
5	B	219/219 (100%)	-0.16	0 100 100	48, 84, 118, 157	0
5	D	219/219 (100%)	-0.17	2 (0%) 81 64	53, 85, 113, 140	0
All	All	2222/2224 (99%)	-0.25	8 (0%) 88 79	27, 74, 124, 193	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	152	PRO	4.2
1	P	192	SER	3.6
5	D	98	LEU	2.4
1	P	151	THR	2.2
1	P	17	VAL	2.2
3	H	212	PRO	2.2
5	D	138	THR	2.0
1	P	144	ILE	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

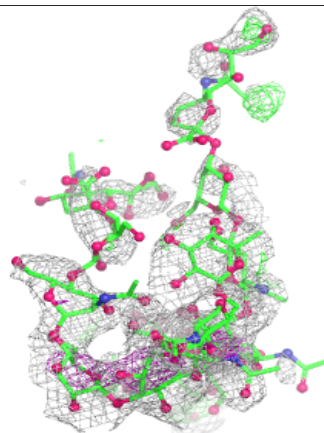
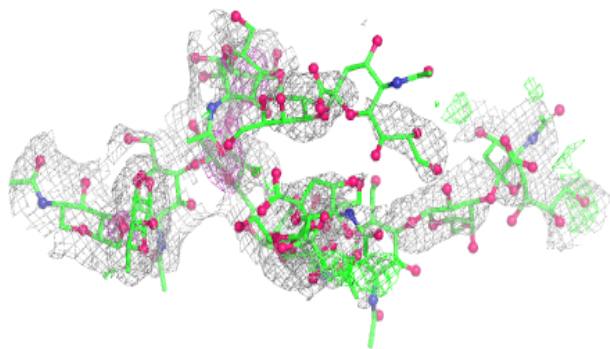
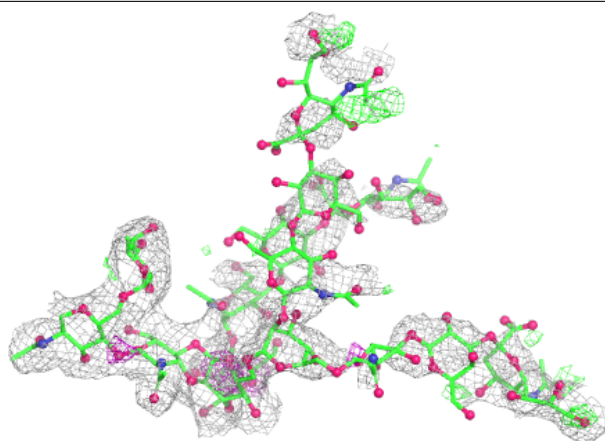
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	E	1	14/15	-	-	73,77,83,89	0
6	NAG	E	2	14/15	-	-	97,99,102,107	0
6	MAN	E	3	11/12	-	-	112,114,118,118	0
6	MAN	E	4	11/12	-	-	120,121,122,122	0
6	NAG	E	5	14/15	-	-	123,123,124,124	0
6	GAL	E	6	11/12	-	-	122,122,123,123	11
6	SIA	E	7	20/21	-	-	117,119,120,120	20
6	MAN	E	8	11/12	-	-	117,119,120,120	11
6	NAG	E	9	14/15	-	-	119,121,121,121	14
6	GAL	E	10	11/12	-	-	118,119,119,119	11
6	SIA	E	11	20/21	-	-	115,119,119,119	20
6	NAG	E	12	14/15	-	-	114,116,117,117	14
6	GAL	E	13	11/12	-	-	111,112,112,112	11
6	SIA	E	14	20/21	-	-	106,108,110,110	20
6	FUC	E	15	10/11	-	-	88,88,89,89	0
7	A2G	F	1	14/15	-	-	60,63,65,65	14
7	GAL	F	2	11/12	-	-	65,66,66,66	11
8	NAG	G	1	14/15	-	-	96,99,101,104	0
8	NAG	G	2	14/15	-	-	112,114,116,120	14
8	MAN	G	3	11/12	-	-	123,124,127,129	0
8	MAN	G	4	11/12	-	-	119,121,122,122	11
8	NAG	G	5	14/15	-	-	115,117,117,118	14
8	GAL	G	6	11/12	-	-	116,117,118,118	11
8	SIA	G	7	20/21	-	-	116,118,118,118	20
8	MAN	G	8	11/12	-	-	130,132,133,134	11
8	NAG	G	9	14/15	-	-	130,131,132,132	14
8	GAL	G	10	11/12	-	-	131,132,132,132	11
8	SIA	G	11	20/21	-	-	131,132,133,133	20
8	NAG	G	12	14/15	-	-	134,136,137,139	14
8	GAL	G	13	11/12	-	-	141,142,143,143	0
8	SIA	G	14	20/21	-	-	144,145,146,146	0
8	FUC	G	15	10/11	-	-	100,101,101,101	0

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

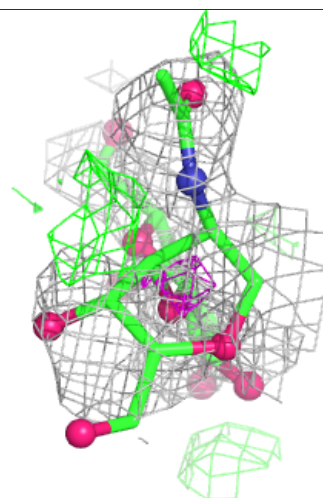
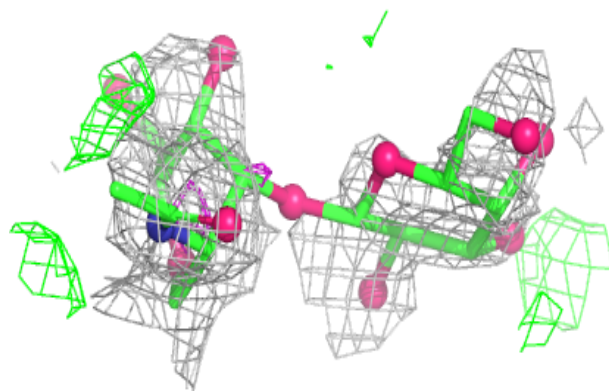
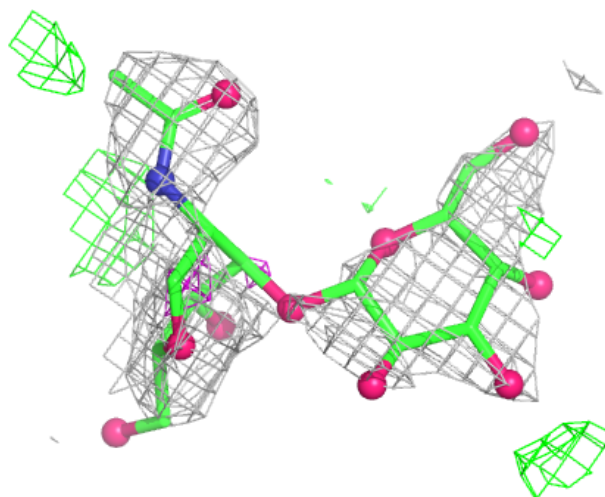
Electron density around Chain E:

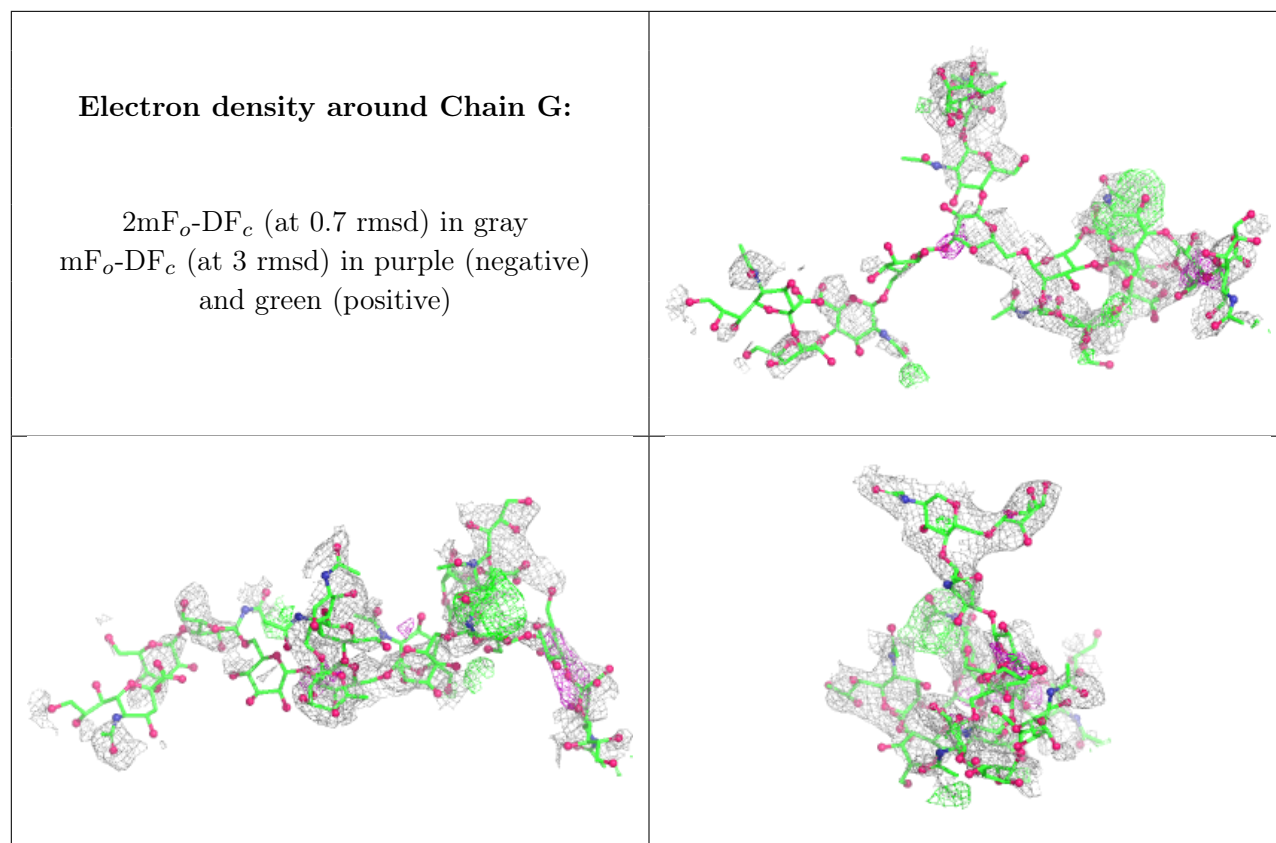
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.